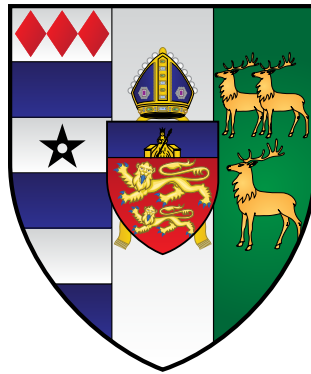


Probing high energy Higgs bosons using $H \rightarrow b\bar{b}$
decays in $\sqrt{s} = 13$ TeV proton-proton collisions at
the ATLAS experiment



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Lincoln College
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Thesis submitted for the degree of
Doctor of Philosophy

Trinity Term, 2021



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Abstract

This thesis presents a novel study of Higgs boson production using $H \rightarrow b\bar{b}$ decays produced with large transverse momentum boosts, with an additional high energy jet in the event, using $\sqrt{s} = 13$ TeV proton-proton collision data collected by the ATLAS experiment, corresponding to an integrated luminosity of 136 fb^{-1} . Higgs boson signal estimates were extracted from candidate jet mass spectra using binned likelihood fits. The Higgs boson signal estimate was probed inclusively using Higgs boson candidate jets with $p_T^{\text{jet}} > 250 \text{ GeV}$. The inclusive Higgs boson production cross-sections were examined in a fiducial region defined by Higgs boson $p_T^H > 450 \text{ GeV}$, and differential bins of $p_T^H = [300, 450] \text{ GeV}$; $[450, 650] \text{ GeV}$; $[650, 1000] \text{ GeV}$; and $> 1000 \text{ GeV}$ inclusively. As sensitivity was not sufficient to make statistically significant measurements of the Higgs boson cross-section, in all cases 95% CL_s limits were set, including a first-time limit set for Higgs bosons with $p_T^H > 1 \text{ TeV}$, $\sigma_H(p_T > 1 \text{ TeV}) < 74 \text{ fb}$. A differential Z boson signal measurement was also made under the same conditions and compared to theoretical predictions. All results were found to be consistent with Standard Model predictions. Particular emphasis is given to the development and validation of the analysis fit model.

Dedicated to my parents – Elvyra and Aivaras

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This degree and the writing of this thesis has been one of the toughest and remarkable journeys I have ever had the privilege to undertake. Many people have contributed to its completion, and granted me the pleasure of their company along the way. I am thankful to all of you. Here, I will attempt to name just a few.

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throughout our time working together. I also must thank Gabriel Facini, Rafael Teixeira de Lima, Francesco Di Bello, Dan Guest, Karol Krizka, Alex Emerman, Ruth Jacobs, and Eleanor Jones for their extensive help, and many an engaging discussion.

This work would also have not been possible without the support from Lincoln College and the University of Oxford, which have funded these studies and financially supported my work travels and training, helped me through hardships, and gave me the privilege to be part of their astounding communities.

I am also immensely grateful to all of the people at the Particle Physics sub-department at the University of Oxford. I must mention Richard Nickerson, who introduced me to laboratory work on ATLAS hardware, which I thoroughly enjoyed; and Tony Weidberg, Daniela Bortoletto, Sue Geddes, Kim Proudfoot and Jennifer Matthews for their support, and many pleasant conversations throughout the years. I also would like to thank Fikri, Santiago, Beojan, Bill, Mike, and Jon for helping me through many a pickle, and always offering useful advice; as well as Aaron, Laurence, Iwan, Alex, Gavin, Andrew, and the rest of my cohort, for many great conversations and laughs.

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Preface

High energy physics is an immensely collaborative field. The work presented in this thesis was done as part of one of the largest scientific collaborations in the world – the *ATLAS collaboration* – with over five thousand current members [1]. The analyses the author contributed to were conducted in large teams, and relied on tools and recommendations from within this scientific community. This thesis aims to provide the reader with a comprehensive insight into the analyses she worked on, with a particular focus on her contributions. Hence, the thesis also includes descriptions of work conducted by other members of these analyses, crucial to contextualise the contributions of the author.

In some cases, internal ATLAS documentation is cited. This is mostly done to credit the work of other analysis members, unless stated otherwise (i.e. to identify the work of the author). In all cases where internal documentation is cited, it is identified as such after the citation.

This section lists the publications to which the author contributed, in chronological order of personal involvement, and briefly outlines her work. More detailed descriptions of her contributions are given at the beginning of each relevant chapter (chapters 4 – 9), either in the introduction or a dedicated section.

Publications

Double- b tagging efficiency calibration in gluon splitting events [2]

(internal, written by author), as part of

Efficiency corrections for a tagger for boosted $H \rightarrow b\bar{b}$ decays in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector (ATLAS Collaboration, 2021, ATL-PHYS-PUB-2021-035) [3]

Chapter 4, contribution: November 2017 – June 2019

Study to calibrate the efficiency of the dedicated tagging tool which identifies highly collimated decays to two b -quarks using gluon splitting ($g \rightarrow b\bar{b}$) events. The author aided the extension of a validation procedure into a calibration, largely through software-based work and validation studies. She updated the calibration software to comply with the latest ATLAS software tools and recommendations used at the time, and studied the differences rising from these changes. The author also integrated the calibration software to the wider flavour-tagging calibration package, documented it for easy future-user access, and did some organisational work for the calibration sub-group.

Search for boosted resonances decaying to two b -quarks and produced in association with a jet at $\sqrt{s} = 13$ TeV with the ATLAS detector (ATLAS Collaboration, 2018, ATLAS-CONF-2018-052) [4]

Not presented in the thesis, contribution: March 2018 – November 2018

A search for light ($m = 70 \text{ GeV} - 230 \text{ GeV}$) beyond Standard Model resonances decaying to two b -quarks at high transverse momentum (p_T), in events with an additional jet in the final state, including a Higgs boson interpretation. It is the precursor for the analysis at the focus of this thesis, described in the following entry. The author made various small contributions to this analysis, including jet mass resolution studies, and inclusion of jet uncertainties to the analysis software.

Study of Higgs-boson production with large transverse momentum using the $H \rightarrow b\bar{b}$ decay with the ATLAS detector (ATLAS Collaboration, 2021, CERN-EP-2021-185) [5]

Chapters 5 – 9, active contribution: December 2018 – November 2020

A study of inclusive Higgs boson production in $H \rightarrow b\bar{b}$ decays at high transverse momentum, where the momentum boost is provided by an external jet in the final state. The author had a large impact on the analysis, as one of the main contributors (3 – 4 people) during the time she was actively involved.

The Higgs boson measurements were made by performing a complex likelihood fit over several data regions. The author of this thesis produced many vital development and validation studies for the measurement fit and framework. She conducted studies on the treatment of signals, backgrounds and systematic uncertainties in the measurement, and implemented the developments stemming from these studies into the technical analysis workflow. She was the main contributor to the fit analysis software (~ 11 thousand lines of code), and as a fit and fit software expert, she also assisted other group members with studies and code implementation. The major areas of contribution were:

- fitting framework implementation and validation;
- $t\bar{t}$ control region inclusion and fit studies;
- differential fit implementation;
- mass template smoothing of nominal processes and systematic uncertainties;
- systematic uncertainty pruning studies;
- systematic uncertainty decorrelation studies;
- measurement fit tests and validation.

“Kelią nueina einantys.”

The journey is completed by those who keep walking.

— Lithuanian Proverb

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Introduction

The experimental discovery of the Higgs boson in 2012 by the Large Hadron Collider (LHC) experiments ATLAS and CMS [6, 7] was the final piece in establishing the validity of the Standard Model (SM). It marked the beginning of a new era in experimental particle physics, as physics beyond the Standard Model (BSM) could now be probed through measurements of theoretically known properties of the Higgs boson, and couplings between the Higgs boson and BSM particles.

The Higgs boson couples to all massive particles in the SM, making it a promising probe for massive BSM particles. However, Higgs bosons are rare, and background reduction methods used in Higgs analyses further reduce the numbers of accessible Higgs boson events. For example, the most abundant Higgs boson decay channel – to two b -quarks ($H \rightarrow b\bar{b}$), is particularly difficult to probe due to large backgrounds in proton-proton (pp) collisions.

The first experimental measurement (with a 5σ statistical significance) of $H \rightarrow b\bar{b}$ decays was made in 2018 [8]. So far, the measurements in this channel have only been made in final states which significantly restrict the total Higgs boson production cross-section, and exclude the most abundant Higgs boson production channel in pp collisions – gluon-gluon fusion (ggF).

The restriction of accessible Higgs boson events poses significant challenges to probing BSM physics through the Higgs boson. Heavy BSM physics effects to Higgs boson production rates are predicted to increase with Higgs boson momentum, and the ggF production mode is expected to be particularly sensitive to such effects due

to the presence of a virtual loop in the process [9, 10].

This thesis presents a novel study of Higgs boson production using $H \rightarrow b\bar{b}$ decays at the ATLAS experiment, which is fully inclusive of all Higgs boson production modes, and was made public in October 2021 [5]. The analysis targeted some of the most energetic Higgs bosons produced at the LHC, by utilising the characteristic collimation of Higgs decay products – the *boosted* decay topology – to reduce immense backgrounds in this final state.

The momentum boost was provided by an additional quark or gluon jet (particle shower created by the hadronisation of these particles) in the event, resulting in a final state of $H(\rightarrow b\bar{b}) + j$, a method developed by BSM particle searches in a similar mass range. The targeted final state takes advantage of the most abundant Higgs boson decay channel and does not restrict Higgs boson production modes, which allows it to be sensitive to highly energetic Higgs bosons.

The analysis aims to probe Higgs boson production both inclusively and in differential momentum bins with a particular focus on high momentum regimes. It was the first Higgs boson study in this channel at the ATLAS experiment, as well as the first ATLAS analysis to target Higgs boson production cross-sections in fiducial volumes with $p_T > 650$ GeV and $p_T > 1$ TeV. Furthermore, the high energy focus and access to the ggF production mode makes the $H(\rightarrow b\bar{b}) + j$ analysis uniquely tuned to study the BSM enhancements in this phase-space, which will be attempted in future iterations of this analysis.

The Higgs boson cross-section measurements were made by performing a complex fit of the reconstructed Higgs boson candidate mass spectra in multiple regions. The author of this thesis made significant contributions across many areas of the fit implementation, development and validation. Furthermore, she also contributed to the calibration of a novel tool – the *boosted double-b tagger* – which combines topological and b -quark identification techniques to recognise boosted $H \rightarrow b\bar{b}$ decays. This tool will aid future studies in this decay channel, and other analyses with

similar final states.

The aim of this thesis is to provide the reader with a comprehensive description of the novel $H(\rightarrow b\bar{b}) + j$ analysis, while placing an emphasis on her contributions. Chapter 1 briefly presents the theoretical background; chapter 2 presents the LHC and the ATLAS experiment; chapter 3 describes the physics object reconstruction techniques utilised in the presented work; chapter 4 presents the identification strategies of the boosted $H \rightarrow b\bar{b}$ topology, and the calibration of the boosted double- b tagger.

Subsequent chapters focus on the $H(\rightarrow b\bar{b}) + j$ analysis. Chapter 5 introduces the analysis, and presents an overview required to contextualise the presented studies; chapter 6 presents the signals and backgrounds considered in the analysis, chapter 7 presents sources of systematic uncertainty in the analysis and their treatment in the measurement fit, studied by the author; chapter 8 delves into fitting studies of the $t\bar{t}$ background; and chapter 9 presents the results of the $H(\rightarrow b\bar{b}) + j$ analysis.

Chapter 1

Theoretical Background

1.1 The Standard Model

The Standard Model (SM) is currently the most complete theory describing fundamental particles and the interactions between them. It was made possible by many extraordinary contributions from scientists throughout the 20th century¹, with most notable contributions by S. Glashow [11], S. Weinberg [12], and A. Salam [13].

In basic terms, it describes three fundamental forces²: the strong force, electromagnetic force (EM), and the weak force; and two classes of elementary particles, grouped by their intrinsic angular momentum – *spin*: *fermions* – particles with half-integer spin, and *bosons*, which have integer spin. The summary of the particles in the SM with details of their masses and charges is given in figure 1.1.

Elementary fermions make up the known matter in the universe, of which there are two groups. *Quarks* make-up composite particles, called *hadrons*, such as protons, neutrons, pions, etc., and interact through all three forces – strong, EM, and weak. There are six flavours of quarks: up, down, strange, charm, bottom, and top.

Leptons – the second fermion group – include three flavours of electron-like lep-

¹ A pleasant read about the history of the Standard Model can be found in [14] – a transcript of a talk by S. Weinberg at the *Symposium on Prestigious Discoveries at CERN* (2003).

² The SM does not include a description of gravity, which is hence omitted from the discussion. Overall, gravity is too weak to influence the studies described in this thesis.

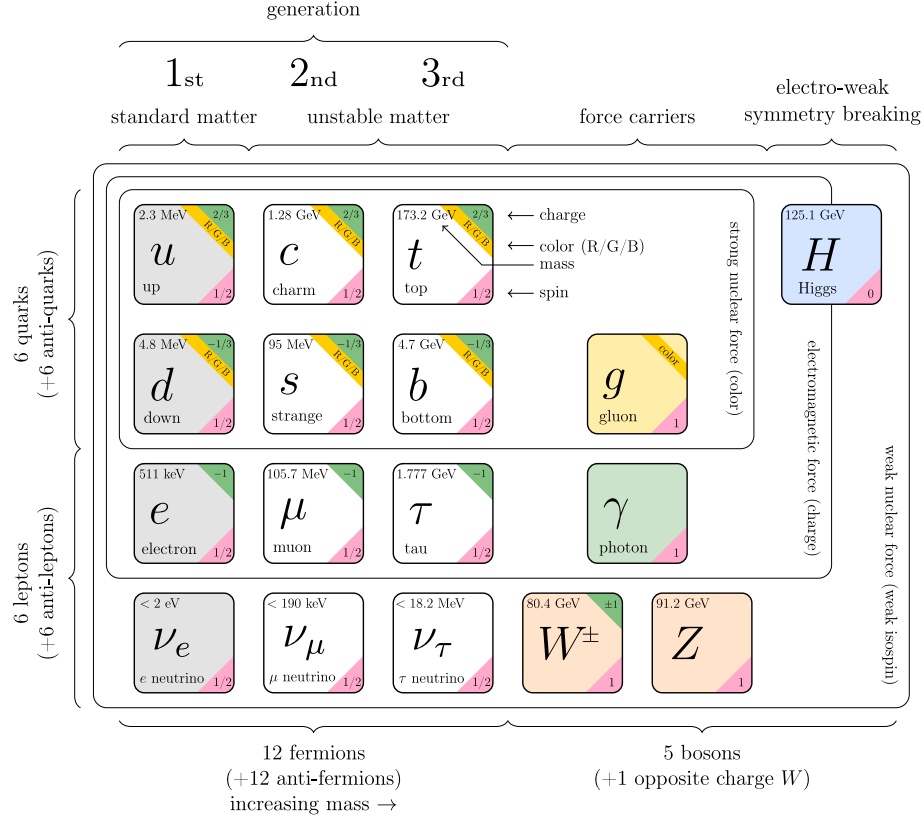


Figure 1.1: Fundamental particles and their basic properties as described by the Standard Model of particle physics. Adapted from [15, 16].

tons: electron, muon and tau, each of which have a counterpart neutrino. All leptons interact through the weak force. The electron-like leptons are charged, and therefore interact through the EM force as well, whereas neutrinos are neutral and only interact via the weak force.

The second class of fundamental particles – bosons – mediate fundamental interactions. Four types of gauge bosons mediate forces: gluons (g) mediate the strong, photons (γ) – EM, and $W^\pm$ and Z bosons – the weak force. Lastly, all particles in the SM acquire mass through the *Brout-Englert-Higgs mechanism* (discussed later), which also implies the existence of a scalar (spin 0) boson, called the *Higgs boson*.

The Standard Model itself is a quantum field theory (QFT) which interprets fundamental particles as excited states of quantum fields, and the dynamics of the theory are described by a Lagrangian. It is a special QFT, called a *gauge theory*,

which must be invariant under certain transformations, collectively called the *symmetry group* of the theory. The symmetry group of the SM is $SU(3) \times SU(2) \times U(1)$.

The symmetries required by each of the sub-groups give rise to the fundamental forces: $SU(3)$ gives rise to the strong force, $SU(2)$ gives rise to the weak force, and $U(1)$ to the EM interactions. The latter two, are known to unify at large energy scales. They are known collectively as the *electroweak* (EW) interaction, and are described by the EW gauge group – $SU(2) \times U(1)$.

1.2 The Higgs Mechanism

To maintain the $SU(2) \times U(1)$ symmetry the bosons mediating the EM and weak forces are required to be massless. This caused a problem in the Standard Model, as, unlike photons, W and Z bosons were predicted (and later observed [17]) to be massive, owing to the short range of the weak force. A solution to this problem was achieved through the Brout-Englert-Higgs mechanism [18, 19] (later – *Higgs mechanism*).

To allow for massive W and Z bosons, the EW symmetry must be spontaneously broken, i.e. the system must have a non-symmetric vacuum solution (ground state). In the SM this is achieved via the Higgs mechanism. It will be briefly described in this section, for further details see [20] and [21].

The Higgs mechanism introduces a complex scalar field ϕ to the SM, which is a $SU(2)$ doublet with two complex (or four real) components:

$$\phi = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix}, \quad (1.1)$$

and enters the SM Lagrangian as

$$\mathcal{L}_H = (\mathcal{D}_\mu \phi)^\dagger (\mathcal{D}^\mu \phi) - V(\phi) + \mathcal{L}_{\text{Yukawa}}. \quad (1.2)$$

The first term is a kinetic term, which describes the interactions between the gauge

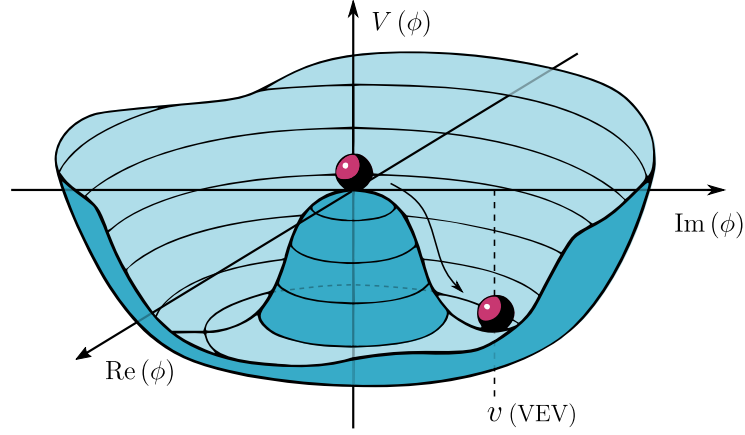


Figure 1.2: Illustration of the Higgs potential. Adapted from [21].

fields via field derivatives, and includes the mass terms of W and Z bosons. The second term describes the field potential, and the last term describes the coupling between the ϕ and fermions.

The breaking of gauge symmetry is built into the field potential, given by:

$$V(\phi) = -\mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2, \quad (1.3)$$

where $-\mu^2$ and λ are real constants. λ must be positive such that $V(\phi)$ has a finite minimum, whereas $-\mu^2$ has to be negative such that the value of ϕ in the minimum energy state, called the *vacuum expectation value* (v , VEV), is non-zero, i.e.³ $\langle \phi \rangle \neq 0$. Under these conditions the potential takes the shape illustrated in figure 1.2, colloquially known as the *Mexican hat potential*.

Without loss of generality, one can choose any orientation of the basis states to define the field in the ground state. By choosing $\langle \phi_3 \rangle = v$, and $\langle \phi_1 \rangle = \langle \phi_2 \rangle = \langle \phi_4 \rangle = 0$, the field in the ground state can be defined as

$$\langle \phi \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}. \quad (1.4)$$

Here, a choice of a particular “direction” of a vacuum state was made. The ability

³ $\langle \phi \rangle$ is used as shorthand for the ground-state $\langle 0 | \phi | 0 \rangle$ in bra-ket notation.

to make a choice of a distinct vacuum state, i.e. the directionality of it, breaks EW symmetry. By minimising $V(\phi)$ (eq. 1.3) the value of the VEV can be found to be

$$v = \sqrt{\frac{\mu^2}{\lambda}}. \quad (1.5)$$

The particle states of a field are described by excitations in the field. In this case, they can be probed by introducing a perturbation in the field $\phi(x)$ in the form of a new scalar field $h(x)$, with $\langle h \rangle = 0$, such that

$$\phi(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h(x) \end{pmatrix}. \quad (1.6)$$

By plugging $\phi(x)$ into equation 1.3, and focusing on the quadratic terms, which, for a scalar field, can be considered to be mass terms, one can find

$$V = \lambda v^2 h^2 + \text{other terms}. \quad (1.7)$$

Hence, the field h is shown to be massive, with $m_h = \sqrt{2\lambda}v$. The EW symmetry breaking mechanism manifests a massive scalar field, called the *Higgs field*, and excitations in this field materialise as scalar particles, called *Higgs bosons*.

The masses for the W and Z bosons are generated in the kinetic term of the Higgs Lagrangian. Interactions with the Higgs field also enable the mass generation for fermions described by the $\mathcal{L}_{\text{Yukawa}}$ term in the Higgs Lagrangian. The coupling constants describing the strength of interactions between fermions and the Higgs field are known as *Yukawa couplings*, and they are directly related to the fermion masses as⁴: $g_f = m_f \sqrt{2}/v$.

1.3 Measuring the Higgs Boson

The Higgs boson discovery in 2012 [6] experimentally completed the Standard Model, but was certainly not the last step in establishing its validity. Since then, studies

⁴ This does not include neutrino masses, which are considered to be beyond-SM physics.

have been dedicated to measure Higgs boson production rates and couplings to various SM particles, and compare them to theoretical predictions.

Furthermore, it is known that the SM is not a complete theory. Many fundamental questions remain unanswered, such as the nature of dark matter, the origin of neutrino masses, etc.. Experimental studies of the Higgs boson could give insight into physics beyond the Standard Model (BSM). Therefore, today, in late 2021, the Higgs boson remains at the focus of the experimental particle physics community, and is the focal point of the work described in this thesis.

1.3.1 Higgs Boson Production and Decays

The Higgs boson is a relatively heavy particle. Currently, the most accurate measurement of the Higgs boson mass is $m_H = 125.25 \pm 0.17$ GeV [22]; hence, large energies are needed to produce a sufficient amount of Higgs bosons to be studied. All Higgs boson experimental studies are currently conducted in pp collisions at the Large Hadron Collider (LHC), which will be presented in chapter 2.

The percentage contributions of the dominant Higgs boson production modes to the total Higgs boson production cross-section at the LHC are given in figure 1.3a. By far the most dominant production mode is gluon-gluon fusion (ggF), expected to contribute 87% of Higgs bosons produced by the LHC, followed by vector boson fusion (VBF) and production in association with a vector boson (VH , $V = W, Z$), which are expected to contribute 7% and 4% of the Higgs bosons, respectively.

Higgs bosons have a very short lifetime ($\tau = 1.6 \times 10^{-22}$ s [23]), and therefore are detected through their decay products. The predicted branching ratios of SM Higgs bosons with $m_H = 125$ GeV are given in figure 1.3b. The most prominent Higgs boson decay (BR=58%), is to two b -quarks ($H \rightarrow b\bar{b}$) – the decay channel of choice for the analysis described in this thesis.

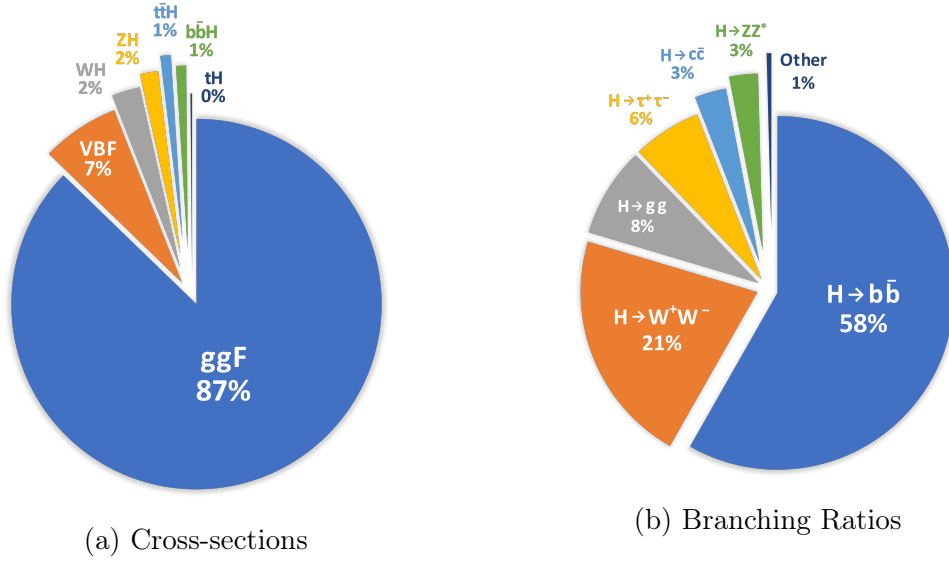


Figure 1.3: Percentage fractions of Higgs boson (a) cross-sections from different production modes in $\sqrt{s} = 13$ TeV pp collisions (total ≈ 56 pb) and (b) branching fractions of different decay channels, as predicted for a SM Higgs boson with $m_H = 125$ GeV. Data from [23].

Higgs Boson Measurements

The most precise Higgs boson mass measurements have been made through measurements of $H \rightarrow ZZ^* \rightarrow 4\ell$ and $H \rightarrow \gamma\gamma$ decays [24, 25]. Despite their relatively low branching ratios, these channels provide exceptionally clean signatures making precise measurements possible. The Higgs boson *signal strength* (μ_H) – the ratio of the observed Higgs boson signal yield (N_{obs}) to its SM expectation (N_{SM}):

$$\mu_H = \frac{N_{\text{obs}}}{N_{\text{SM}}}, \quad (1.8)$$

has so far been measured inclusively, in Higgs boson decays to $\gamma\gamma$, ZZ^* , WW^* , $b\bar{b}$, $\tau\tau$, $\mu\mu$ and $Z\gamma$, and all results were seen to be in good agreement with the SM (as shown in figure 13 of [26], and figure 2 of [27]).

Measurements of Higgs boson production cross-sections inclusively and in differential bins of Higgs boson transverse momentum⁵ (p_T) have also been made in most

⁵ Higgs boson momentum transverse to the collision direction, discussed in section 2.2.

of the prominent Higgs boson production channels: ggF , VBF , WH , ZH and $t\bar{t}H$. All observations made so far were also in agreement with the SM (figures 2 and 9 of [28]). However, all inclusive results were dominated by low p_T contributions (< 300 GeV), and the most extreme regions of Higgs boson p_T so far probed by differential measurements by the ATLAS experiment have been in a fiducial region with $p_T^H > 450$ GeV (figure 9 in [28]).

Higgs boson measurements have been largely focused on signatures including leptons, photons or missing energy (neutrinos) in the event, which help reduce immense quark and gluon backgrounds from proton-proton collisions. However, this comes at the cost of restricting production modes, or choosing final states with low branching ratios.

Higgs boson production is extremely rare, with a Higgs boson produced roughly once every 10^9 inelastic pp collisions⁶ at the LHC. Furthermore, Higgs boson production cross-sections reduce dramatically with Higgs boson transverse momentum, as shown later, in figure 1.4. This is because higher energy particles are harder to produce; and the constituent particles of the proton, between which collisions occur, are more likely to carry small (rather than large) fractions of the proton's energy. Therefore, in order to access high p_T regions of Higgs boson momentum, it is important to probe the most prominent Higgs boson decay, $H \rightarrow b\bar{b}$, and reduce limitations on its production modes.

1.3.2 Boosting the Higgs Boson

The analysis described in this thesis specifically targets high energy $H \rightarrow b\bar{b}$ decays using their unique topology. High energy quarks and gluons are observed in the detectors as collimated showers of particles, called *jets* (discussed in section 3.2). When a Higgs boson decays at high energy to two b -quarks, the two b -quark jets

⁶ The total inelastic pp cross-section measured in $\sqrt{s} = 13$ TeV pp collisions at the ATLAS experiment is ~ 80 mb [29].

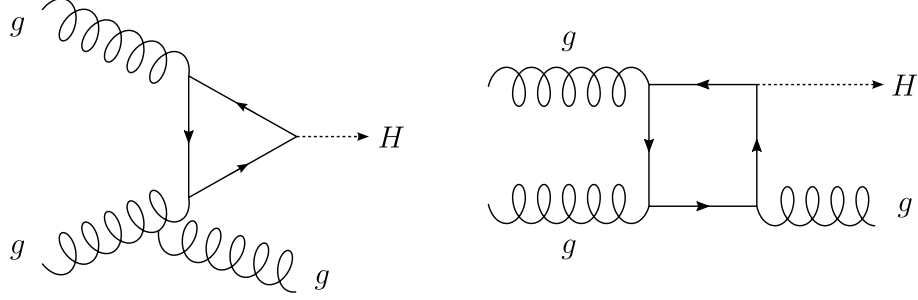


Figure 1.4: Higgs boson production through gluon-gluon fusion with an additional gluon from (left) initial state radiation, and (right) radiated from the virtual loop.

collimate, and can be reconstructed as a single *Higgs jet* with a two-prong substructure. This substructure can be combined with *b*-quark identification methods to identify Higgs jets and substantially reduce backgrounds. This type of decay topology, where multiple quark decays collimate into one large jet with a multiple-prong substructure, is called a *boosted decay*.

The momentum boost is provided by another jet in the event. This final state does not impose restrictions on Higgs boson production modes, and is written as $H(\rightarrow b\bar{b}) + j$. The dominant Higgs boson production mode with this signature is gluon-gluon fusion, in which case the additional jet can be a gluon radiated from one of the initial state gluons or the virtual loop. Feynman diagrams depicting such events are shown in figure 1.4. The jet could also be produced by decays of *W* or *Z* bosons (collectively *V* bosons) to quarks ($V \rightarrow qq$) from the VH production mode, quarks in vector-boson-fusion (VBF), and top quarks in $t\bar{t}H$ production modes.

Figure 1.5 shows the cumulative Higgs boson cross-sections

$$\Sigma(p_T^{\text{cut}}) = \int_{p_T^{\text{cut}}}^{+\infty} \frac{d\sigma}{dp'_T} dp'_T \quad (1.9)$$

(from p_T^{cut} to $+\infty$), of each Higgs boson production mode, and their fractional contributions as a function of Higgs boson p_T . Throughout most of the Higgs boson p_T spectrum, the ggF production mode is dominant, but its contribution decreases

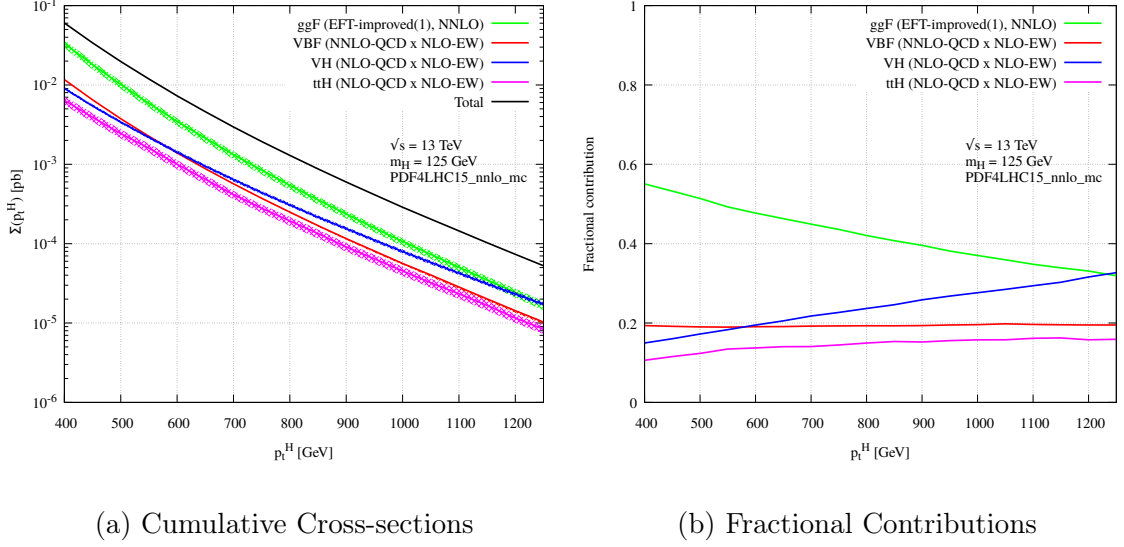


Figure 1.5: The (a) cumulative Higgs boson production cross-sections $\Sigma(p_T^{\text{cut}}) = \int_{p_T^{\text{cut}}}^{+\infty} (d\sigma/dp_T') dp_T'$ (from p_T^{cut} to $+\infty$), and (b) fractional contributions of Higgs boson production modes to $\Sigma(p_T^{\text{cut}})$ as a function of Higgs boson p_T [30].

at high p_T . Hence, it is beneficial to develop a high p_T Higgs boson analysis to be inclusive of all production modes.

The $H(\rightarrow b\bar{b}) + j$ analysis is the first ATLAS analysis to be sensitive to the ggF production mode, and to target Higgs boson production at $p_T^H > 650$ GeV [28]. More details on Higgs jet reconstruction and identification will be given in chapters 3 and 4, and a deeper discussion on the experimental advantages of measuring the Higgs boson in this final state will be given in section 5.1.

1.3.3 The Boosted Higgs Boson — A Portal to New Physics

In the Standard Model, all massive particles acquire mass through interactions with the Higgs field, and thus are expected to couple to Higgs bosons. If massive BSM particles do exist, Occam's razor would suggest that they could also acquire mass through interactions with the Higgs field, and would also be expected to couple to Higgs bosons.

As the scientific community has not yet observed any indications of new heavy

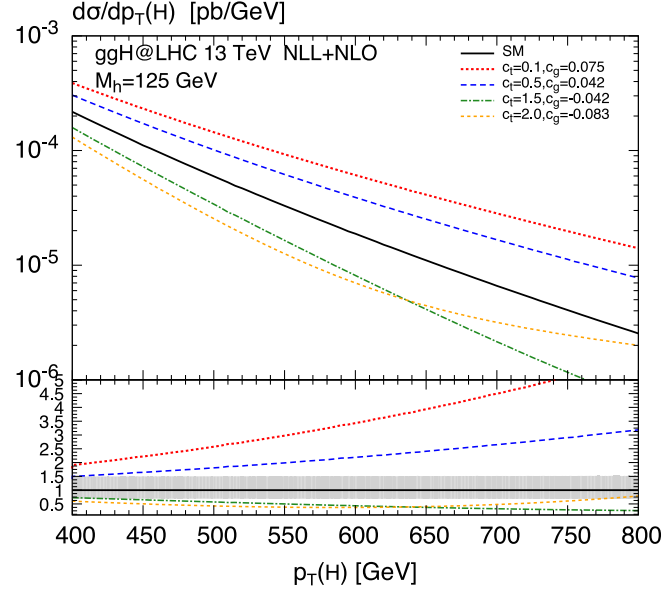


Figure 1.6: The transverse momentum spectrum of a Higgs boson between 400 GeV and 800 GeV in the SM compared with spectra with various BSM modifications [9]. The coefficients c_g and c_t correspond to BSM modifications to Higgs boson interactions with gluons, and the top Yukawa coupling (in SM $c_g = 0, c_t = 1$). The bottom panel shows the ratio of modified cross-sections and the SM. The variations were chosen such that the inclusive cross-section is within 20% of the SM, which roughly was the experimental uncertainty on the measured Higgs cross-section at the time of the studies.

particles directly, they are also searched for via their impact on known processes. For this reason, Higgs production through gluon-gluon fusion is a particularly interesting production mode to study. Higgs bosons do not couple to massless gluons directly, instead interacting through a virtual quark loop, dominated by top quarks, because of their heavy mass. In this virtual loop, energy does not need to be strictly conserved, owing to the uncertainty principle, and scales much higher than the electroweak scale can be accessible (e.g. heavy BSM particles).

Such effects should be more pronounced at higher Higgs boson momentum, as the heavy virtual particles would in effect be less defiant of energy conservation, i.e. be less “off-shell”. Figure 1.6 shows possible modifications to the ggF production

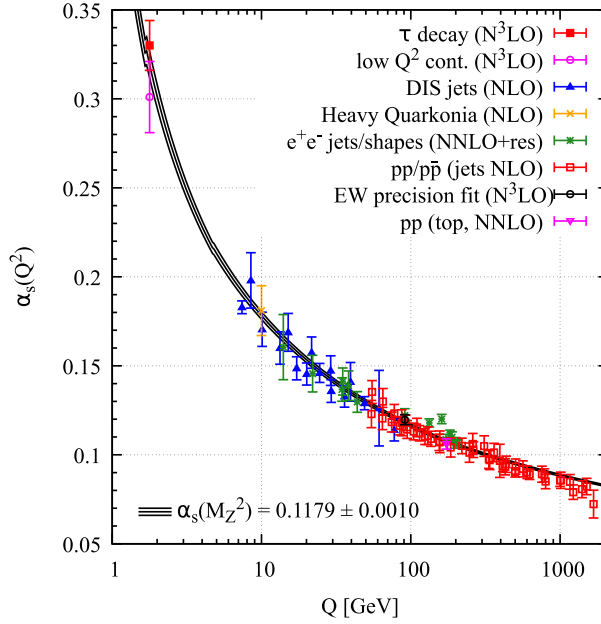
cross-section as a function of Higgs boson transverse momentum (p_T), as found by a 2016 study [9]. The coefficients c_g and c_t describe BSM modifications to the effective Higgs boson coupling to gluons and the top Yukawa coupling (SM $c_g = 0$, $c_t = 1$), and were chosen such that the inclusive cross-section would not deviate from the SM by more than 20%, which was roughly the experimental uncertainty on it at the time. It is seen that BSM contributions become more prominent as a function of Higgs boson p_T , which makes these regions particularly interesting to study. Furthermore, the study observed that large changes in total Higgs boson cross-section were not required to obtain significant modifications to the cross-section p_T spectrum, further motivating the aim to probe higher regions of Higgs boson p_T .

Measuring the Higgs boson production cross-section through ggF at high Higgs boson p_T would provide a model-independent way of probing BSM physics. The analysis at the focus of this thesis is the first analysis at the ATLAS experiment to target extremely high energy Higgs bosons in a final state sensitive to ggF .

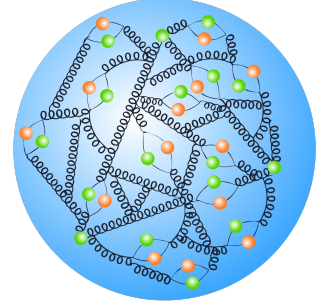
1.4 Quarks and Gluons in Final States

The $H(\rightarrow b\bar{b}) + j$ final state is entirely comprised of quarks and gluons, which are *colour charged* particles. Colour charge is the quantum number possessed by particles interacting through the strong force. As the name implies, the strong force is the strongest of fundamental forces and dominates the behaviour of colour charged particles. The theory governing strong interactions is called Quantum Chromodynamics (QCD). More information on QCD in the context of high energy physics and pp collisions can be found in [31].

The strength of the strong interactions is described by the strong coupling constant α_s . However, calling α_s a constant is, in fact, a misnomer, as it decreases as the interaction energy scale increases. The relationship between α_s and momentum transfer in the interaction Q is shown in figure 1.7a.



(a)



(b)

Figure 1.7: (a) The strength of the strong coupling constant α_s as a function of the energy scale Q of the interaction [32]. The points depict different experimental measurements made using theoretical predictions with differing degrees of precision, and the lines indicate the average. (b) An artistic illustration of the proton structure. Green circles represent quarks, orange – anti-quarks, and coiled lines represent gluons. Adapted from [33].

At large energy scales, the coupling becomes very weak, and strongly interacting particles behave as free particles. This phenomenon is called *asymptotic freedom*, which is the case for quarks and gluons in *hard scattering events* – where momentum transfer is large, such as pp collisions at the LHC.

As the available energy decreases, for example, when final state quarks and gluons move away from the interaction point, the coupling strength rapidly increases, to the point where it becomes energetically favourable to manifest quark pairs out of the vacuum, such that composite colour-neutral particles – hadrons – are created, a process called *hadronisation*⁷. In a high energy collision, the produced hadrons will have enough energy to split and hadronise further, forming a particle shower in the

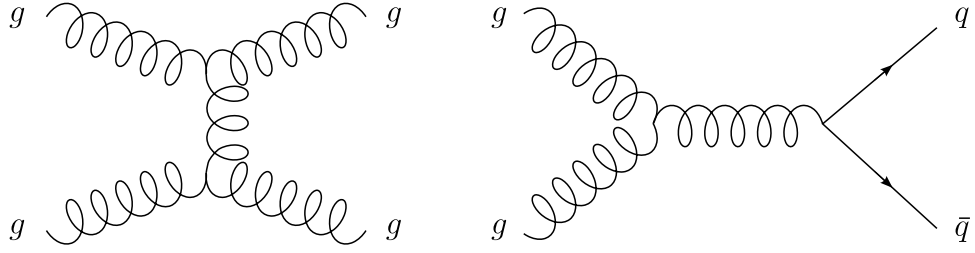


Figure 1.8: Examples of (left) gluon-gluon scattering and (right) gluon splitting events, common in pp collisions. Such events are known collectively as QCD events.

direction of the original quark or gluon, called a *jet*.

Due to the large α_s values at natural energy scales, no free colour-charged particles are currently known to exist in nature. This phenomena is called *confinement*. Quarks and gluons form colour-neutral hadrons in which quarks are bound together through exchange of quarks and gluons between them. An artistic illustration of a hadron is given in figure 1.7b

Decays to quarks or gluons are called *hadronic decays*. Other types of decays mentioned in this thesis are *leptonic* decays, such as $W \rightarrow \ell\nu$, or $t \rightarrow Wb$, where the W boson decays leptonically; and *semi-leptonic* decays of top pair production ($t\bar{t}$) where one top quark decays hadronically, and the other leptonically.

The analysis is performed using data from proton-proton collisions. Protons are hadrons, made up of quarks and gluons, hence, in their collisions the most common events involve scattering between these particles. Examples of such events: $gg \rightarrow gg$ and $gg \rightarrow q\bar{q}$, are given in figure 1.8. Events of this type are collectively called *QCD events*, and make up the largest type of background for the $H(\rightarrow b\bar{b}) + j$ analysis and many other physics analyses at pp colliders.

⁷ Due to their short lifetime, top quarks do not hadronise, and almost always instead decay weakly $t \rightarrow Wb$ [22].

1.5 Chapter Overview

This chapter has given a brief overview on the fundamental forces and particles described by the Standard Model, in section 1.1, and the key role that the Higgs mechanism, and by extension – the Higgs boson plays in the SM, in section 1.2.

Section 1.3 discussed the Higgs boson in an experimental context. An overview of Higgs boson production and decays was given. Currently, most Higgs boson measurements are dominated by low energy Higgs boson contributions, which show good agreement with the Standard Model. However, the production of Higgs bosons at high energies (quantified by transverse momentum, p_T) is not yet thoroughly explored and could be enhanced by BSM physics.

This thesis focuses on Higgs boson production at high energy, by studying $H \rightarrow b\bar{b}$ decays with large momentum boosts provided by an external particle jet. Motivations for this choice of final state are introduced in section 1.3.2, and will be discussed further in section 5.1. As the final state of this analysis consists of quarks and gluons, section 1.4 discussed the behaviour of quarks and gluons in pp collisions and introduced the concept of *jets*.

Chapter 2

The ATLAS Experiment

2.1 The Large Hadron Collider

The 1970s were a decade abundant with particle physics achievement. Many significant discoveries were made throughout the decade, solidifying the Standard Model as the most probable theory of its time, such as evidence of asymptotic freedom, the observation of neutral current interactions, the discovery of charm quarks through the measurement of J/ψ mesons, and others [34].

However, many of the key components of the Standard Model still needed to be verified. The top-quark and the τ -neutrino were yet to be observed, little was known about the behaviour of quark-gluon plasma, and there was still no evidence of the existence of the Higgs boson – the key component of electro-weak symmetry breaking and thus – the Standard Model itself. The energy scales needed to study these phenomena were far from accessible for the experiments of the time, but a large hadron accelerator capable of reaching them was already on the minds of scientists. It was first mentioned in 1977 by Sir John Adams – at the time, the Director General of the European Organisation for Nuclear Research (CERN¹) [35], and the scientific potential of such a hadron machine was consolidated by the discovery of W and Z bosons by the UA1 and UA2 experiments at the Sp $\bar{p}$ S proton-anti-proton collider

¹ French: Conseil Européen pour la Recherche Nucléaire.

($\sqrt{s} = 540$ GeV) in 1983 [17].

More than three decades later, in 2009, the largest particle accelerator in the world – the Large Hadron Collider (LHC) – began operation at CERN in Geneva, Switzerland. It is a circular accelerator, with a circumference of 27 km straddling the territories of Switzerland and France. It currently accelerates protons to 6.5 TeV and collides them at a centre-of-mass energies of 13 TeV – the highest energy scale particle collisions achieved so far.

The LHC operates in multiple-year-long periods of activity called *runs*, during which data is taken almost continuously, interspersed with 2–3 month long technical stops at the end of each year for maintenance work. Long periods of inactivity – *long shutdowns* – are scheduled in between the runs for large-scale maintenance and upgrades. The findings discussed in this thesis were made using the data gathered from 2015 to 2018 – the entire span of *Run 2* of the LHC (later shortened to *Run 2*).

To reach these high energies, protons from an ionised hydrogen source are accelerated to 450 GeV by a succession of smaller accelerators shown in figure 2.1, before being injected to the LHC. The protons circulate in two ultra-high vacuum beampipes, travelling in opposite directions. The beams are crossed at 4 collision points, called *interaction points* (IP), rigged with various detectors constituting the LHC experiments. The four main experiments at these interaction points are ALICE, LHCb, CMS and ATLAS, also shown in figure 2.1. Details on the LHC design and operation in *Run 2* can be found in [38] and [39], respectively.

Within the beams, the protons are grouped in bunches of approximately 10^{11} protons. The bunches are spaced such that the collisions at the crossing points happen every 25 ns. It is unfeasible to record all collisions produced at such high rates, therefore the experiments usually have hardware and/or software based systems to discern and only record potentially interesting collisions, called *events*, by indicating – *triggering* on – certain physics objects. The ATLAS Trigger System is described later in section 2.2.4.

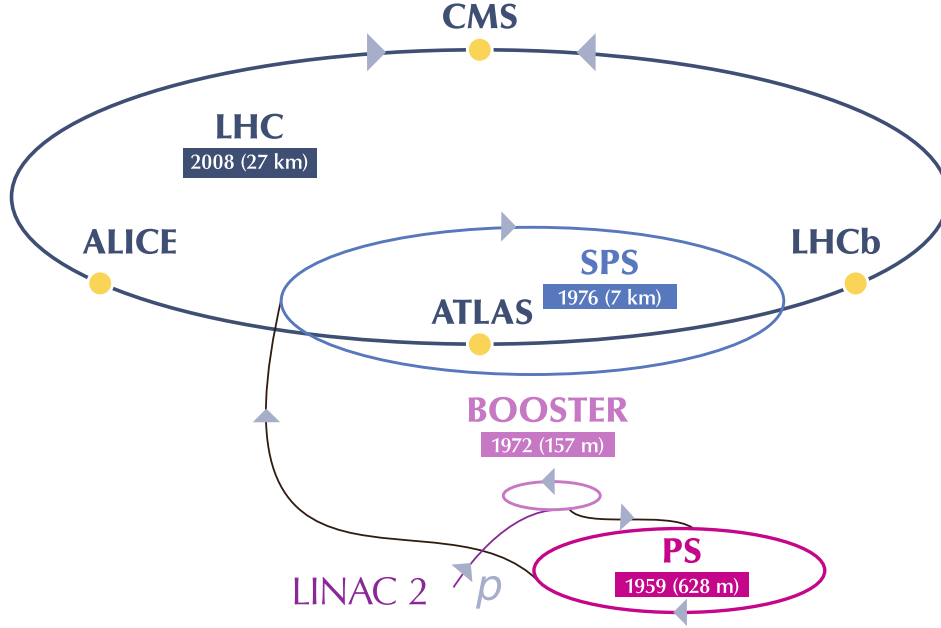


Figure 2.1: A diagram of the LHC part of the CERN accelerator complex. Protons are first accelerated to 50 MeV by the linear accelerator *Linac 2*, followed by three consecutively larger circular accelerators: the *Proton Synchrotron Booster*, the *Proton Synchrotron* (PS) and the *Super Proton Synchrotron* (SPS), each accelerating the protons to 1.4 GeV, 25 GeV and 450 GeV, respectively [36]. Adapted from [37].

To compare theoretical predictions with experimental findings, it is vital to know the expected number of events of interest produced by an experiment. At any point in time the rate at which events with a cross-section σ occur is given by

$$\frac{dN}{dt} = \sigma \mathcal{L}, \quad (2.1)$$

where $\mathcal{L}$ is the *instantaneous machine luminosity* of the experiment – a machine quantity. The total number of interesting events can be found by integrating equation 2.1. The time integral of $\mathcal{L}$, is more simply referred to as *integrated luminosity* or *luminosity* (L). The cumulative proton-proton (pp) collision luminosity delivered by the LHC and recorded by the ATLAS experiment in *Run 2* is shown in figure 2.2 [40]. To be used in physics analyses (in figure: *Good for Physics*), the data has to be collected while all detectors are fully operational, and assessed to be of good quality.

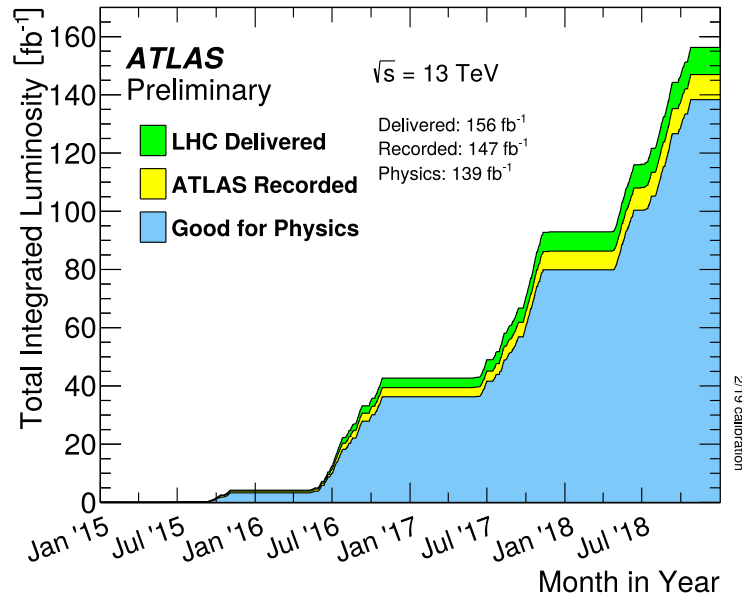


Figure 2.2: The cumulative luminosity delivered by the LHC (green), recorded by the ATLAS experiment (yellow) and approved for use in physics analyses (blue) in *Run 2* (2015-2018). Data shown include special runs for detector calibration and machine commissioning [40].

Interesting events used in LHC analyses are usually rare. High luminosity is desirable to increase the chances of producing rare events. One way higher luminosities are achieved at the LHC is by maximising the number of protons in each bunch. However, as well as increasing the luminosity, this increases the chances of more than one pp collision occurring per bunch crossing. Additional interactions in a bunch crossing are called *in-time pileup*. Pileup contributes low energy deposits which cause adverse effects on event reconstruction [41].

Another source of pileup is *out-of-time* pileup originating from the slow response time of some detectors. In some cases the signal integration time of a detector is slower than the 25 ns bunch spacing. This does not cause concern as events of interest which leave signatures in these detectors are rare enough that they are not expected to happen more than once within the response time. However, because of the slow response, residual signals from neighbouring bunch crossings can be

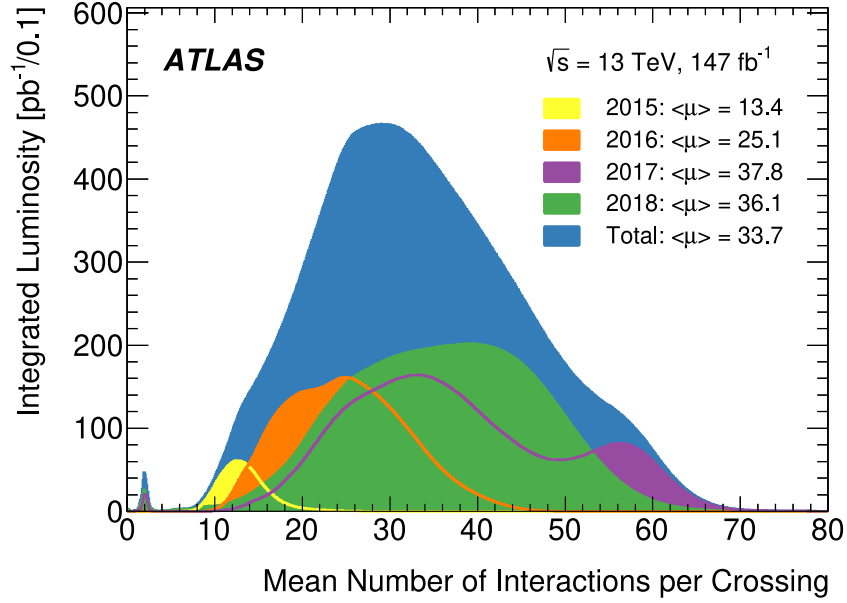


Figure 2.3: Luminosity-weighted distributions of the mean number of interactions per bunch crossing – μ – over *Run 2*, yearly and collectively. The yearly and total *Run 2* averages of mean interactions per crossing are given in the legend. Data shown includes special runs for detector calibration and machine commissioning [40].

recorded, resulting in pileup.

The occurrences of pileup are stochastic in nature, so the amount of pileup is described by the *mean number of interactions* per bunch crossing

$$\mu = \mathcal{L}_{\text{bunch}} \times \frac{\sigma_{\text{inel}}}{f_r} \quad (2.2)$$

where $\mathcal{L}_{\text{bunch}}$ is the instantaneous per bunch luminosity, σ_{inel} is the inelastic pp cross-section (80 mb for 13 TeV collisions), and f_r is the LHC revolution frequency [40]. The values of μ throughout *Run 2* are shown in figure 2.3. The average number of simultaneous interactions per bunch crossing over all years (i.e. average μ over all years in *Run 2*) is just below 34 [40].

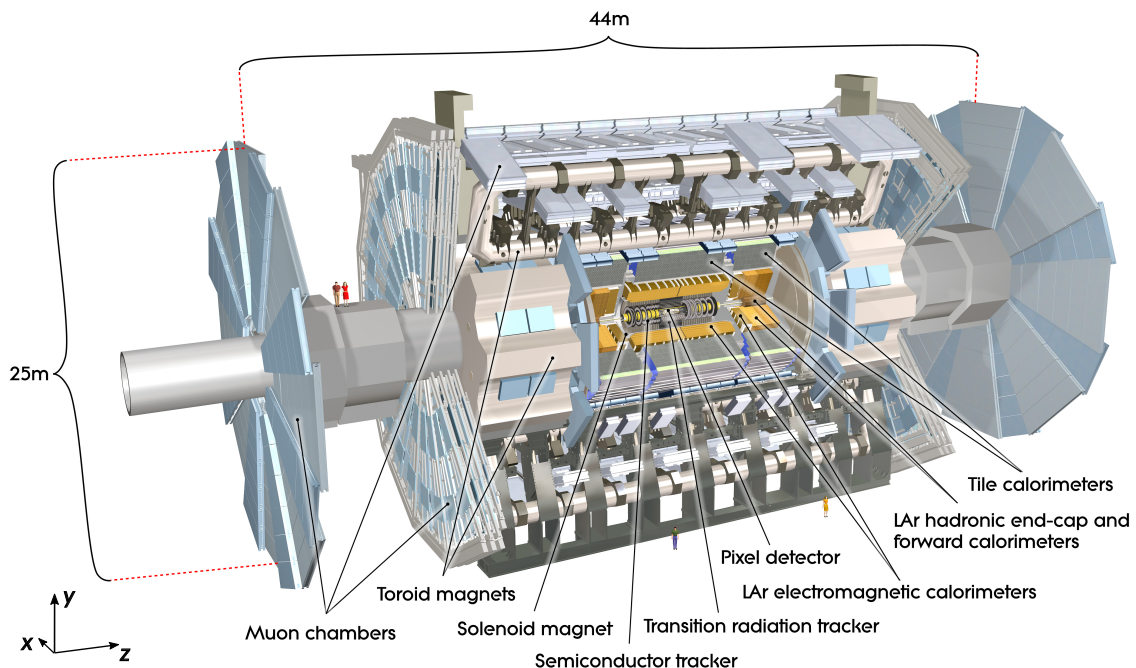


Figure 2.4: A diagram of the components of the ATLAS Experiment at CERN [42]. The Cartesian coordinate definition is shown in the bottom left. The people are included for scale and are not part of the detector system.

2.2 The ATLAS Experiment

Placed at one of the LHC interaction points is the ATLAS (A Toroidal LHC ApparatuS) experiment – the largest general-purpose particle detector in the world. *General purpose*, in this case, means that the experiment is designed such that a variety of analyses, covering a range of physics topics, could be possible using the data recorded by it. The ATLAS experiment is also one of the largest collaborative efforts in the world with approximately 3000 scientific authors from 181 institutions worldwide [1].

The experiment consists of a system of detectors, collectively called the *ATLAS detector*, arranged in concentric cylindrical layers around the interaction point, with nearly 4π solid angle coverage. A diagram of the ATLAS detector is shown in figure

2.4. The cylindrical part of the ATLAS detector is called the *barrel*, and the circular bases – the *endcaps*. The following is a short overview of the ATLAS detector components. An in-depth description of the detector sub-systems is given later in this chapter. The information throughout this chapter is largely based on the official ATLAS Experiment description [42].

Closest to the interaction point is a set of *tracking detectors* used for capturing the trajectories of passing particles, collectively called the *Inner Detector* (section 2.2.1). In order of proximity to the interaction point, these are: the Silicon Pixel Detector, the Semiconductor Tracker (SCT), and the Transition Radiation Tracker (TRT). The Inner Detector is surrounded by a superconductive solenoid magnet producing a 2 T magnetic field.

Outside the Inner Detector is the *Calorimetry System* (section 2.2.2), which is used for energy measurement. It is comprised of a liquid argon (LAr) electromagnetic (EM) calorimeter; and a hadronic calorimeter, comprised of a steel and scintillator tile calorimeter in the barrel region and a LAr calorimeter in the endcap region; and a LAr forward calorimeter. Placed around the calorimeters is a sophisticated muon detection system – the *Muon Spectrometer* (section 2.2.3), which utilises several different tracking technologies within toroidal magnets.

The Coordinate System

ATLAS analyses use a standardised coordinate system [42]. The definition of the Cartesian coordinates is indicated in the ATLAS detector diagram shown in figure 2.4. The z -axis is defined by the beam direction, and the circular cross-section of the detector is in the $x - y$ plane. The x -axis is pointing towards the centre of the LHC ring, and the y -axis is pointing upwards.

As the detector is cylindrical it is more useful to use cylindrical coordinates. The radial distance from the origin is denoted by r . The azimuthal angle ϕ is in the $x - y$ plane, and the polar angle θ is between the $x - y$ plane and the z -axis. Both are

defined in terms of directional momentum components:

$$\tan \phi \equiv \frac{p_y}{p_x}, \quad \text{and} \quad \cot \theta \equiv \frac{p_z}{p_T}. \quad (2.3)$$

where p_T is the momentum component in the $x - y$ plane, i.e. transverse to the beam. This definition of *transverse* will be used throughout the thesis unless stated otherwise. The polar angle is expressed in terms of pseudorapidity

$$\eta \equiv -\ln \left[\tan \frac{\theta}{2} \right], \quad (2.4)$$

which goes to 0 when the direction is perpendicular to the beamline (in the $x - y$ plane), and ∞ when the direction is along the beamline ($\theta = 0$).

2.2.1 The Inner Detector

ATLAS tracking detectors capture “images” of particle paths, called *tracks*. Electromagnetically charged particles passing through the tracking detectors leave small energy deposits, called *hits*, which are combined to make tracks.

The detectors operate within a strong magnetic field. Charged particles travelling within magnetic fields experience a perpendicular force causing their trajectories to curve. The radius (r) of the curve is related to the particle momentum (p) as

$$p = q|\mathbf{B}|r \cdot \sin \angle (\mathbf{v} \times \mathbf{B}), \quad (2.5)$$

where q and $\mathbf{v}$ are the charge and velocity of the particle, and $\mathbf{B}$ is the magnetic flux density. In the transverse case $\mathbf{v}$ is always perpendicular to $\mathbf{B}$, simplifying the expression²

$$p_T = q|\mathbf{B}|r. \quad (2.6)$$

The ATLAS Inner Detector (ID) is comprised of three sub-detectors shown in figure 2.5: the Silicon Pixel Detector, the Semiconductor Tracker (SCT), and the

² The given expression is general (i.e. in SI units). To get p_T in [GeV], the expression $p_T = 0.3q|\mathbf{B}|r$ can be used with q in units of electron charge $|e|$, $|\mathbf{B}|$ in [T], and r in [m].

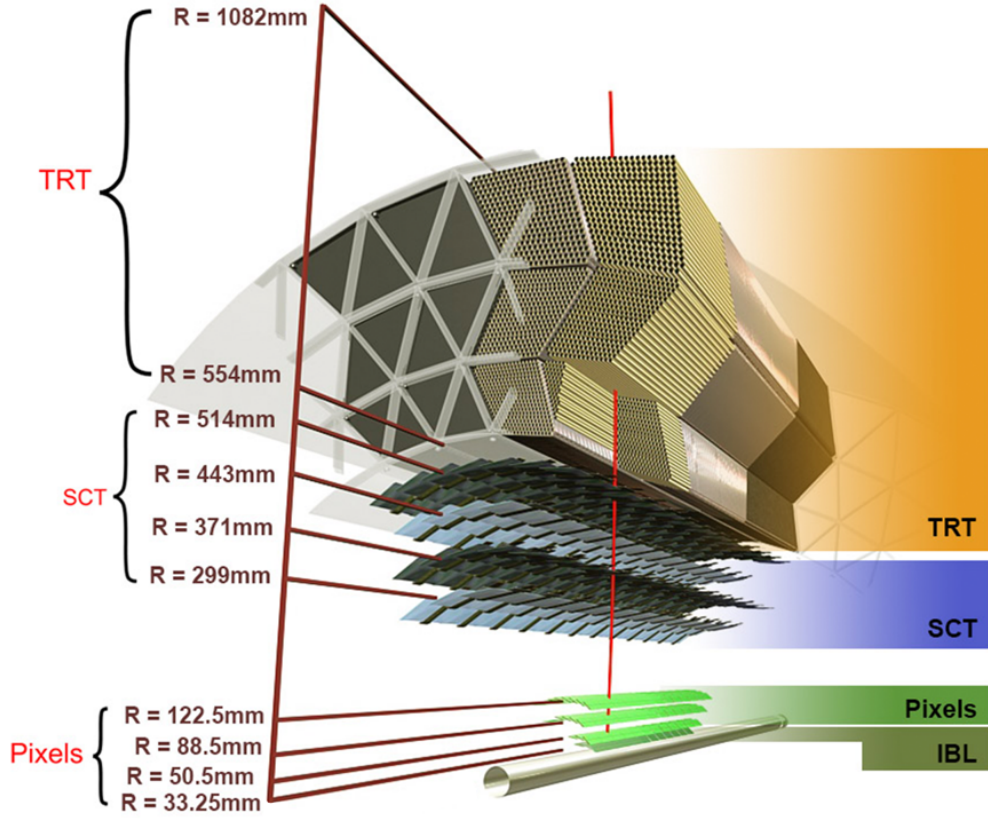


Figure 2.5: A diagram of the barrel cross-section of the ATLAS Inner Detector, and its components [44].

Transition Radiation Tracker (TRT). It is surrounded by a solenoid magnet generating a 2 T magnetic field. The ID spans 3512 mm on either side of the interaction point, has a radius of 1150 mm, can make measurements within $|\eta| < 2.5$, and was designed with a minimum momentum resolution requirement of $\sigma(p_T)/p_T \leq 0.05\% \text{ GeV}^{-1} p_T \oplus 1\%$ (table 1.1. in [42]).

The spatial resolutions³ of the three detector groups are: $10 \times 115 \mu\text{m}^2$ for the Silicon Pixel Detector, $17 \times 580 \mu\text{m}^2$ for the SCT, and $130 \mu\text{m}$ in the $r - \phi$ direction for the TRT. The Pixel Detector on average provides 4 spatial hits per track, the SCT provides 8, and the TRT – around 30 [43].

³ Areas here and later in the section are quoted as $(r - \phi) \times z$.

The Silicon Pixel Detector

The Silicon Pixel Detector is the closest detector to the interaction point, consisting of four barrel layers and three endcap disks. Its primary use is to accurately measure primary and secondary interaction vertices, which is particularly important for the identification of b -quarks, discussed in chapter 3. The detector has to be very close to the interaction point and offer high granularity, therefore silicon pixels are used.

The inner-most barrel layer, called the *Inner B-Layer* (IBL) has been added during Long Shutdown 1, improving vertex reconstruction and tracking [45]. The IBL is placed at an average radius of 33.25 mm from the beam pipe, and has ~ 12 million $50 \times 250 \mu\text{m}^2$ pixels in total, implemented using two different silicon sensor types with $\mathcal{O}(200 \mu\text{m})$ thicknesses.

Other barrel layers and endcap disks use $250 \mu\text{m}$ thick silicon wafer sensors with 46080 pixels of $50 \times 400 \mu\text{m}^2$ dimensions. One sensor with its readout electronics makes a *module*. Each module has an intrinsic accuracy of $10 \mu\text{m}$ in the $r - \phi$ direction in all regions, and $115 \mu\text{m}$ both in the z direction in the barrel and in the r direction in the endcap disks (table 4.1 in [42]).

In the barrel layers, the modules are installed in staves arranged in a petal formation at a 20° azimuthal angle. Each staffe has 13 modules. The layers are at radial distances of 50.5 mm, 88.5 mm and 122.5 mm, with 22, 38 and 52 staves, respectively. The endcap disks are each divided into 8 sectors with 6 modules per sector. Combined, the three barrel layers and six endcap disks amount to 1744 pixel modules, or over 80 million pixels.

The Semiconductor Tracker

Outside the Pixel Detector, the Semiconductor Tracker (SCT) provides four spatial particle track points within $|\eta| < 2.5$, using silicon micro-strip sensors. Strip sensors are used as they offer high granularity for precision track reconstruction at a lower cost and less complex implementation than pixel sensors.

The detector consists of four barrel layers and nine disks at each endcap. In the barrel region the layers are placed at radial distances of 299 mm, 371 mm, 443 mm, and 514 mm. All layers use modules with identical micro-strip sensors glued on both sides of a baseboard, aligned with a small stereo angle of 40 mrad, enabling a point-in-space measurement.

The SCT has 4088 sensors, each with 1536 readout channels, amounting to more than 6 million readout channels in total. The intrinsic accuracy of point-in-space measurements for a single module are $17\,\mu\text{m}$ in the $r - \phi$ direction in both barrel and endcap regions, $580\,\mu\text{m}$ in the z direction in the barrel region, and $580\,\mu\text{m}$ in the r direction in the endcaps (table 4.1 in [42]).

Transition Radiation Tracker

The Transition Radiation Tracker (TRT) is the outermost detector in the ID, spanning radially between 554 mm and 1082 mm, consisting of $\sim 300\,000$ straw tubes with a diameter of 4 mm. It provides a large number of hits per track, around 30 on average [43], within its $|\eta| < 2$ acceptance, as well as particle identification capabilities.

The straw tubes in the barrel region are placed parallel to the beam, and span the length of the TRT detector⁴ (144 cm). They are arranged in three cylindrical rings, with 73 layers in total. In the endcaps the straw tubes are 36 cm long, arranged in wheels, pointing radially outward in the azimuthal ($r - \phi$) direction, with 160 layers of straws per end-cap [46]. Because the wires in the barrel do not have fine segmentation along the z -axis, the TRT detector only provides track information in the $r - \phi$ direction with an intrinsic accuracy of $130\,\mu\text{m}$ [42].

The TRT also is used to discriminate between electrons and pions through the use of transition radiation [47], which is emitted by charged relativistic particles passing a boundary between two media with different dielectric constants. The

⁴ The wires are electrically split into 2 – 3 parts, depending on proximity to the interaction point, to reduce occupancy.

transition radiation emitted by the particle amplifies the signal in the detector. On average, electrons produce more transition radiation in the TRT compared to pions, which can be used to differentiate between the two. This function of the TRT is not used in the work described in this thesis. More information on particle identification with the TRT can be found in [46].

2.2.2 The Calorimetry System

Calorimeters are detectors which measure particle energy through the interactions between the particle and the detector material. When particles come in contact with the detector material, they produce a *particle shower*. The energy of the initial particle can be deduced by measuring the energy deposited in the calorimeter material by the secondary shower particles.

The dominant types of interactions between traversing particles and matter are energy dependent [47]. High energy photons and electrons shower solely through EM interactions, creating an EM cascade primarily progressing through pair production ($\gamma \rightarrow e^+e^-$) and photon bremsstrahlung ($e^{+/-} \rightarrow e^{+/-}\gamma$), called an *electromagnetic shower*. As the shower develops, the shower particles lose energy, until they primarily interact through ionisation and excitation of the detector material, rather than pair production and bremsstrahlung, stopping the cascade. Hadrons produce much more complex showers, called *hadronic showers*, which progress through strong and secondary EM interactions.

The rate at which particles within the shower lose energy in a material determines the length of the shower and therefore is one of the most important shower characteristics. For electromagnetic showers this is characterised by *radiation length* X_0 , which is the length an electron has to travel in a material to lose $1 - 1/e$ ($\sim 63\%$) of its initial energy through bremsstrahlung. Likewise, photons have to travel $\frac{9}{7}X_0$ to lose the same amount of intensity through pair production [48]. The longitudinal shower profile of hadronic showers is characterised by the mean free path for a

hadron in a material, called the *nuclear interaction length* λ [48].

Both radiation and nuclear interaction lengths are material characteristics, and for most materials $\lambda > X_0$, for example in lead $X_0 = 0.56$ cm, whereas $\lambda = 17.59$ cm [49]. Therefore, hadronic showers are typically much longer and broader. Due to the different properties of EM and hadronic showers, calorimeters are often designed to target one type of shower, with measurement accuracy and full shower containment in mind. In general purpose experiments, such as ATLAS, EM calorimeters are placed in front of the hadronic calorimeters and should contain the full EM shower, with only hadronic showers entering the hadronic calorimeters. The hadronic calorimeters are also designed to be denser and larger so as to contain most hadronic showers.

Calorimeters measure energy using *active materials*, which convert some of the shower energy to signals, either via ionisation of electrons in the material, which induce a current with the use of electric fields, or by converting the excitations to light through scintillation, which is collected using photosensitive devices.

To make an accurate measurement, it is paramount that most of the created showers are captured. To increase the longitudinal progression of the showers, layers of dense *absorber materials* can be used, which do not provide an energy measurement, but induce much quicker shower development. Calorimeters which consist of alternating layers of active and absorber materials are called *sampling calorimeters*, as the energy measurement is made by interpolating between signals registered in the active material layers. All ATLAS calorimeters are sampling calorimeters.

A view of the ATLAS calorimetry system is shown in figure 2.6. It consists of three main sub-systems: the liquid argon (LAr) EM calorimeter, the hadronic calorimeter combining LAr calorimeters in the endcaps and plastic tile calorimeters in the barrel, and the LAr forward calorimeter. Detailed parameters of the calorimeter system can be found in table 1.3 of [42].

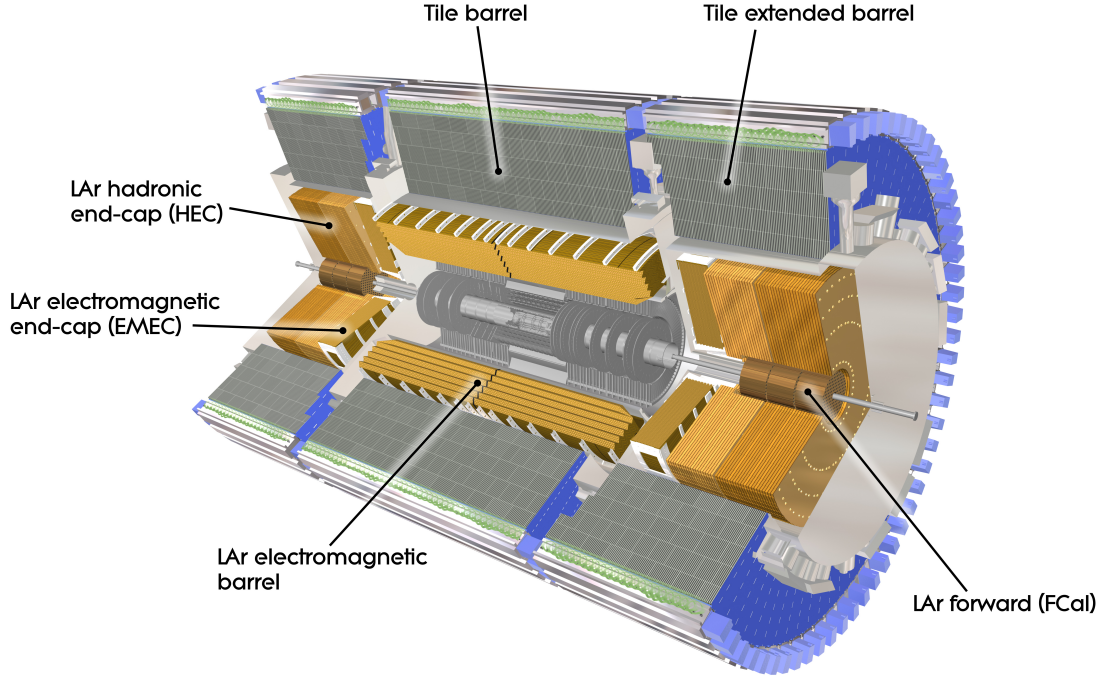


Figure 2.6: Diagram of the ATLAS calorimetry system components [42].

Energy Resolution of ATLAS Calorimeters

The fractional energy resolution of calorimeters can be parameterised as

$$\frac{\sigma_E}{E} = \frac{a}{\sqrt{E}} \oplus \frac{b}{E} \oplus c, \quad (2.7)$$

where a is the *stochastic* term rising from the random nature of the showering process; b is the *noise* term describing the contribution of electronic noise from the readout chain; and c is the *constant* term grouping all non-energy-dependent contributions [48].

The energy resolution of the ATLAS EM calorimeter was measured in electron test-beams [50], and found to be

$$\frac{\sigma_E}{E} = \frac{2.8\% \sqrt{\text{GeV}}}{\sqrt{E}} \oplus \frac{0.12 \text{ GeV}}{E} \oplus 0.3\%. \quad (2.8)$$

The hadronic calorimeter energy resolution measured in pion test-beams [50] was

found to be

$$\frac{\sigma_E}{E} = \frac{52.9\% \sqrt{\text{GeV}}}{\sqrt{E}} \oplus 5.7\%, \quad (2.9)$$

with a negligible electronic noise term.

ATLAS Electromagnetic Calorimeter

The ATLAS EM calorimeter is a sampling calorimeter using liquid argon as the active material and lead as the absorber. The detector consists of cavities filled with liquid argon interspersed with accordion-shaped electrodes and lead plates. This geometry allows for ϕ symmetry without azimuthal cracks [42].

The barrel and endcap parts of the calorimeter cover $|\eta| < 1.475$ and $1.375 < |\eta| < 3.2$, respectively. The barrel detector is made up of two half-barrels with a small gap at $z = 0$, and the endcap calorimeters consist of two coaxial wheels (outer: $1.375 < |\eta| < 2.5$, and inner: $2.5 < |\eta| < 3.2$) [42]. The barrel calorimeter and the outer endcap wheel – covering the precision physics η -range ($|\eta| < 2.5$) has three radial layers each, whereas the inner endcap wheel has two radial layers and coarser lateral granularity. Figure 2.7 shows a diagram of a barrel module displaying the accordion-shaped electrode and absorber geometry, and the three radial layers.

ATLAS Hadronic Calorimeter

The hadronic calorimeter consists of LAr calorimeters at the endcaps, behind the EM disks, and plastic tile calorimeters in the barrel and around the LAr endcaps. The hadronic tile calorimeter uses scintillating plastic tiles as the active material, layered with steel absorber. The scintillation photons are collected by *wavelength shifting fibres*, placed at the edges of tiles, which transmit the light to photomultiplier tubes.

The tile calorimeter consists of three components (shown in figure 2.6): the *barrel* – covering $|\eta| < 1.0$, and two *extended barrels* placed around the end-cap calorimeters, covering $0.8 < |\eta| < 1.7$. All components of the tile calorimeter are

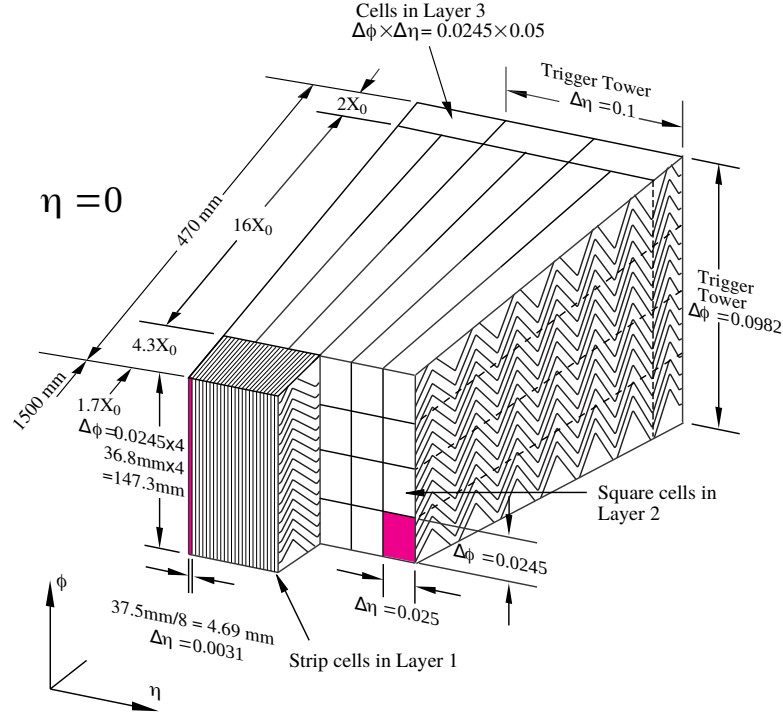


Figure 2.7: Diagram of an ATLAS liquid argon (LAr) barrel calorimeter module, showing three radial layers, the accordion shaped electrode and absorber geometry, and the size of a trigger tower (discussed in section 2.2.4) [42]. X_0 denotes a unit of EM shower length defined in [48].

segmented into three radial layers.

The hadronic endcap calorimeter (HEC) uses liquid argon as the active material interspersed with copper absorber plates arranged in a flat geometry. The HEC consists of four disks in total – two at each endcap, placed one behind the other – and covers a pseudorapidity range of $1.5 < |\eta| < 3.2$. Each disk is segmented into two radial layers, resulting in four layers per endcap.

ATLAS Forward Calorimeters

The forward calorimeters provide ATLAS with nearly 4π calorimeter coverage by extending the pseudorapidity of the ATLAS calorimetry system from $|\eta| < 3.2$ to $|\eta| < 4.9$ (covering $3.1 < |\eta| < 4.9$). A large calorimetry coverage is crucial for studies with invisible final state particles, relying on accurate missing energy

estimation in the event. The forward calorimeters are integrated into the hadronic endcap calorimeters (one at each endcap), starting around 5 m from the interaction point. They are liquid argon calorimeters, made up of three 45 cm deep (z) modules each. The module closest to the IP uses copper absorber and focuses on EM shower measurement, and the remaining two use tungsten to contain hadronic showers.

The work described in this thesis focuses on events within $|\eta| < 2.5$ (within the acceptance of the tracking system), and therefore does not use data collected by the ATLAS Forward Calorimeter. More information on the ATLAS forward calorimeter can be found in [51].

2.2.3 The Muon Spectrometer

In the presented work, muons are only used for triggering and event identification purposes, and are not investigated as physics objects beyond this. Hence, this section offers a only a brief description of the ATLAS muon tracking system – the Muon Spectrometer (MS). A diagram showing the components of the Muon Spectrometer is given in figure 2.8. More information on the MS, and the technologies used in each detector subsystem can be found in [42].

Muons lose relatively little energy through interactions with matter at $\mathcal{O}(\text{GeV})$ energy scales [47], and pass through the calorimeters without stopping. Hence, the muon spectrometer is the outermost ATLAS detector system. It can measure muon momentum within $|\eta| < 2.7$, and trigger on energetic muons within $|\eta| < 2.4$.

The Muon Spectrometer consists of four different muon tracking chambers. *Monitored Drift Tube* (MDT) chambers cover the entire pseudorapidity range of the MS, and offer the best tracking resolution. In the forward region ($|\eta| > 2$), where signal rates are higher, multiwire proportional chambers, called *Cathode Strip Chambers* (CSC) are installed, which offer higher granularity.

Muon triggering capabilities are provided by two types of fast trigger chambers:

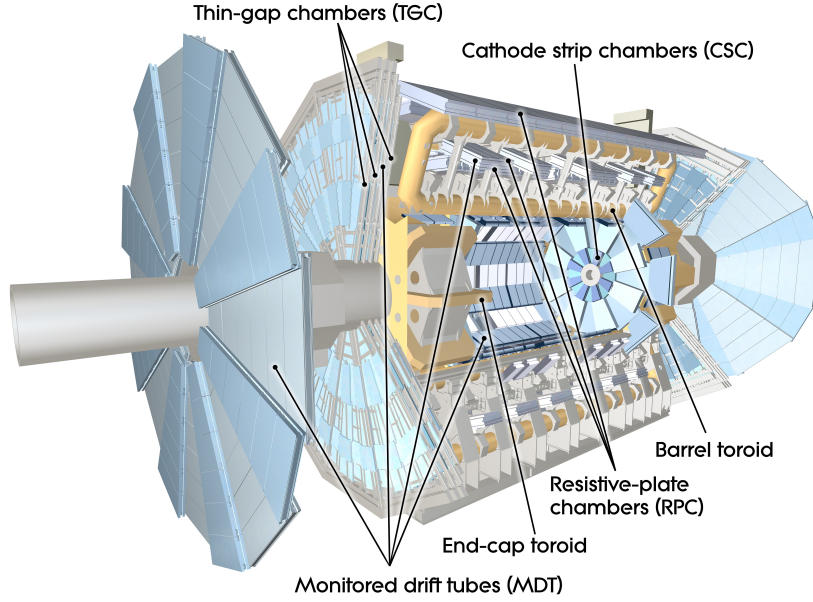


Figure 2.8: A diagram of the ATLAS Muon Spectrometer [42].

Resistive Plate Chambers (RPC) in the barrel region ($|\eta| < 1.05$), and Thin Gap Chambers (TGC) in the endcaps ($1.05 < |\eta| < 2.4$). They also provide additional space points for tracking purposes.

To bend the tracks of the muons, magnetic fields are provided by three large 4 T toroid magnets – one in the barrel region covering $|\eta| < 1.4$, and one at each endcap, covering $1.6 < |\eta| < 2.7$. The magnetic field in the region between $1.4 < |\eta| < 1.6$ is induced by both the barrel and endcap fields. Toroid magnets provide contained magnetic fields, which remain perpendicular to the particle paths even at small angles. The induced magnetic fields are approximately 0.5 T in the barrel region, and 1 T in the endcap regions [42].

2.2.4 The Trigger System

Collisions at ATLAS happen every 25 ns, which translates to 4×10^7 collisions per second (40 MHz frequency). The average event size is ~ 1 MB [52], meaning that if every collision were to be recorded by ATLAS, such data rates would exceed the

estimated storage capabilities of the world in 2007 [53] in 84 days. Hence, a system is needed to identify potentially interesting events, and record them for later analysis.

The systems used for the recognition are called *triggers*, and the action of recognition – *triggering*. The selections are made by looking for signatures of a number of certain objects (e.g. muons, jets, presence of b -quarks, etc.) passing predetermined energy thresholds. The ATLAS *Run 2* Trigger System has two levels: a hardware-based *Level 1* trigger (L1), and a software-based *High-Level* trigger (HLT). More information on the ATLAS trigger system in *Run 2* can be found in [52, 54].

In broad terms, the selection for each type of object, is based on a chain of selection criteria in the L1 trigger and HLT, called a *trigger chain*. The list of trigger chains used in data taking is called a *trigger menu* [52]. The details of the *Run 2* trigger menu can be found in [54].

The L1 trigger has a fixed decision time of $2.5 \mu\text{s}$ and reduces the event rates to $\sim 100 \text{ kHz}$ using information from ATLAS calorimeter and muon systems. The signals from the calorimeter and muon systems are formed into reduced granularity objects called *trigger towers*. An example of the trigger tower size and geometry in the ATLAS EM calorimeter is shown in figure 2.7. The trigger towers are then used to form *Regions of Interest* (RoI): in the calorimeters they are formed by scanning for characteristic energy deposits in neighbouring towers [54], and in the muon system – by looking for hit-coincidences within a “road” tracking the path of the muon [42].

The calorimeter and muon trigger output is treated separately, as well as fed into a topological trigger to form selections based on geometric or kinematic association between the two systems. Information from these three trigger subsystems is used by the *Central Trigger Processor* for decision making. The RoI information of events passing the L1 trigger is sent to the HLT. The HLT consists of ~ 40 thousand processor cores which make decisions in $\sim 200 \text{ ms}$, and reduce data rates to $\sim 1 \text{ kHz}$ [52].

Events passing the HLT are written into *data streams* depending on their in-

tended use. For example the *physics stream* is intended for physics analysis use, and stores full detector information, leading to large event sizes, whereas the *calibration streams* are intended for detector calibrations, which only require partial information from relevant detectors, and allow to maximise the event rates required for calibrations.

Some types of interesting events are more frequent than the maximum data rate, such as those used for background or QCD studies, meaning that not all of them can be read out. This is dealt with by triggering on only a fraction of such events. The factor by which the trigger rate is reduced is called a *prescale*, and triggers using prescales are called *prescaled triggers*. Events used for pile-up studies have to be gathered with minimal event selection. Loose prescaled triggers, called *minimum bias* triggers [55], are used to gather such events, called *minimum bias* events.

Chapter 3

Physics Object Reconstruction in ATLAS

The focus of this thesis is the identification and measurement of high energy $H \rightarrow b\bar{b}$ decays. The b -quarks hadronise in the detector, forming hadronic particle *jets* (introduced in section 1.4), and the momentum boost is provided by another jet in the event. Hence, all objects in an $H(\rightarrow b\bar{b}) + j$ event are jets, making them the most important objects in this thesis. A large part of this chapter is dedicated to jets, presented in section 3.2.

Furthermore, jets initiated by heavy quarks have characteristic signatures in the tracking detectors, which can be used to identify b -quark jets (b -jets). The experimental identification of jet flavour is called *flavour tagging*, or in this case – *b -tagging*, and will be discussed in section 3.3.

In proton-proton (pp) collisions, energetic muons are mainly produced in weak decays. Hence, in some cases discussed in this thesis, they are used as indicators of top-quark or heavy flavour hadron decays to lighter states ($t/b \rightarrow qW$, $W \rightarrow \mu\nu$). A brief overview of muon reconstruction is given in section 3.4. This chapter starts, however, by presenting an invaluable instrument in particle physics analyses and tool development – simulations of processes in pp collisions.

3.1 Simulation of Proton-proton Collisions

Particle production and decays are stochastic processes, hence it is fitting to simulate them using a stochastic method – the *Monte Carlo* (MC) *method*. The software used to produce these simulations are called *Monte Carlo generators*.

The MC method is based on pseudo-random sampling to simulate desired processes on an event-by-event basis. The sampling is based on theoretical predictions of the processes in question. The simulations are done iteratively, starting with the initial process of interest, following through the evolution of the particle-level state, and lastly, modelling the detector effects.

The simulated event information without detector effects is called *truth-level information*. The particles in the event record are called *truth-particles* and their kinematic variables in this state are – *truth-variables* (e.g. *truth- p_T*). The kinematic variables of particles after detector simulation is applied, or in data, are called *reconstructed variables*.

A brief overview of the truth-level simulation process is presented in this section, written with the aid of [56–58]. All detector simulations used in this thesis were done using GEANT4 [59] simulation software, according to ATLAS guidelines [60]. The details of detector simulation are beyond the scope of this thesis.

Truth-level Event Simulation

A diagram of a proton-proton collision is given in figure 3.1. As discussed previously, *pp* collisions are in fact collisions between constituent quarks or gluons - collectively called *partons*. The simulation begins by estimating the cross-section of a selected *hard scattering process*¹ - the highest energy interaction in the event. In the example shown in figure 3.1 the hard scattering is $gg \rightarrow t\bar{t}H$ (shown in red circles).

¹ Simulations are usually performed for each hard scattering process of interest individually, as most events in *pp* collisions are not interesting.

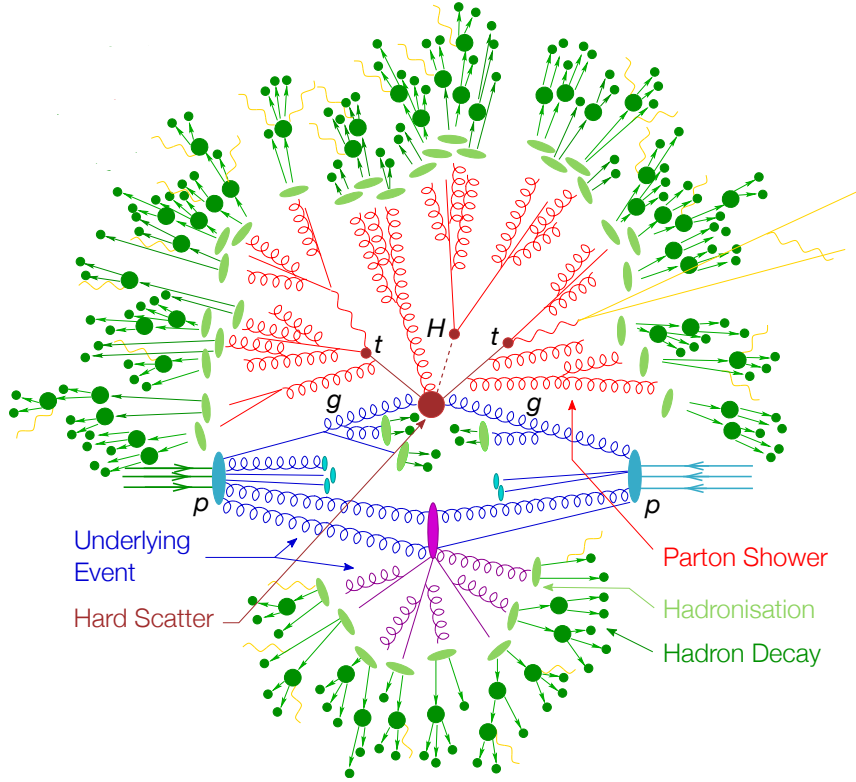


Figure 3.1: An illustration of a proton-proton collision, resulting in a $gg \rightarrow t\bar{t}H$ hard scattering process (dark red circle), in the context of a simulation procedure. The red lines represent the radiative *parton shower* stage. Light green ovals represent parton *hadronisation* and dark green circles represent further hadron decay, both simulated using hadronisation models. Blue lines indicate interactions between proton remnants and a secondary hard scattering event is shown in purple, together making up the *underlying event*. Adapted from [61].

Due to the large energy transfer in the hard scattering process, the partons in the collision can be considered to be free particles. This allows the cross-section of the hard scattering process to be calculated perturbatively, using *matrix element*² *generators*. Usually the calculations are done to leading order (LO) or next-to-leading order (NLO) perturbative expansion terms in α_s , the strong coupling constant. Another input required to simulate a hard scattering process is a *parton distribution*

² Matrix element ($\mathcal{M}$) is the amplitude of transition from initial to final state, cross-section $\sigma \propto |\mathcal{M}|^2$.

function (PDF), which models the distribution of the proton energy between the proton constituents.

The partons in the initial and final states of the hard scatter have large enough energies to radiate other coloured particles (red lines in figure 3.1), which are equivalent to higher-order perturbative terms. Estimating exact outcomes from first principles would be extremely computationally strenuous. Hence, a simplified probabilistic method, called *parton shower* [57], is used to sequentially simulate the cascades.

As the parton shower stage progresses, the partons lose energy. At some point the energies become so low, that the partons start to hadronise (green circles in figure 3.1), and can no longer be considered to be free particles. Due to the complex nature of QCD processes at low energy scales, the processes cannot be modelled using perturbation theory and require empirical modelling.

The secondary interactions between the proton constituents which did not participate in the hard scattering event, are collectively called the *underlying event*, and can involve both hard and soft (high and low energy) processes. These processes are simulated by a separate procedure, and are included in the final model at a later stage of the simulation process.

All simulation stages which require approximate modelling – parton shower, hadronisation, underlying event simulation – involve free parameters in the approximate descriptions. The optimised sets of the free parameters, called *tunes* [62], are taken as input by the MC generators.

3.2 Jets

Jets are showers of particles, and appear as such in the detectors. They are comprised of hadrons, many of which are charged and leave signatures in both tracking detectors and calorimeters. This leads to two types of jet objects to consider: *track jets* – formed using tracks in the tracking detectors, and *calorimeter jets* – formed

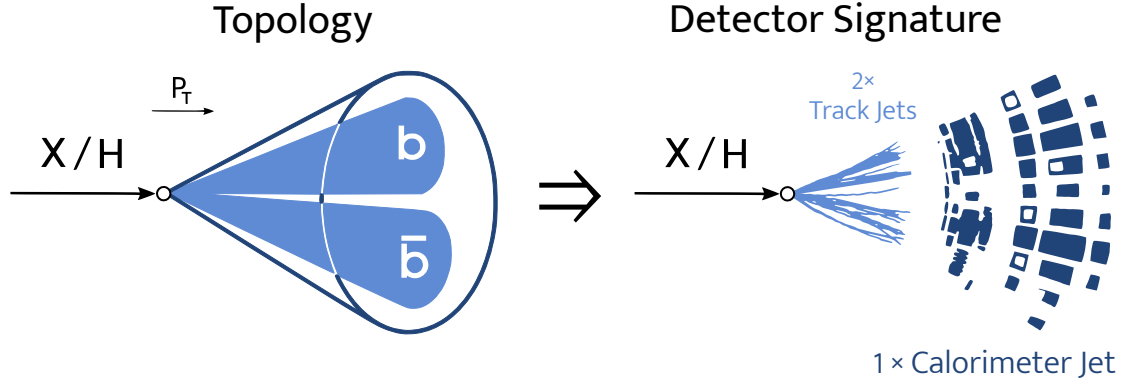


Figure 3.2: (Left) a diagram showing the topology of a Higgs boson or other particle (X) decaying to two b -quarks at high momentum, creating two collimated b -jets. (Right) a stylised illustration of the signature of such a decay in the ATLAS detector. Calorimeter deposits are depicted by rectangular shapes, and tracks are represented by curved lines near the interaction point.

using energy deposits in the calorimeter. The $H(\rightarrow b\bar{b}) + j$ analysis utilised both kinds of jets.

3.2.1 The Higgs Jet

Higgs boson decays to two b -quarks at high p_T have a distinct topology, shown in the left panel of figure 3.2. The momentum boost makes the b -jets collimate. The angular separation of objects in the detector is expressed by:

$$\Delta R = \sqrt{\Delta\phi^2 + \Delta\eta^2} \quad (3.1)$$

where η is the pseudorapidity and ϕ is the azimuthal angle in the detector (introduced in section 2.2). The angular separation of the decay products of a Higgs boson at high momentum can be approximated [63] by

$$\Delta R \approx \frac{2m_H}{p_T}, \quad (3.2)$$

where m_H and p_T are the mass and transverse momentum of the Higgs boson. This means that at Higgs boson transverse momentum $p_T^H > 250$ GeV, the decay products

will be collimated within $\Delta R < 1.0$, with the collimation increasing with p_T^H .

Due to the better spatial resolution of the tracking detectors, track jets can be much smaller than calorimeter jets³. Therefore, it was convenient to define a *Higgs boson jet* (later – *Higgs jet*) as a single large calorimeter jet with two track jets within it, as illustrated in the right panel of figure 3.2. Higgs boson kinematics were described by the calorimeter jet, and the characteristic $b\bar{b}$ decay was identified using track jet information.

3.2.2 Jet Clustering

Jets are comprised of many particles and result in large dispersed signals within the ATLAS detector. This is illustrated in an event visualisation of a ZH event candidate, shown in figure 3.3 where the Z candidate decays to two muons (left), and the H candidate decays to two b -quarks forming jets (right). The jet signal deposits are seen to cover large areas, as opposed to muons⁴, which leave narrow localised deposits.

Jet clustering algorithms are used to reconstruct jets from single fundamental particles using detector deposits. The most commonly used algorithm at the ATLAS experiment, and the algorithm used for all jets in the studies presented in this thesis, is the *anti- k_t* algorithm. It is part of a family of *sequential recombination algorithms* which iteratively combine “nearby” energy deposits until all deposits are clustered into jets (or a desired number of jets is reached). Such algorithms start with a set of N deposits, and define two types of distance variables:

d_{ij} – between two deposits i and j ;

d_{iB} – between deposits i and the beam.

The algorithm looks for the shortest distance out of all deposit combinations $\{d_{ij}, \dots,$

³ Minimum jet sizes at ATLAS are $R_{\min}^{\text{track}} = 0.02$ for track jets, and $R_{\min}^{\text{calo}} = 0.4$ for calorimeter jets, where R is the angular size parameter of the jet, discussed in section 3.2.2.

⁴ And other particles which do not interact through the strong force.

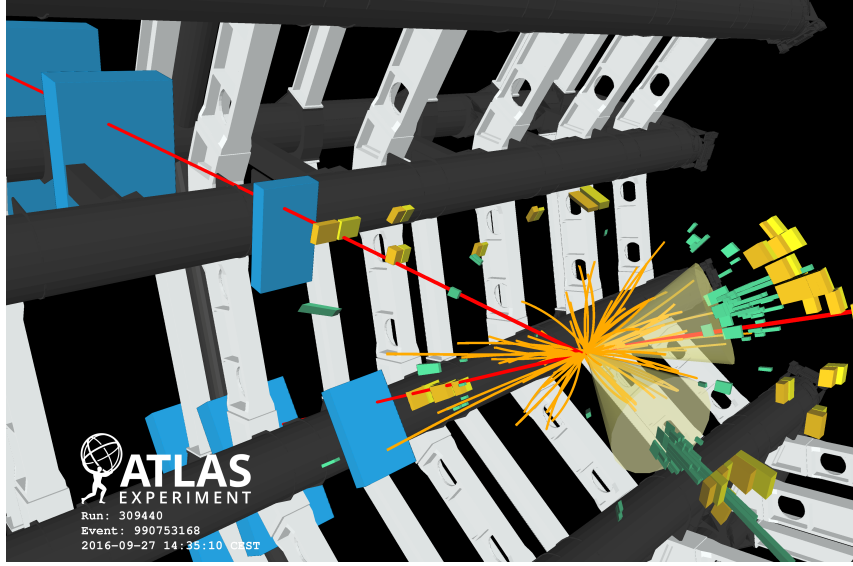


Figure 3.3: A visualisation of a ZH event at ATLAS [64]. Two b -jets are compatible with an $H \rightarrow b\bar{b}$ decay (right); two muons opposite the jets are compatible with a $Z \rightarrow \mu\mu$ decay (left), and another muon is associated with one of the b -jets. Identified jets are represented by yellow cones, and muons – by red lines. Orange lines indicate tracks in the tracking detectors, green and yellow bars – deposits in EM and hadronic calorimeters, and blue panels indicate hits in the muon detectors.

$d_{mn}, d_{iB}, \dots, d_{nB}\}$. If the shortest distance is d_{ij} , deposits i and j are combined and re-entered into the set. If the shortest distance is d_{iB} , i.e. deposit i is “isolated”, then deposit i is determined to be a formed *jet* and is removed from the set. The procedure is continued until no deposits remain in the set.

The anti- k_t algorithm defines the distance variables as

$$d_{ij} = \min \left(\frac{1}{p_{Ti}^2}, \frac{1}{p_{Tj}^2} \right) \frac{\Delta_{ij}^2}{R^2}; \quad (3.3a)$$

$$d_{iB} = \frac{1}{p_{Ti}^2}; \quad (3.3b)$$

where R is the desired jet size parameter (chosen by the user), and Δ_{ij} is the angular distance between the deposits, expressed as

$$\Delta_{ij}^2 = \Delta\eta_{ij}^2 + \Delta\phi_{ij}^2. \quad (3.4)$$

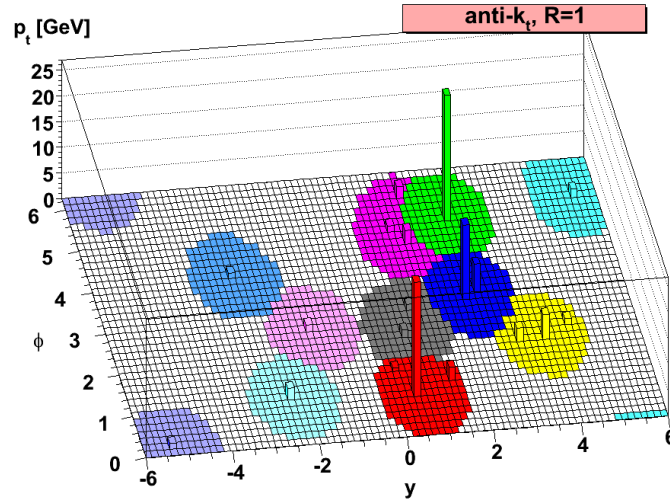


Figure 3.4: Jet areas, as clustered using the anti- k_t algorithm on a sample set of parton events [65].

$\Delta\eta$ and $\Delta\phi$ are the pseudorapidity and the azimuthal angle differences between the two deposits. This definition preferentially chooses high p_T deposits to seed the clustering, and clusters nearby high p_T deposits first, resulting in largely conical jet shapes, as shown in figure 3.4, with an angular span $\Delta R \approx R$.

As the jets are created by many particles, it is important that the jet definition is *infra-red safe* – robust against soft radiation by the particles within the jet, and *collinear safe* – robust against collinear splitting of particles in the jet. The anti- k_t algorithm is safe in both respects: the jet shape is dominated by high p_T deposits, such that any soft radiation is inconsequentially absorbed; and any collinear splitting would be clustered immediately as $d_{ij} \propto \Delta_{ij}^2 \rightarrow 0$. More information on the anti- k_t algorithm can be found in [65].

3.2.3 Calorimeter Jets

In this thesis, the reconstructed kinematic properties of Higgs boson candidates are given by the kinematic properties of their representative calorimeter jets. Because

of the large areas of the jets, they are sensitive to contamination by soft radiation from pileup and underlying event (UE). Many of the calorimeter jet reconstruction choices are focused on reducing such effects in order to increase the accuracy of the jet measurements.

Calorimeter jets used in this analysis were formed using the anti- k_t jet clustering algorithm (implemented using the FASTJET software package [66]) described in the previous section. It is beneficial to strategically group the calorimeter cells before passing them to the jet clustering algorithm to reduce the noise input and the algorithm computation time. The inputs given to the anti- k_t algorithm were three-dimensional groups of calorimeter deposits, called *topological cell clusters* (later, *topoclusters*), presented in the following.

Topoclusters

Topoclusters are three dimensional collections of cells, built around large energy deposits. The clustering is based on cell signal-to-noise ratio,

$$\varsigma = \frac{E}{\sigma_{\text{pileup}} \oplus \sigma_{\text{electronic}}} . \quad (3.5)$$

The calorimeter cells are sorted into three categories: *seed cells* with $\varsigma > 4$, *growth cells* with $\varsigma > 2$, and *other cells* with $\varsigma > 0$.

The topocluster building procedure starts with the highest ς seed cell and proceeds through all unclustered seed cells in descending order. The proto-cluster is a seed cell and its neighbouring cells. If any of those neighbouring cells pass the growth criterion ($\varsigma > 2$), their neighbours are included as well. The growth procedure continues until the borders of the topoclusters are made up completely of cells which do not pass the growth criterion. An illustration of formed topoclusters is given in figure 3.5. More information on topoclusters can be found in [67].

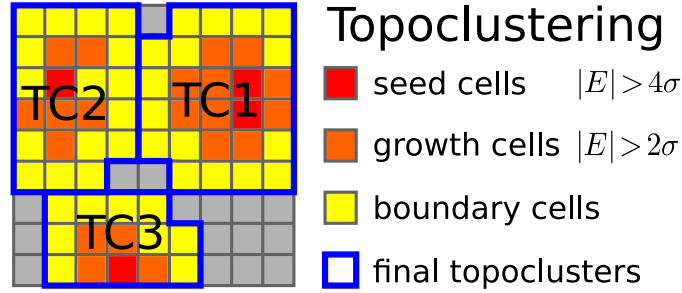


Figure 3.5: An illustration of topocluster formation [68]. The cells are in $\eta - \phi$ space, and the cell size for the hadronic calorimeter is 0.1×0.1 in $\eta - \phi$.

Jet Size

There are two main types of calorimeter jet used in ATLAS. *Small- R* jets, constructed with a size parameter of $R = 0.4$ are mainly used to represent standalone quarks and gluons. *Large- R* jets, built with $R = 1.0$, are generally used for more complex objects with sub-structure, such as Higgs bosons, weak bosons or top-quarks.

It was shown previously, using equation 3.2 that the decay products of a Higgs boson with $p_T^H > 250$ GeV would collimate within $\Delta R < 1.0$ of the original Higgs boson. By defining Higgs boson candidates as a single large- R calorimeter jet with two track jets within it, the studies presented in this thesis were able to study Higgs bosons with $p_T^H > 250$ GeV using the boosted topology to identify them.

Small- R jets were only used in this thesis as recoil objects in the double b -tagging calibration study (section 4.2). Hence, this section is focused on large- R calorimeter jets.

Jet Trimming

Due to their large area, large- R jets are particularly subject to soft radiation contamination from pileup and the UE. Several *jet grooming* techniques, aiming to

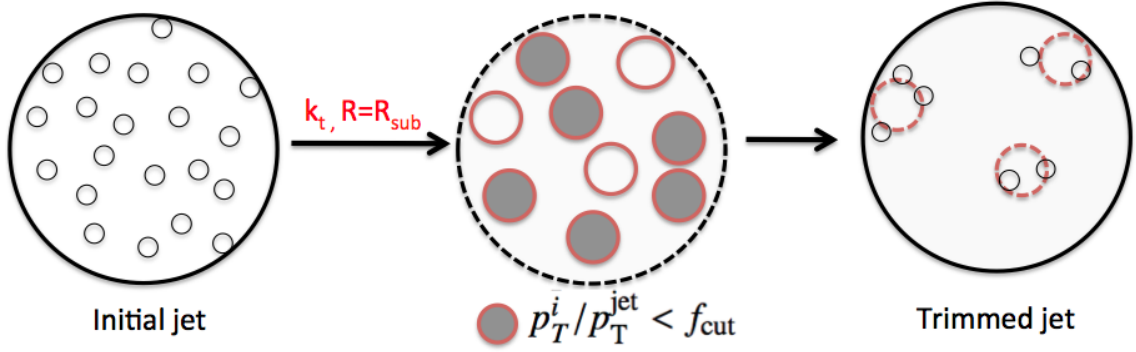


Figure 3.6: An illustration of the trimming procedure [69]. The initial large- R jet inputs are re-clustered using the k_T algorithm into sub-jets with size parameter R_{sub} (0.3), and sub-jets carrying less than f_{cut} of the total jet momentum are removed. The remaining sub-jets form the trimmed large- R jet.

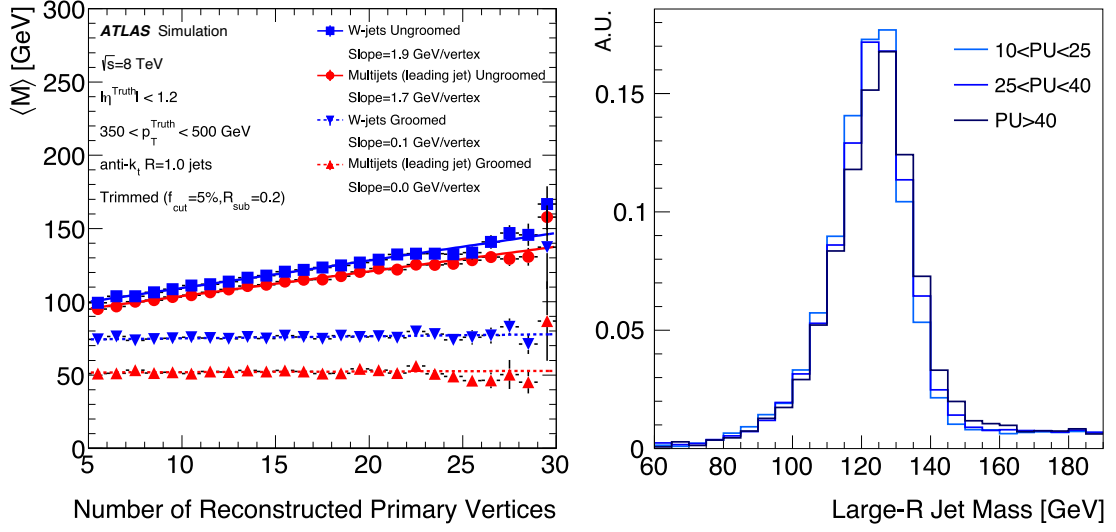
mitigate this issue, have been studied by the ATLAS collaboration [69, 70], and *jet trimming* [71] is the recommended grooming technique, which was utilised in the object reconstruction used in this thesis.

Jet trimming procedure is illustrated in figure 3.6. First, the inputs of the large- R jets are re-clustered using the k_T [72] jet clustering algorithm (described later) into small sub-jets with the size parameter $R_{\text{sub}} = 0.2$. The sub-jets containing less than $f_{\text{cut}} = 5\%$ of the original jet p_T are discarded, and the remaining sub-jets make up the new trimmed large- R jet. The selected R_{sub} and f_{cut} values are a common recommendation for ATLAS analyses [70].

The k_T algorithm is a “conjugate” of the anti- k_t algorithm. In the k_T algorithm the p_T terms in the distance variables (equation 3.3) have powers of 2 instead of -2 , such that the algorithm clusters soft deposits first. The k_T algorithm distributes energy between sub-jets more evenly than the anti- k_t algorithm⁵, and therefore is more suited for use in the trimming procedure.

The trimming procedure significantly reduces the jet mass dependence on pileup.

⁵ The anti- k_t algorithm would allocate most of the energy to the hardest sub-jet, which would make it more likely for all other softer sub-jets to be removed [71].



(a) Optimisation Study [70]

(b) $H(\rightarrow b\bar{b}) + j$ Analysis

Figure 3.7: (a) The mean jet mass $\langle M \rangle$ distributions of $W \rightarrow qq'$ and QCD multi-jet events, against number of primary vertices in the event N_{PV} [70]. The slopes of linear fits to the distributions are given in the legend. (b) Higgs boson jet mass distributions in bins of total pileup (PU) in simulated ggF events from the $H(\rightarrow b\bar{b}) + j$ analysis at the focus of this thesis [73] (internal).

Figure 3.7a shows the mean jet mass $\langle M \rangle$ dependence on the number of primary vertices in the event⁶ N_{PV} in simulated $W \rightarrow qq'$ and QCD events with multiple jets (i.e. *multi-jet* events). Before trimming $\langle M \rangle$ has a clear correlation with N_{PV} , whereas after trimming is applied the correlation is seen to be mitigated. A cross-check of the Higgs jet mass dependence on the total pileup⁷ was made by the $H(\rightarrow b\bar{b}) + j$ analysis team in simulated ggF events, shown in figure 3.7b. No significant dependence was observed.

⁶ A measure of in-time pileup.

⁷ The mean number of interactions per proton bunch crossing μ , presented in section 2.1, here labelled as PU.

Jet Mass

In general, jet variables are derived by summing the four-vectors of the constituent topoclusters. The topoclusters are assumed to be massless, but due to the angular spread of the inputs, this results in a massive final jet. However, due to the relatively coarse granularity of the calorimeter, the jet mass resolution deteriorates at high jet momentum [74]. This is remedied by using a *combined mass* definition m^{comb} , where the calorimeter derived mass definition m^{calo} is supplemented by more granular track information.

The track-based mass of the jet m^{track} is derived by summing the four-vectors of all tracks associated⁸ with the large- R jet (with mass assumptions of $m_{\text{pion}(\pi)}$). As only charged particles leave signatures in the tracking detectors, m^{track} has to be corrected using calorimeter information collected from both charged and neutral particles. The *track-assisted jet mass* definition [74] is

$$m^{\text{TA}} = \frac{p_T^{\text{calo}}}{p_T^{\text{track}}} \times m^{\text{track}}, \quad (3.6)$$

where p_T^{calo} and p_T^{track} are the jet transverse momenta, derived by summing the four-momenta of jet calorimeter inputs, and tracks associated with the jet, respectively.

To achieve the best possible resolution, the calorimeter-based mass definition and track-assisted jet mass definition are combined as a weighted sum

$$m^{\text{comb}} = w^{\text{calo}} m^{\text{calo}} + w^{\text{TA}} m^{\text{TA}}, \quad (3.7)$$

where the weights (w^{calo} , w^{TA}) are optimised to minimise the mass resolution [74]. The combined jet mass definition m^{comb} is used widely across ATLAS analyses. More information can be found in [74]. The comparison between different jet mass definitions in simulated W and Z boson events is shown in figure 3.8. The combined mass definition delivers the best mass resolution throughout most of the investigated jet p_T spectra.

⁸ Using the *ghost association* method described in section 3.2.6.

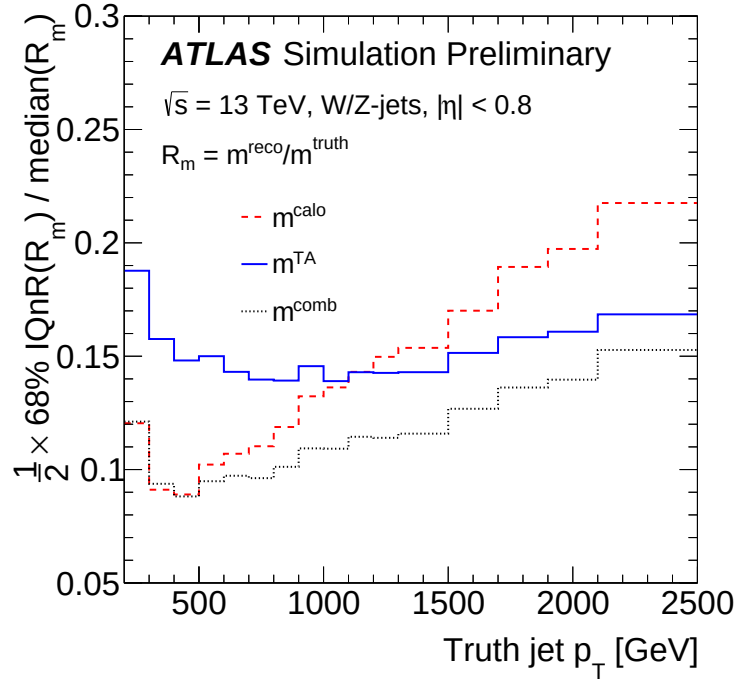


Figure 3.8: Fractional jet mass resolution as a function of jet p_T from simulated high energy $W/Z \rightarrow qq$ events with different jet mass definitions: calorimeter-based jet mass (m^{calo}), track-assisted jet mass (m^{TA} , eq. 3.6), and combined jet mass (m^{comb} , eq. 3.7) [74].

3.2.4 Calorimeter Jet Calibration

Large- R jets used in this thesis went through three calibrations, which will be briefly discussed in this section⁹. More information on the calibrations can be found in [67, 75, 76]. A diagram of the jet reconstruction process highlighting the calibration stages is shown in figure 3.9.

The jet calibrations serve several purposes. The reconstructed jet properties must be representative of the properties of the particles which initiated them, and simulated jet properties must agree with the jet properties in data. In general terms, the calibrations are performed by comparing a *probe* dataset (uncalibrated)

⁹ Small- R ($R = 0.4$) calorimeter jets only have a minor role in this thesis, as the recoil object in the double b -tagging calibration, presented in section 4.2. Hence, their calibration will not be discussed. Details on small- R jet calibration can be found in [77].

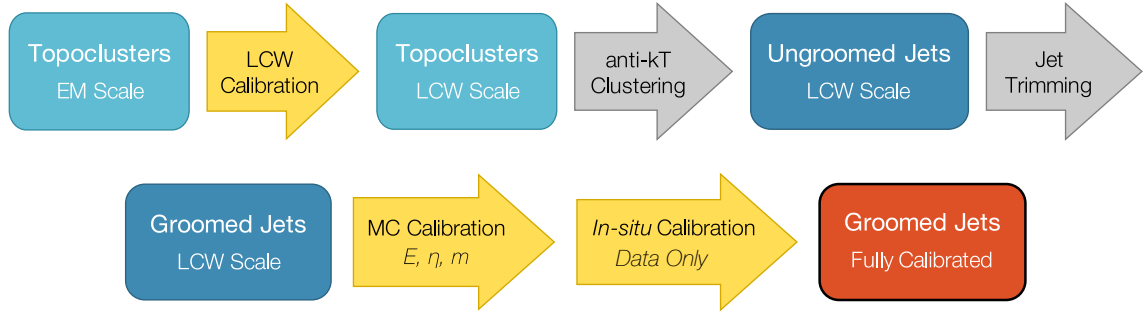


Figure 3.9: A flowchart of large- R calorimeter jet reconstruction and calibrations. Calibrations are shown in yellow, and are presented in this section. For *LCW Calibration* see “EM-to-Hadronic Scale Calibration” passage. Adapted from [76].

to a *reference* dataset (understood), and deriving response ratios for distributions of interest (such as E , p_T , m , etc.), called – *calibration scale factors*. The scale factors are used to weight the distributions of interest to the desired scale.

The calibrations are often performed in central (small $|\eta|$) regions of the detector, where measurements can be made more accurately, so a dedicated calibration must also be made to make the jet η response uniform. The calibrations also have associated uncertainties. As they are performed sequentially, the uncertainties are propagated across each procedure, to form a final set of jet uncertainties.

EM-to-Hadronic Scale Calibration

The topoclusters presented at the beginning of this section are formed using calorimeter cell deposits. The energy values of these deposits are said to be on the *electromagnetic* (EM) *scale*, i.e. as measured by the calorimeters. This name is chosen as the calorimeters are *non-compensating*, i.e. their response to EM particles is better than their response to hadrons.

Furthermore, jet energy (signal) can be lost due to the noise mitigation in the clustering method, and inactive material. To correct for all three sources of energy

loss, a *local hadronic cell weighting* (LCW) calibration is performed, using simulated charged and neutral pion events. The calibrated topoclusters are used to form large- R jets. The procedure is complex and beyond the scope of this thesis, more information can be found in [67].

Detector-to-Particle Jet MC-based Calibration

Once the jets are formed and groomed the jet four-momenta need to be calibrated to represent *particle-level jets*. The calibration is done in simulated QCD events with two jets in the final state (*di-jet*) events. The calibration compares the average energy and mass responses between reconstructed and particle-level jets¹⁰, $R_X = \langle X_{\text{reco}}/X_{\text{particle}} \rangle$, where $X = \{E, m\}$, as functions of X_{reco} in bins of η .

The jet energy and mass scale (JES and JMS) calibration scale factors are the inverses of these ratios $c_{\text{JES}} = R_E^{-1}$, $c_{\text{JMS}} = R_m^{-1}$. First, the JES scale factors are derived and applied to reconstructed jet four-vectors, correcting jet E , p_T , m , and η ; after this, the JMS scale factors are derived and applied to jet mass. More information can be found in [75, 76].

Data-to-MC *in-situ* Calibrations

Simulations do not perfectly represent reality, limited by assumptions made for computational purposes, or modelling capabilities of complex physics processes, detectors, and detector response. Such differences are corrected through *in-situ* calibrations, which rely on well-known (calibrated) objects in data to provide a reference point for the calibration. The following briefly describes large- R jet *in-situ* calibrations, more information can be found in [75, 76]¹¹.

The *in-situ* jet calibrations were performed to correct the jet mass and energy

¹⁰ The particle-jets were constructed using particle-level information from the simulation record, following the same clustering and trimming procedures as detector jets.

¹¹ The jet mass scale calibration is done in di-jet events as described in [76], however, unlike the description in [76], it does not include the *forward folding* technique, and is done directly after the MC-based calibration, as described in [75]. This is following ATLAS recommendations for winter 2019 analyses.

scales. Generally, data and MC are compared in terms of the average response between jet properties (X_{jet} , where $X = \{p_T, m\}$) and properties of well calibrated reference objects (X_{ref}) in the same event: $R^X = \langle X_{\text{jet}}/X_{\text{ref}} \rangle$. The scale data-to-MC factors are then defined as $\text{SF} = (R_{\text{data}}^X/R_{\text{MC}}^X)^{-1}$, derived as functions of X .

Jet Mass Scale Calibration: calorimeter jet mass is calibrated *in-situ* in di-jet events, using the R_{trk} method [75, 76]. The method compares the average calorimeter-to-track jet mass response $R_{\text{trk}}^m = \langle m^{\text{calo}}/m^{\text{track}} \rangle$ in data and MC. No assumption is made on whether one definition is more correct than the other, and uncertainties are derived for both mass definitions. As the combined jet mass definition (m^{comb}) is dependent on jet p_T , m^{calo} and m^{track} , the combined mass values are calculated after both mass and energy calibrations are made.

Jet Energy (p_T) Calibration: The JES calibration is performed in two parts. The first part is **η —intercalibration**, where forward jets ($0.8 < |\eta| < 2.5$, small angle to the beam) are calibrated against central jets ($|\eta| < 0.8$, large angle to the beam), such that the jet p_T response is uniform across the full η spectrum. Di-jet events are used, where a forward jet is recoiling against a central jet. Then, an absolute p_T calibration is performed using events of jets recoiling from Z bosons, photons and multiple small- R jets.

The *in-situ* calibrations only correct mass and energy scale effects, but do not calibrate jet mass or energy resolution (JMR or JER). JER uncertainties were derived through comparisons in simulation, as part of the MC-based calibration. The jet mass resolution uncertainties were derived by varying detector geometry in simulation [75]. Both are considered to be conservative estimates. At the time of writing (2021), methods of in-situ calibration for mass and energy resolution have been developed [78], which will be used in the future.

3.2.5 Track Jets

The key functionality of track jets in this thesis is to identify two b -jets in a highly collimated $H \rightarrow b\bar{b}$ decay. The process of identifying b -quark jets – *b-tagging* (discussed in section 3.3) – relies on track information, so it is important to correctly assign tracks between near-by jets.

Track jets are built from inner detector (ID) tracks in two steps. First the anti- k_t algorithm is used to cluster tracks passing a set of tight pileup mitigation requirements, described in section 4 of [79], with $p_T > 0.5$ GeV¹² and $|\eta| < 2.5$. This defines the track jet cone size and direction. Next, tracks passing looser selection requirements [80] are associated to the track jets in order to efficiently perform jet flavour identification. The association is based on ΔR separation between the jet axis and tracks, with ΔR threshold reducing with jet p_T [81, 80].

Variable Radius Jets

The studies described in this thesis use *variable radius* (VR) jets [82, 83], where the jet radius parameter R in the anti- k_t algorithm is allowed to vary with jet p_T as

$$R = \frac{\rho}{p_T}. \quad (3.8)$$

The parameter ρ controls the rate of change of the cone size with p_T . The variable-radius approach exploits the fact that jets with higher p_T will be more collimated. Taking this into account when forming jets reduces jet overlap in cases with multiple nearby jets as shown in figure 3.10.

All studies presented in this thesis use variable radius track jets with $\rho = 30$ GeV, minimum size parameter $R_{min} = 0.02$ (determined by the detector resolution), maximum size parameter $R_{max} = 0.4$, with $p_T > 10$ GeV and $|\eta| < 2.5$. This selection is standard across ATLAS analyses using variable radius jets. The optimisation

¹² The $p_T > 0.5$ GeV threshold is an updated recommendation used in the $H(\rightarrow b\bar{b}) + j$ analysis. [79] quotes an earlier $p_T > 0.4$ GeV recommendation, which was used in the double b -tagging calibration presented in section 4.2.

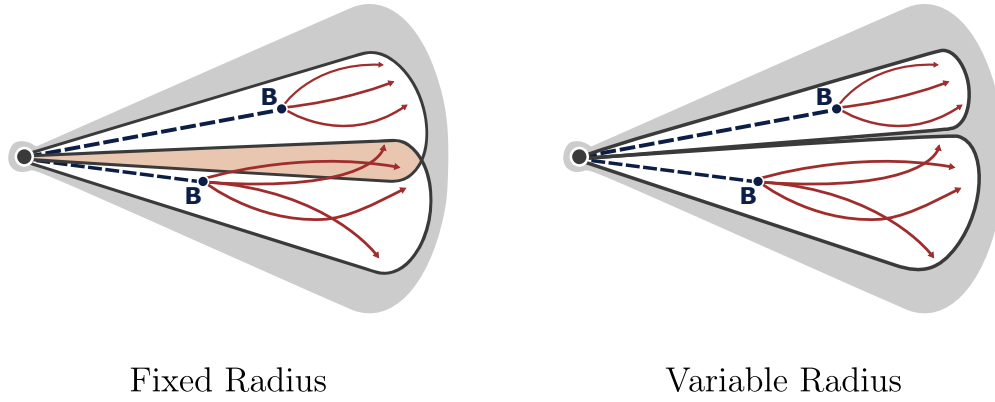


Figure 3.10: An example of track jets from two nearby b -quarks reconstructed with fixed radius and variable radius jet size parameters.

of these values can be found in [83].

VR Track Jet Performance

A jet initiated by a b -quark should, in reality, contain a b -hadron in the decay chain, and b -tagging relies on identifying these b -hadron decays. Hence, it is important, that the b -hadron is within the track jet object to begin with. Figure 3.11 compares the efficiency of associating¹³ truth b -hadrons to track jets reconstructed with fixed radius ($R = 0.2$) and variable radius size parameters in simulated boosted $H \rightarrow b\bar{b}$ decays [83]. The fixed- R track jet performance falls rapidly at high Higgs jet p_T , whereas VR track jets perform better overall with the optimal value of $\rho = 30$ GeV.

Overlap Removal

Due to the dense environment of a boosted topology, the track jets within a large- R jet are susceptible to overlap. Strong overlap can make the assignment of looser tracks to the track jets (as needed for b -tagging) ambiguous, so events where the

¹³ The association is done by finding a b -hadron within $\Delta R < 0.3$ of the track jet, described in detail in section 3.3.2.

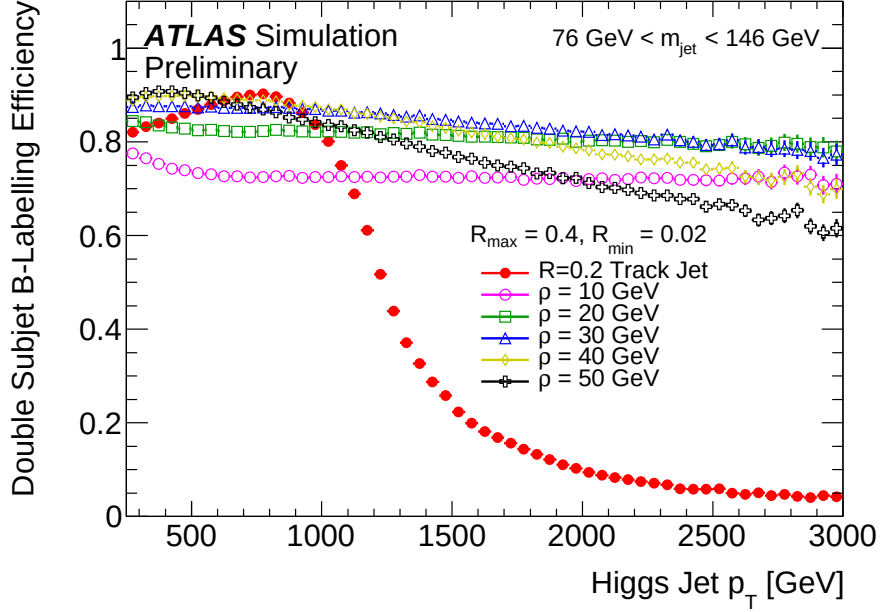


Figure 3.11: Efficiency of associating truth-level b -hadrons to two leading p_T track jets within a Higgs jet, for fixed- R track jets, and VR track jets with different rate-of-change parameters ρ , as found in simulated boosted $H \rightarrow b\bar{b}$ events [83].

angular distance ΔR between two track jets ($j_{i/j}$) is smaller than the smaller jet size parameter (R) of the two,

$$\Delta R(j_i, j_j) < \min[R_i, R_j] , \quad (3.9)$$

are discarded. This check is performed for all track jets considered for b -tagging, against all track jets passing a looser p_T requirement of $p_T > 5$ GeV [3] (note, $j_{\text{tag}} \subset j_{\text{loose}}$). In the $H(\rightarrow b\bar{b}) + j$ analysis this results in $\sim 7\%$ reduction in Higgs boson efficiency [73] (internal).

3.2.6 Jet Association

The Higgs jets were built by associating track jets to a large- R jet. The separation between objects in the detector is usually expressed in terms of angular distance ΔR . However, in this case the track jets and tracks were used to determine important

qualities of the Higgs boson candidates – track jets were used to identify the $H \rightarrow b\bar{b}$ decay topology, and track information was used in the Higgs jet mass definition and calibration. Therefore, for such purposes, a less ambiguous association technique is used, called *ghost association* [84, 85, 69].

In this method, infinitesimally soft *ghosts* of the track jets¹⁴ are formed by setting the track jet p_T to be infinitesimal, and keeping only the direction information of the track jets. The ghosts are associated to large- R jets by running the same jet clustering algorithm with the un-groomed large- R jet inputs *and* track jet ghosts. As the ghosts are point-like entities in direction only, this does not change the final large- R jets, and only gives information on which track jets are associated with which large- R jet¹⁵. Using ghost association to associate track jets to calorimeter jets to form boosted topologies is standard throughout ATLAS [3].

3.3 Identification of b -quark Jets (b -tagging)

Heavier quarks decay into lighter quarks through the weak interaction, which is much slower than EM or strong interactions. Because of this, at relativistic energies b -quarks have time to travel measurable distances in the detector before decaying¹⁶. The delayed decays result in characteristic displaced vertices from the interaction point, called *secondary vertices* (SV). Moreover, b -quark decays have high track multiplicities compared to light quarks. Figure 3.12 shows a diagram of a b -quark decay.

At ATLAS, software-based tools - *taggers* - are designed to identify jets likely to have been initiated by b -quarks and *tag* them as b -jets, in a process called *b-tagging*. The studies presented in this thesis use a b -tagging algorithm based on

¹⁴ This example is given in terms of associating track jets to the large- R jets, but any entities (tracks, small calorimeter jets, etc.) can replace the track jets in this technique.

¹⁵ These un-groomed ghost-associated large- R jets are only a by-product of the association processes. Analyses use groomed large- R jets.

¹⁶ A 50 GeV b -quark will on average travel 5 mm in the detector before decaying.

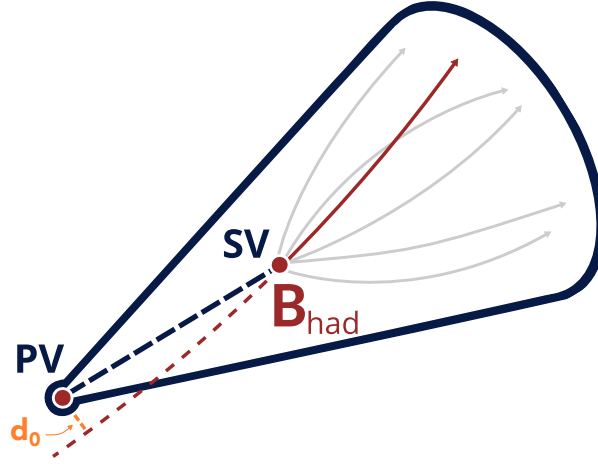


Figure 3.12: A diagram showing a characteristic b -hadron decay within a track jet. The hadron travels a measurable distance from the primary vertex (PV) before decaying, creating a secondary decay vertex (SV). An example of the transverse impact parameter d_0 of a track from the b -hadron decay is shown.

machine-learning (ML), called MV2.

ML-based algorithms are called *high-level taggers*. The MV2 algorithm uses discriminants, produced by targeted *low-level b*-tagging algorithms, as input. The low-level algorithms used by the MV2 tagger are: IP2D and IP3D, which use characteristic track and impact parameter¹⁷ information; SV2, based on secondary vertex reconstruction; and JETFITTER – a b -quark decay chain reconstruction algorithm. All mentioned algorithms have been developed by the ATLAS collaboration, more information can be found in [86, 87].

The MV2 algorithm assigns a value between -1 and 1 to each jet, depending on how *non-b-jet-like* (-1) or *b-jet-like* (1) it determines the jet to be, based on its training. This value is called the *discriminant* of the algorithm. The MV2 algorithm is trained on a hybrid sample of $t\bar{t}$ and Z' events¹⁸, where $m_{Z'}$ is set to 4 TeV, to

¹⁷ The distance of closest approach between the extrapolated track and the primary vertex.

¹⁸ Z' is a postulated BSM particle, which can decay to quark pairs, often used to generate MC samples of high energy jets.

provide a sufficient amount of high p_T b -jets.

The passing requirement for the jet to be considered a b -jet is defined in terms of b -tagging *efficiency working points* – the value of the MV2 discriminant corresponding to a desired b -tagging efficiency. The b -tagging *efficiency* is defined as:

$$\epsilon_{b\text{-tag}} = \frac{\text{b-tagged } b\text{-jets}}{\text{all } b\text{-jets}}. \quad (3.10)$$

The studies described in the thesis use the 77% efficiency working point.

The tagging algorithms were compared in terms of background rejection. Rejection is quantified as the inverse of the efficiency at which background events pass the tagging condition, i.e. are *mis-tagged* as b -jets. Figures 3.13a and 3.13b show the light-jet (u, d, s quark) and c -jet rejection by various algorithms, as a function of $\epsilon_{b\text{-tag}}$. The MV2 tagger was seen to reject backgrounds more efficiently than all shown low-level taggers throughout the entire range of $\epsilon_{b\text{-tag}}$. Another ML-based tagger – DL1 – was shown to perform slightly better in light-jet rejection at the selected working point, but the MV2 algorithm was chosen to be used in the $H(\rightarrow b\bar{b}) + j$ analysis due to its maturity during the development of the event selection.

3.3.1 Calibration

Differences in b -tagging efficiency between data and simulation can arise from challenges in theoretical and detector modelling. Hence, the b -tagging efficiency needed to be calibrated using true b -jets in data. A $t\bar{t}$ sample enriched with fully leptonic decays was used. The calibration in the cited reference [88] was performed by associating tracks to $R = 0.4$ calorimeter jets, however, a more recent calibration using VR track jets was also made, yielding similar results.

The calibration utilised both top candidates in the $t\bar{t}$ events, and the calibration scale factors were derived in bins of jet p_T . Four regions were defined depending on the expected dominant flavours of the two top candidates (leading and sub-leading jets in p_T): $j_i j_j = bb, bl, lb, ll$, where l denotes a jet with no associated

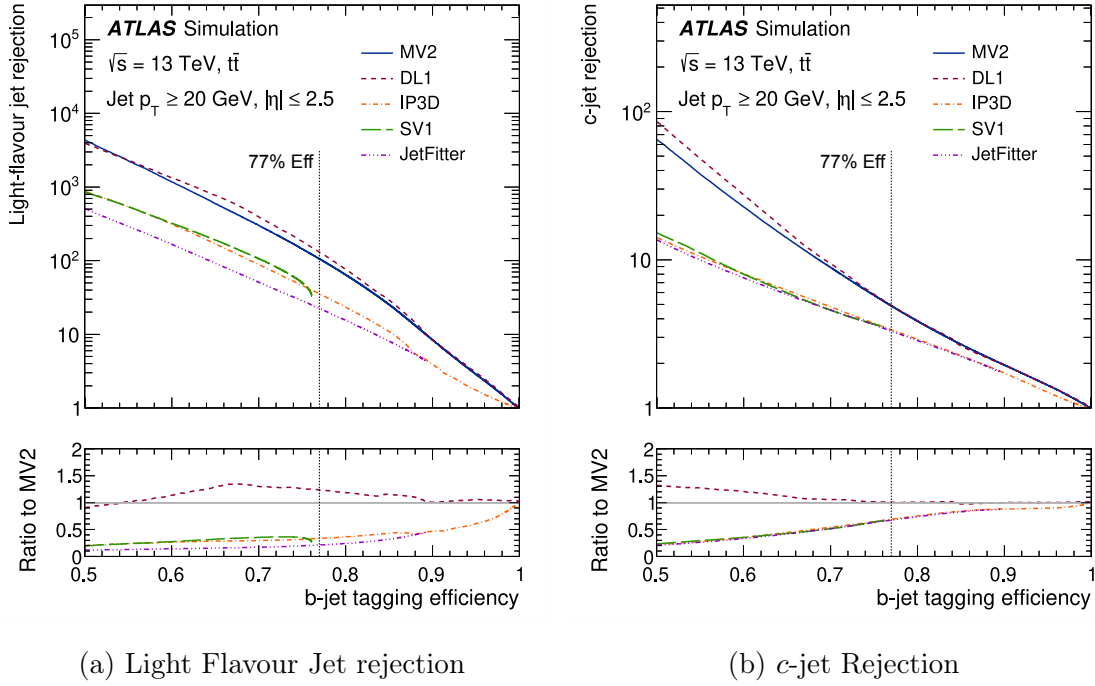


Figure 3.13: Rejection of (a) light-flavour jets and (b) c -jets by various b -tagging algorithms, as a function of b -tagging efficiency in simulated $t\bar{t}$ events enriched in fully leptonic $t\bar{t}$ decays [88]. *Note:* The comparisons were made by associating tracks to $R = 0.4$ calorimeter jets. Similar studies have been made internally using VR track jets, showing equivalent findings.

b -hadron. The bb region was further subdivided into bins of MV2 discriminant, and the remaining regions were used to aid the estimate the flavour composition in data.

The flavour composition of the MC samples was determined using the truth labelling procedure described in section 3.3.2. A binned likelihood fit was performed across all bins to estimate the b -tagging efficiencies¹⁹ (ϵ_{data}) in data. The b -tagging efficiency in MC (ϵ_{MC}) was found using the pre-fit estimates. The calibration scale factors were the data-to-MC efficiency ratios: $\text{SF} = \epsilon_{\text{data}}/\epsilon_{\text{MC}}$, and were applied to the simulated samples when used in analysis. More information on the b -tagging calibration can be found in [88].

¹⁹ The fit measures b -tagging probabilities in each MV2 discriminant bin, which are summed to give total efficiencies.

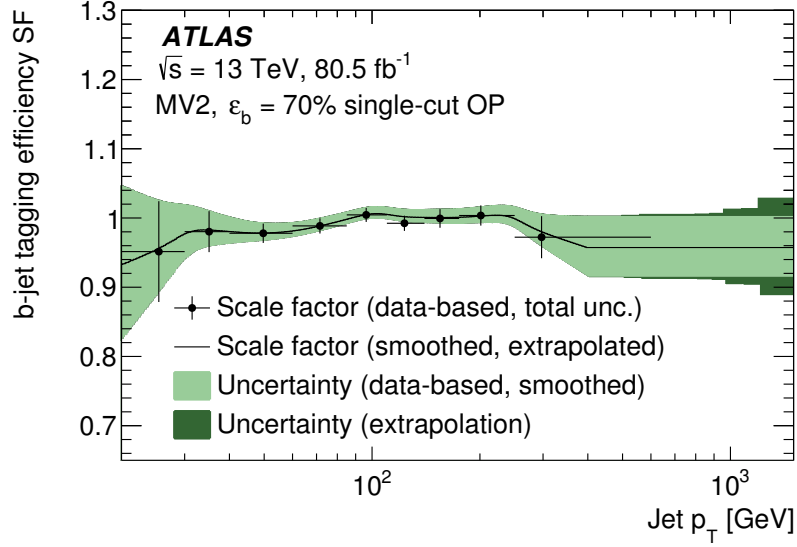


Figure 3.14: Data-to-MC b -tagging efficiency scale factors derived in $t\bar{t}$ events, enriched in fully leptonic decays, for the MV2 b -tagging algorithm at a 70% efficiency working point [88].

The scale factors derived by this calibration at the 70% efficiency WP, are shown in figure 3.14. Overall, the agreement between data and MC was good – the scale factors were within 2σ (standard deviations) of unity. Few data events with $p_T^{\text{jet}} > 400$ GeV were present in the data, so an MC-based extrapolation (described in section 10.2 of [88]) was performed to extrapolate the scale factors to higher p_T regions. The procedure resulted in an additional extrapolation uncertainty, also shown in figure 3.14. The extrapolation uncertainty was relatively small for $p_T^{\text{jet}} < 1$ TeV, but non-negligible, and increased with p_T^{jet} . The scale factors for VR track jets at a 77% WP were seen to behave analogously, with uncertainties of a similar extent.

Similarly, c -jet and light-jet mis-tagging rates also have to be calibrated. The c -jet mis-tagging rate was calibrated in semi-leptonic $t\bar{t}$ decays [89], and the light-jet mis-tagging rate was calibrated using di-jet events [90]. The double b -tagging calibration study presented later, in section 4.2, used b -tagging scale factors derived by an earlier calibration in semi-leptonic $t\bar{t}$ events [91].

3.3.2 Truth Labelling

As seen throughout this chapter, the matching of simulated jets to truth-level b -quarks – *truth labelling* – is used to assess the performance of b -tagging strategies and track jet definitions. The *truth-flavour* of a simulated track jet is determined by searching for truth-particles within $\Delta R < 0.3$ of the track jet axis.

First this is done for b -hadrons ($p_T > 5$ GeV). If there is a successful match the track jet is labelled as a b -jet. If no b -hadrons are matched, the procedure is repeated for c -hadrons, and τ -leptons sequentially. If a particle is matched with multiple jets, the nearest jet is labelled. If a jet has no matches it is labelled as a light-jet [88].

3.4 Muon Reconstruction

In some cases presented in this thesis, muons were used for triggering, and in event selection to indicate weak decays of heavy quarks. This section gives a brief overview on the reconstruction of muons used in the studies presented in this thesis. As muon kinematics are not studied in this thesis, the calibration of muon kinematic variables will not be discussed. More information on muon reconstruction and calibration can be found in [92].

The ATLAS collaboration has multiple methods to identify muons. The muons used in the presented analyses were reconstructed from inner detector (ID) and muon spectrometer (MS) information, as illustrated by figure 3.15. This method of muon reconstruction is called *combined muon* reconstruction. First, muons are reconstructed by building segments from hit patterns in different layers of the MS, and fitting the segments to build track candidates. Then muon tracks from the MS are extrapolated inward to match with tracks in the ID.

A range of selection criteria are applied in order to reduce background muons, mainly originating from light hadron (pion and kaon) decays. Several groups of muon selection criteria are provided to cater to the needs of different physics analyses at

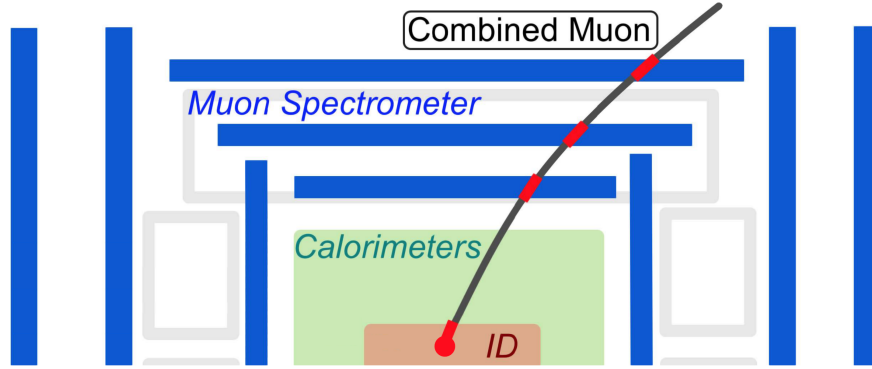


Figure 3.15: A diagram showing the path of a muon in the ATLAS detector, and detector signals used in the *combined muon* reconstruction (shown in red). Adapted from [93].

ATLAS. The selections (described in [92]) include hit thresholds, geometrical and kinematic requirements, and use goodness-of-fit information. The $H(\rightarrow b\bar{b}) + j$ analysis used *medium* muons – the default muon selection at ATLAS, whereas the double b -tagging calibration study presented in section 4.2 used *loose* muons, which maximises muon reconstruction efficiency, to increase the available sample size.

In all presented studies muons were required to have $p_T > 10$ GeV and $|\eta| < 2.4$. In some cases muons were required to be *isolated*, i.e. well separated from other objects in the event. The isolation criteria are based on ID track and calorimeter information. Thresholds are placed on the sums of track momentum ($\sum p_T^{\text{track}}$) and topocluster transverse energy ($\sum E_T^{\text{topo}}$) in cones around the direction of the muon transverse momentum (p_T^μ). All available muon isolation working points are listed in table 2 of [92]. Where isolated muons were required in the presented studies, the *FixCutLoose* thresholds were used.

3.5 Chapter Overview

This chapter reviewed the ingredients needed to build the $H(\rightarrow b\bar{b}) + j$ analysis. Section 3.1 presented the simulation process of proton-proton collisions, section 3.2

presented jets – the principal objects in this thesis. It introduced the Higgs jet object, and discussed its components – calorimeter jets and track jets. Section 3.3 presented the b -jet identification technique used in this thesis, and section 3.4 presented the reconstruction of muons, used in some event selections.

The next chapter will explore the combination of b -tagging and jet sub-structure techniques to identify the boosted $H \rightarrow b\bar{b}$ decay topology, and a dedicated calibration of the double b -tagging procedure used to identify boosted $H \rightarrow b\bar{b}$ decays.

Chapter 4

Identification of Boosted Double- b Decays

4.1 Double b -tagging

The focus of this thesis are $H \rightarrow b\bar{b}$ decays, which, at high momentum, manifest as large- R jets with two nearby b -jets within them. This boosted topology allowed the combination of b -tagging and jet substructure techniques to reduce the immense QCD backgrounds.

An ATLAS study [63] compared various b -tagging approaches for a boosted $H \rightarrow b\bar{b}$ topology, using the MV2 b -tagging algorithm described in section 3.3. In this study, a *Higgs jet* was defined by a large- R ($R = 1.0$) calorimeter jet associated with at least one or two $R = 0.2$ fixed radius track jets¹, depending on whether single or double b -tagging was used.

Standard double b -tagging required the two leading p_T track jets to pass the same single b -tagging working points² (WP). *Asymmetric b -tagging* also required the two leading p_T associated track jets to be b -tagged, but in this case one sub-jet had to pass a fixed WP, while the other was varied in the studies. *Single b -tagging* required any one track jet associated to the large- R jet to be b -tagged, and the *leading single*

¹ Note, the $H(\rightarrow b\bar{b}) + j$ analysis at the focus of this thesis used variable radius track jets due to their better performance, as discussed in section 3.2.5.

² The b -tagging working points, b -tagging efficiency and background rejection are defined in section 3.3.

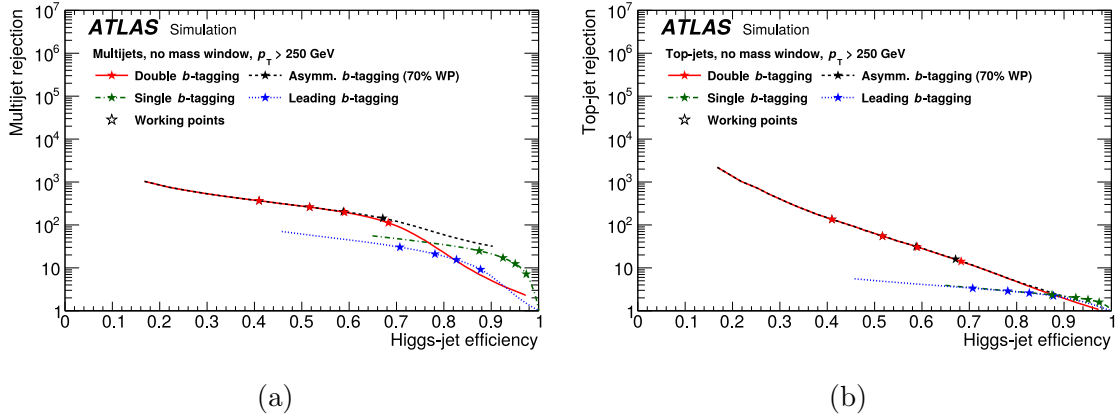


Figure 4.1: The (a) QCD and (b) top background rejection as a function of Higgs boson efficiency in simulated events for different b -tagging schemes [63]. The stars identify the standard b -tagging efficiency working points (for which calibrations were provided), corresponding to 60%, 70%, 77% and 85% single b -jet efficiency.

b -tagging required the leading p_T associated track jet to be b -tagged.

Figure 4.1 shows the QCD (4.1a) and top (4.1b) background rejection as a function of Higgs jet efficiency for jets with $p_T > 250$ GeV. In both cases the double b -tagging and asymmetric b -tagging gave the best background rejection for a wide range of Higgs jet efficiencies. Single b -tagging performed better at very high Higgs jet efficiency values, because double b -tagging schemes would require very loose thresholds to reach such high efficiencies.

The $H(\rightarrow b\bar{b})+j$ analysis used the double b -tagging scheme because of its simplicity, great performance and background rejection as compared to the other b -tagging schemes. The $H(\rightarrow b\bar{b})+j$ analysis also utilised variable radius (VR) sub-jets, described in section 3.2.5, due to their better performance compared to fixed radius track jets.

The MV2 single b -tagging algorithm was used for the b -tagging of the individual track jets. The analysis used calibration scale factors derived for the MV2 algorithm with VR track jets, which were applied twice. The validity of this treatment was independently confirmed in boosted $g \rightarrow b\bar{b}$ events, and boosted $Z \rightarrow b\bar{b} + \gamma$ events

(sections 7 and 8 of [63], respectively).

A dedicated double b -tagging calibration in boosted $g \rightarrow b\bar{b}$ events is an ongoing effort within ATLAS to which the author has significantly contributed during its initial development. The following sections introduce the early calibration procedure and relates it to the current developments of the calibration effort.

4.2 Double b -tagging Calibration in $g \rightarrow b\bar{b}$ Events

This section presents the double b -tagging calibration procedure in $g \rightarrow b\bar{b}$ events. The calibration is described as it was in its earlier stages, more closely familiar to the author. The differences with regard to the calibration in its current state are described where relevant.

QCD events, where gluons split into two b -quarks, are the largest source of boosted $b\bar{b}$ decays at ATLAS. The calibration used $g \rightarrow q\bar{q}$ events with a selection focusing on enriching the samples with $b\bar{b}$ decays, as the $g \rightarrow b\bar{b}$ decays could not be completely isolated. The procedure was derived from the previously mentioned double b -tagging validation studies in the same channel (section 7 in [63]). Section 4.2.1 further expands on the motivation for this calibration, and section 4.2.2 presents the author's contributions to this effort. Sections 4.2.3, 4.2.4, and 4.2.5 present the data and simulated samples used, the event selection, and the considered systematic uncertainties, respectively.

The boosted double b -tagging calibration in $g \rightarrow b\bar{b}$ events is an *in-situ* calibration. It used $b\bar{b}$ events in data to derive scale factors used to correct discrepancies between double b -tagging efficiencies in MC and data, rising from mismodelling. As $g \rightarrow b\bar{b}$ events could not be completely isolated, a data-driven method was used to extract the flavour composition of data, presented in section 4.2.6.

Section 4.2.7 outlines the calibration procedure, and section 4.2.8 presents the preliminary results. Section 4.2.9 summarises the new developments made since

these results were produced, and section 4.2.10 describes the next steps and future outlook for this calibration.

4.2.1 Motivation

Boosted $b\bar{b}$ decays are an object of interest in many ATLAS analyses. At the time of writing, analyses were recommended to apply the calibration scale factors derived for single b -tagged jets twice. The validation of kinematic jet quantities in $g \rightarrow b\bar{b}$ events, from which this calibration was derived, showed that this was a reasonable approach [63]. However, double b -tagging efficiency scale factors derived in a dedicated *in-situ* calibration would take into account possible effects rising from a highly collimated and busy tracking environment.

Furthermore, as mentioned in section 3.3.1, the single b -tagging scale factors and uncertainties for track jets with $p_T \geq 400$ GeV had to be derived using an MC-based extrapolation³. Boosted $b\bar{b}$ decays are a source of extremely high momentum b -jets, so a calibration in this topology could be used as a crosscheck for the currently recommended extrapolations, and as a potential framework for future calibrations at high momentum.

Recently, a Machine-Learning-based double- b -tagging algorithm (D_{Xbb} , or *the D_{Xbb} tagger*) has been developed by ATLAS. It was shown to outperform the standard double b -tagging approach, which uses two single b -tags [81]. The D_{Xbb} tagger can only be calibrated using a dataset of boosted $b\bar{b}$ decays. Therefore, the development of a calibration in this topology is crucial.

The D_{Xbb} tagger is designed to discriminate between light jets, jets initiated by top quarks, and jets initiated by Higgs bosons, therefore, it will be important to develop calibrations based on these processes. Preliminary calibrations of the D_{Xbb} tagger in $Z(\rightarrow b\bar{b}) + \gamma$ and $Z(\rightarrow b\bar{b}) + j$ events have been published for the first

³ At the time this work was done, the calibration was only done for jets with $p_T \leq 250$ GeV, requiring extrapolation beyond this point [91].

time in August 2021 [3]. This section presents the double b -tagging calibration in $g \rightarrow b\bar{b}$ events, which has been ongoing since 2017, and as of October 2021 is yet to be finalised.

4.2.2 Author's Contributions

The author of this thesis made a significant contribution to this calibration in its initial stages (2017-2019), as the validation method was extended towards a calibration. Her contributions were largely focused on software-related work which was crucial for the calibration to proceed.

Software used and written by analysis groups at ATLAS usually relies on baseline ATLAS software. This software is periodically updated, and the versions are called *software releases*. Every few years a new major software release is produced, involving updates to simulation and reconstruction software and various other performance improvements. A move to a new ATLAS software release induces a chain of necessary software updates throughout the entire collaboration to accommodate change in tools, data structure and formatting.

The principal task of the author was to update the extensive data preparation and analysis software frameworks to use the new ATLAS software release. She also aligned and integrated the data preparation software of the $g \rightarrow b\bar{b}$ calibration into a central ATLAS package allowing for easier maintenance in the future, and wrote extensive documentation on the calibration, to provide easy access to new users, vital to reduce hand-over times which occur frequently at such analyses.

The author also updated the analysis to use the most up-to-date selection and uncertainty recommendations provided by other ATLAS groups at the time, and studied the changes arising from the updated software and recommendations, which she documented in an internal ATLAS communication note [2] (internal).

An issue affecting the samples which were used by the author was found after her

departure from the effort, hence the plots shown in this chapter have been produced by a student to whom she passed on her work, but would not have been possible without her contributions. In all, the author successfully performed the software migration, integrated the software into a wider ATLAS infrastructure, and wrote extensive internal documentation on the effort, software, and her work.

4.2.3 Data and Simulated Samples

The double b -tagging calibration used ATLAS data at a pp collision energy of 13 TeV passing all data quality requirements. Studies shown were performed using data gathered over 2017 corresponding to an integrated luminosity of 44.3fb^{-1} . Current ongoing studies (as of 2021) are performed using the full *Run 2* data set.

Two types of simulated multi-jet samples were used: an inclusive sample containing all generated events needed for a sufficient amount of light-light ($u/d/s$) quark final states; and a sample generated with a muon-in-event requirement with $p_T > 3$ GeV and $|\eta| < 2.8$ to have a sufficiently large sample of multi-jet events with heavy (b, c) quarks.

Both MC samples were generated with the PYTHIA8 [94] generator with a leading order NNPDF2.3 [95] parton distribution function (PDF) set and the A14 [62] underlying event tune⁴. In both cases the EvtGen [96] package was used to accurately model b and c hadron decays. Pileup effects were included by overlaying simulated minimum-bias events on each hard scatter event. The minimum-bias events were simulated using the PYTHIA8 generator with the NNPDF2.3 PDF set and the A3 [97] tune.

⁴ Parton distribution functions and generator tunes are described in section 3.1.

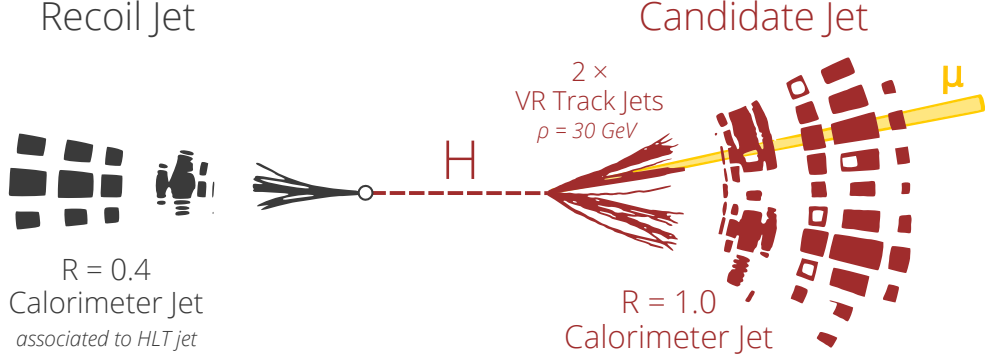


Figure 4.2: A stylised diagram showing the structure of an event of interest. Calorimeter deposits are depicted by rectangular shapes, and tracks are represented by curved lines near the interaction point.

4.2.4 Event Selection

This calibration is focused on boosted $g \rightarrow b\bar{b}$ events with a boosted $X \rightarrow b\bar{b}$ topology. The momentum boost is provided by another high energy jet in the event, which is also used for triggering. A diagram of the event can be seen in figure 4.2. The data used in this calibration were collected with an unprescaled HLT trigger requiring a single small- R ($R = 0.4$) calorimeter jet with a 420 GeV jet p_T threshold. The HLT jet had to be within $\Delta R < 0.4$ of a reconstructed small- R calorimeter jet in the event, called the *trigger jet* (j^{trig}).

A primary vertex (PV) with at least two $p_T > 0.5$ GeV tracks was required, and the primary vertex with the largest $\sum p_T^2$ was used. At least one large- R calorimeter jet with $p_T > 500$ GeV and $|\eta| < 2.0$ with at least two ghost-associated variable radius track jets (j^{trk}) was required, together forming the *candidate jet*.

The details of calorimeter and track jets used are given in sections 3.2.3 and 3.2.5, respectively. In addition to the track jet track selection requirements described in section 3.2.5, each track was also required to pass loose impact parameter thresholds: a transverse impact parameter threshold of $|d_0| < 5$ mm, and a longitudinal impact

parameter threshold of $|z_0 \sin(\theta)| < 3$ mm, to further reduce pileup contributions.

The samples were enriched with $b\bar{b}$ decays by requiring one of the track jets associated with the large- R jet to have an associated muon, which was indicative of a heavy quark undergoing weak decay. The muon had to pass the *loose* selection criteria, and be within $\Delta R < 0.2$ of the track jet axis. The muon selection criteria are described in section 3.4.

Two jets out of all of the track jets associated to the large- R jet were chosen for the analysis. First, the leading p_T jet with an associated muon was selected as the *muon jet* (j_μ^{trk}). Then, the leading p_T jet out of all remaining track jets, regardless of muon-matching, was selected as the *non-muon jet* ($j_{\text{non-}\mu}^{\text{trk}}$). The jet axes of the trigger jet and the muon jet had to be separated by at least $\Delta R(j^{\text{trig}}, j_\mu^{\text{trk}}) > 1.5$ to ensure the independence of the two objects.

The double b -tagging definition investigated in this study required both investigated track jets to pass the MV2 70% efficiency working point. Track jet flavour in MC was determined by looking for truth particles within $\Delta R < 0.3$ of the track jet axis, described in more detail in section 3.3.2 on *truth labelling*.

Each candidate jet will have two flavours associated with it – one for each sub-jet. Since the two sub-jets were not identical this resulted in nine candidate flavour combinations:

Flavour types:	$g \rightarrow b\bar{b}$ candidate	$j_{\text{non-}\mu}^{\text{trk}}$		
		B	C	L
B - bottom (b quarks)	B	BB	BC	BL
C - charm (c quarks)	C	CB	CC	CL
L - light ($u/d/s$ quarks)	L	LB	LC	LL

The current calibration effort has moved to calibrating the ML-based tagger due to its better performance. The ML-based tagger algorithm considers up to three largest p_T track jets associated to the large- R jet, which is reflected in the current event selection – at least two track jets are required, and up to three are considered.

4.2.5 Systematic Uncertainties

Three major systematic uncertainty sources were considered in the calibration: *large- R jet* uncertainties, *flavour tagging* uncertainties, and *modelling* uncertainties. The large- R jet uncertainties were derived in the calibrations⁵ described in section 3.2.4. The b -tagging efficiency, and c -jet and light-jet mis-tagging uncertainties were provided by calibrations described at the end of section 3.3.1. The modelling uncertainties are presented in this section.

The correction scale factors from the flavour tagging calibrations were applied to the simulated samples in these studies, as it makes it easier to observe mismodelling effects in the development stages of the calibration.

MC Generator Modelling Uncertainties

The validation study from which this calibration was derived used simulated samples produced with a HERWIG++ MC generator to estimate a generator modelling uncertainty, by taking a bin-by-bin difference between distributions produced with the base and alternative generator.

At the time of these studies equivalent alternative generator samples were not available, thus generator modelling uncertainties were not present in the results, however they will be included in the finalised calibration.

Impact Parameter Modelling Uncertainties

Photon conversions, hadronic material interactions with the ID material, and light long lived particle decays such as K or Λ can produce displaced vertices or tracks with non trivial impact parameters. These effects were difficult to model and required additional modelling uncertainties which were derived by weighting events containing tracks from photon conversions by $\pm 10\%$, from hadronic material inter-

⁵ Note, this work used earlier uncertainty derivations than those cited in section 3.2.4, which can be found in [98].

actions by $\pm 10\%$, and from light long lived particle decays by $\pm 30\%$. This treatment was taken from the light-jet mis-tagging calibration [90].

The transverse impact parameter resolution – $\sigma(d_0)$ – depends on various difficult-to-model detector effects. More accurate estimates of $\sigma(d_0)$ were made using minimum-bias, di-jet and Z+jets events [99] in bins of track p_T and η . A systematic uncertainty related to this procedure was included.

Fake Muon Modelling

The MC samples produced with a truth-muon requirement did not have a sufficient amount of fake muons. The impact of this mismodelling was estimated by an uncertainty in which events containing fake muons in the muon-filtered samples were scaled up a factor of 2 as was recommended internally in ATLAS at the time.

4.2.6 Flavour Composition Estimate Fit

The double b -tagging efficiency $\epsilon_{b\bar{b}}$ is the fraction of true $b\bar{b}$ jets, which are tagged as $b\bar{b}$ jets

$$\epsilon_{b\bar{b}} = \frac{N_{b\bar{b}, \text{tagged}}}{N_{b\bar{b}, \text{all}}}, \quad (4.1)$$

where $N_{b\bar{b}}$ is the number of $b\bar{b}$ jets. However the samples used in this calibration were not pure in $b\bar{b}$ decays, thus the fraction of $b\bar{b}$ events in the data had to be estimated. The flavour composition of the multi-jet data could not be extracted directly from simulation, as QCD processes are difficult to accurately model due to their complex nature. Therefore a data-driven method was used.

The flavour composition in data was extracted by fitting flavour-sensitive – *signed transverse impact parameter significance* (s_{d_0}) – distributions with expectations from MC. The post-fit expectations were seen to be representative of data. This section describes the flavour composition fitting procedure. The extraction of double b -tagging efficiencies from these results will be described in the following section.

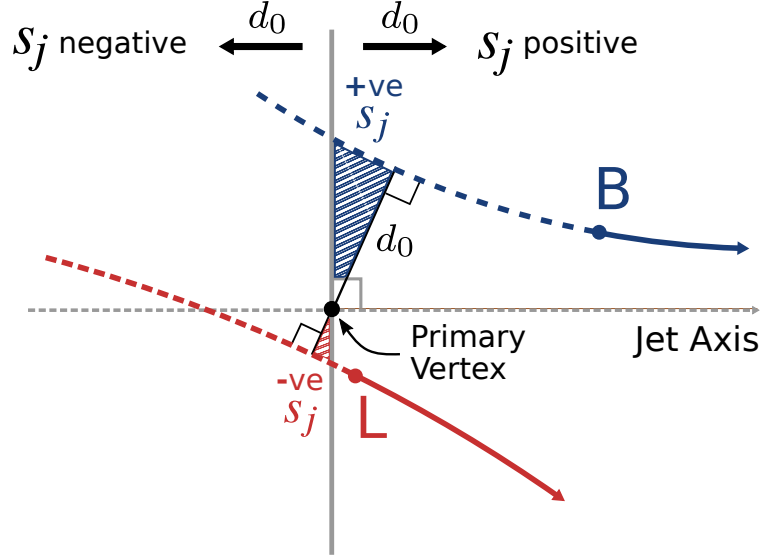


Figure 4.3: A graphical illustration of tracks left by a light ($u/d/s$) quark and the decay of a b quark, depicting transverse impact parameters d_0 , and the definition of s_j – sign indicating whether or not d_0 is in the jet direction.

Signed Transverse Impact Parameter Distributions

The signed transverse impact parameter significance is defined as:

$$s_{d_0} = \frac{|d_0|}{\sigma(d_0)} s_j, \quad (4.2)$$

where $\sigma(d_0)$ is the transverse impact parameter resolution, and s_j is a sign indicating whether d_0 is on the same side of a plane perpendicular to the jet axis and going across the primary vertex, as the jet, i.e. whether d_0 is in the direction of the jet. If d_0 is in the jet direction – s_j is positive, and negative otherwise. A diagram depicting d_0 and s_j is shown in figure 4.3.

The signed transverse impact parameter significance is sensitive to jet-flavour in two ways. Heavy flavour quarks take a longer time to decay, therefore their tracks will have larger impact parameters (d_0) and a broader s_{d_0} spectra. Also, s_j will tend to be positive for heavy flavours, since heavy quarks have time to travel a measurable distance in the jet direction before decaying. The measured s_j of light flavour tracks

is mostly governed by resolution effects and thus have no strong positive or negative skew.

The mean s_{d_0} of the three highest p_T tracks in a given track jet ($\langle s_{d_0} \rangle$) was used as the discriminating variable. It provided additional discrimination between heavy flavour track jets and light track jets with tracks with large d_0 from light long lived particle decays, like Λ or K_S .

An earlier b -tagging validation study in $g \rightarrow b\bar{b}$ events [100] using similar methodology, found that BC, CB, LB and LC combinations made up less than 1% of the samples, which was insufficient for accurate fitting of $\langle s_{d_0} \rangle$ shapes. These flavour components were merged into larger flavour components with the most similar shape resulting in 5 effective flavour combinations:

			$g \rightarrow b\bar{b}$		$j_{\text{non-}\mu}^{\text{trk}}$		
			candidate		B	C	L
BC	<i>merged into</i>	BL	j_{μ}^{trk}	B	BB		BL
CB	<i>merged into</i>	CL		C		CC	CL
LB and LL	<i>merged into</i>	LL		L			LL

The similarity deduction is described in section 6.7 of [100]. This approach was used in the double b -tagging validation study from which this calibration was derived, and kept in the calibration. The yields of the small flavour components were reviewed and found to be smaller than 1%, which was consistent with the previous study. At the time of writing, new flavour merging studies are ongoing to accommodate the changed candidate jet definition with up to three associated sub-jets.

The $\langle s_{d_0} \rangle$ shapes for j_{μ}^{trk} and $j_{\text{non-}\mu}^{\text{trk}}$ in simulation are shown in figure 4.4. The described s_{d_0} behaviour can be seen in both samples. The heavier flavour jets have wider distributions with a skew in the positive direction, and the behaviour was noticeably more prominent for the b jets as opposed to c jets. A slight skew in the positive direction was also seen for the light jets due to light long-lived particles (such as K or Λ).

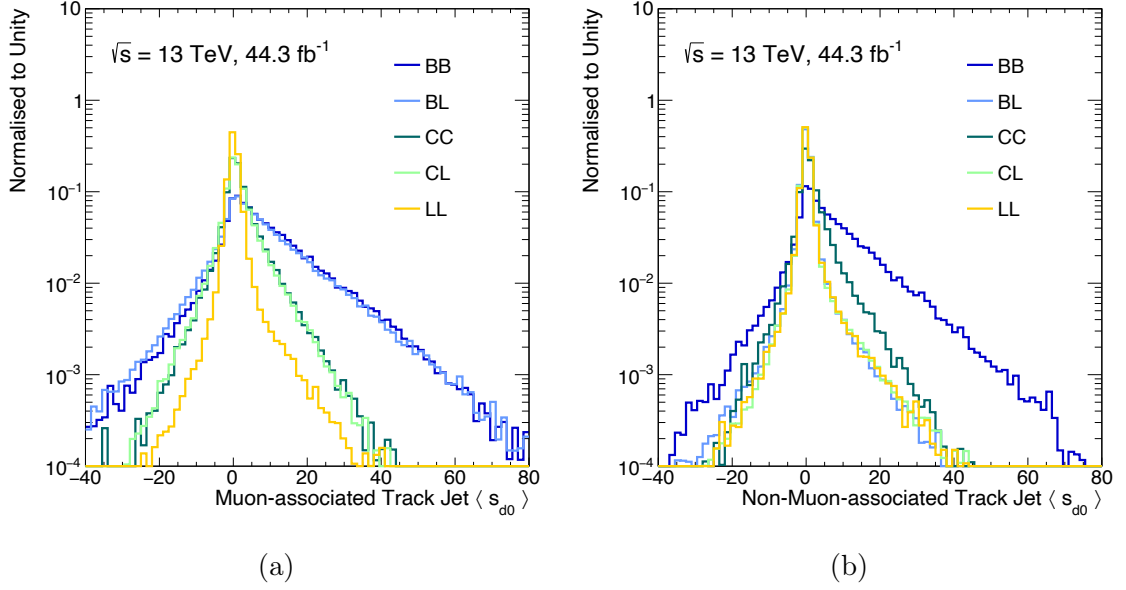


Figure 4.4: Simulated $\langle s_{d_0} \rangle$ shapes of (a) j_{μ}^{trk} and (b) $j_{\text{non-}\mu}^{\text{trk}}$ for each flavour component. All distributions are normalised to unity. *Note:* The first and second letter of each flavour pair indicates the flavour of j_{μ}^{trk} and $j_{\text{non-}\mu}^{\text{trk}}$, respectively.

Fitting the Flavour Composition

The flavour composition of data was estimated with a binned likelihood fit of the $\langle s_{d_0} \rangle$ distributions for j_{μ}^{trk} and $j_{\text{non-}\mu}^{\text{trk}}$ simultaneously. The likelihood definition is:

$$\mathcal{L} = \prod_{i=1}^n p(y_i | \boldsymbol{\theta}) , \quad (4.3)$$

where n is the number of bins, y_i is the number of data events in bin i . $\boldsymbol{\theta}$ is a vector of length k , containing the number of total estimated events for each flavour component, and k is the number of flavour components in the fit, which in this case was 5 (9 – 4 merged).

The probability distribution $p(y_i | \boldsymbol{\theta})$ was assumed to be a Poisson distribution:

$$p(y_i | \boldsymbol{\theta}) = \frac{e^{-\boldsymbol{\theta} \cdot \mathbf{x}_i} (\boldsymbol{\theta} \cdot \mathbf{x}_i)^{y_i}}{y_i!} , \quad (4.4)$$

where $\mathbf{x}_i$ is a vector of length k , containing the fractions of estimated events of each

certain flavour component in bin i

$$x_{ij} = \frac{\text{number of } j^{\text{th}} \text{ flavour component events in bin } i}{\theta_j} \quad (4.5)$$

The templates were binned in variable-size bins, such that the relative MC statistical uncertainty in each bin was smaller than 25%. As flavour composition could vary with sub-jet p_T , the fits were performed in separate sub-jet p_T bins:

$$\begin{array}{ll} j_{\mu}^{\text{trk}} & : \quad p_T < 100 \text{ GeV}; \quad \left| \quad 100 \text{ GeV} < p_T < 200 \text{ GeV}; \quad \right| \quad p_T > 200 \text{ GeV}; \\ j_{\text{non-}\mu}^{\text{trk}} & : \quad p_T < 100 \text{ GeV} \quad \left| \quad 100 \text{ GeV} < p_T < 200 \text{ GeV}; \quad \right| \quad 200 \text{ GeV} < p_T < 300 \text{ GeV}; \quad \left| \quad p_T > 300 \text{ GeV}; \end{array}$$

giving 12 $j^{\text{trk}} p_T$ regions. Minuit fitting software [101] was used to perform the fits.

Examples of the $\langle s_{d_0} \rangle$ distributions for j_{μ}^{trk} in a single p_T bin before and after the fit are shown in figures 4.5a and 4.5b, respectively. The ratio plots shown in the bottom panels of the figure show an overall improvement in the agreement between data and simulation after the fit.

The flavour composition fit produces a *correction factor*, c_f^r , for each flavour component ($f = bb, bl, cc, cl, ll$) in each $j^{\text{trk}} p_T$ region – r . The correction factors were applied to the simulated events, such that they could be used to estimate the bb flavour components in data, as presented in the following section.

4.2.7 Calibration Procedure

The double b -tagging calibration scale factors describe the differences of double b -tagging efficiency ($\epsilon_{b\bar{b}}$, equation 4.1) in data and MC.

$$\kappa_{b\bar{b}} = \frac{\epsilon_{b\bar{b}}^{\text{data}}}{\epsilon_{b\bar{b}}^{\text{MC}}} . \quad (4.6)$$

In simulation the truth flavour of the track jets was known, therefore the definition of $\epsilon_{b\bar{b}}^{\text{MC}}$ was straight forward:

$$\epsilon_{b\bar{b}}^{\text{MC}} = \frac{N_{b\bar{b}, \text{tagged}}^{\text{MC}}}{N_{b\bar{b}, \text{all}}^{\text{MC}}} , \quad (4.7)$$

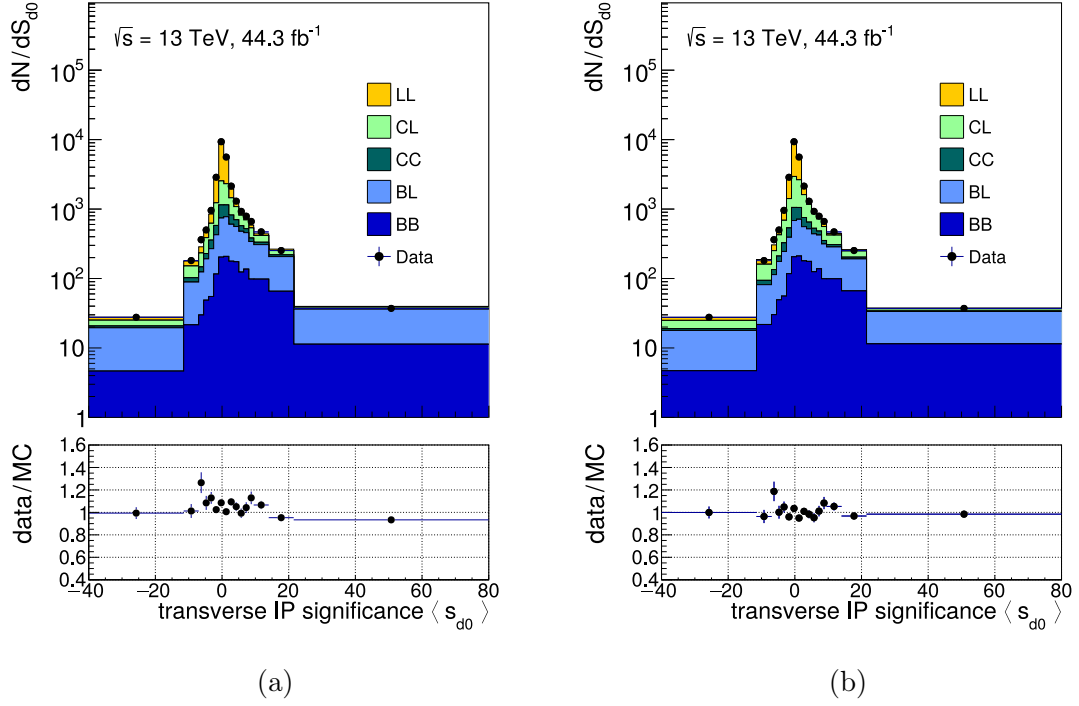


Figure 4.5: $\langle s_{d0} \rangle$ distributions in data and MC (a) before and (b) after the flavour composition fitting procedure in $p_T(\mu\text{-jet}) = [100; 200]$ GeV; $p_T(\text{non-}\mu\text{-jet}) = [100; 200]$ GeV momentum bin.

It did not matter if $\epsilon_{b\bar{b}}^{\text{MC}}$ is calculated using the simulated samples before or after the flavour composition correction described in section 4.2.6, as the correction factors would cancel out in the equation. In data there was no convenience of knowing the truth flavour of track jets, thus the fraction of $b\bar{b}$ jets used in the definition of $\epsilon_{b\bar{b}}^{\text{data}}$ was estimated by making two assumptions:

1. MC samples after the flavour correction and *before* double b -tagging accurately represent data before tagging, i.e. before tagging:

$$N_{b\bar{b}, \text{all}}^{\text{data}} = N_{b\bar{b}, \text{all}}^{\text{corrected MC}}; \quad (4.8)$$

2. after the flavour correction⁶ and *after* double b -tagging the differences between data and MC were contained in the BB jet fraction, i.e. after tagging:

$$N_{b\bar{b}, \text{ tagged}}^{\text{data}} = N_{\text{all}, \text{ tagged}}^{\text{data}} - N_{\text{non-}b\bar{b}, \text{ tagged}}^{\text{corrected MC}}. \quad (4.9)$$

The first assumption could be made because the MC was corrected such that it would represent data as accurately as possible. The second assumption could be made because after double b -tagging the non-BB components were small enough that their mismodelling would not have a significant impact on the scale factors.

Using the assumptions, the double b -tagging efficiency can be expressed as

$$\epsilon_{b\bar{b}}^{\text{data}} = \frac{N_{b\bar{b}, \text{ tagged}}^{\text{data}}}{N_{b\bar{b}, \text{ all}}^{\text{data}}} = \frac{N_{\text{all}, \text{ tagged}}^{\text{data}} - N_{\text{non-}b\bar{b}, \text{ tagged}}^{\text{corrected MC}}}{N_{b\bar{b}, \text{ all}}^{\text{corrected MC}}}. \quad (4.10)$$

The scale factors were derived in the same p_T bins of j_{μ}^{trk} and $j_{\text{non-}\mu}^{\text{trk}}$ as the normalisation factors for flavour composition correction described in section 4.2.6.

Fit Uncertainties

To account for the intercorrelations of the fit uncertainties on each flavour component, the fit uncertainties for variables in large- R jet bins were extrapolated using a pseudo-experiment method. A more detailed description can be found in section 5.5.1 of [102].

A nominal large- R jet distribution for a variable of interest (such as large- R jet p_T) was created by summing all events in all p_T regions multiplied by their corresponding flavour correction factor c_f^r . The fit uncertainties on each large- R jet variable of interest were derived by creating 2000 pseudo-distributions in the same way as a nominal distribution would be, but the flavour correction factors c_f^r were varied by a Gaussian-distributed random variable which was bound by the

⁶ The flavour correction was always applied before double b -tagging, no further correction was made after double b -tagging was applied.

eigenvalues and eigenvectors of the fit covariance matrix. This resulted in 2000 varied pseudo-distributions.

The fit uncertainties for a distribution of interest were then derived bin-by-bin by fitting a Gaussian distribution to all 2000 values of the pseudo-experiments within that bin. The standard deviation of the fitted Gaussian distribution was said to represent the total fitting uncertainty of said bin.

Systematic Uncertainty Extrapolation

The uncertainty extrapolation method used in the studies shown was not developed by the author. It is important to note that it was a preliminary method, not used in the final published version of the validation studies or the calibration.

The systematic uncertainties were extrapolated by repeating the flavour correction fit for each systematic variation to produce flavour-corrected systematic variations. The total extent of all uncertainties was estimated by adding the extent of each uncertainty in quadrature for each bin of a distribution of interest. Two significant caveats were present with this treatment: firstly, the possible correlations between uncertainties were not taken into account; and secondly, as the flavour correction preserved the total yield of the data, and imposed it on the sum of total sum of all flavour components, suppressing the normalisation aspect of the systematic uncertainties. The uncertainties shown in theses studies should be taken as an indication of the extent of uncertainties, rather than a finalised quantity.

The uncertainty treatment has since been improved as the calibration has moved to using new fitting software allowing the inclusion and correlation of systematic uncertainties in the fit.

4.2.8 Results

Figure 4.6 shows the candidate jet p_T distributions before (4.6a) and after (4.6b) double b -tagging. As mentioned previously, the single b -tagging correction factors

were applied to the samples, such that any differences were clear while the calibration was in development. The simulated templates shown in the plots were flavour-corrected, hence, any differences between data and MC could be assumed to be due to discrepancies specific to double b -tagging response.

After the double b -tagging was applied, the sample was expected to be largely dominated by jets from two b -quarks (i.e. $b\bar{b}$ jets). The agreement between data and simulation was seen to be within 1σ over the entire p_T range. The increase in uncertainties at low large- R jet p_T , was caused by the preliminary uncertainty propagation method, which imposed a constant fixed yield on all uncertainties. The yield restriction created a “pivot point” in the total uncertainty around the weighted mean of the distribution.

Figure 4.7 shows the p_T distributions for j_μ^{trk} and $j_{\text{non-}\mu}^{\text{trk}}$ after flavour correction and double b -tagging. In both cases the agreement was seen to slightly deteriorate at very high track jet momentum. At the time of these studies the MV2 b -tagging algorithm was trained using fixed radius $R = 0.2$ track jets. At high p_T , the VR track jet cone becomes much smaller than $R = 0.2$. For example, a 450 GeV track jet will have an effective cone size of $R_{\text{eff}} = 0.075$. Fewer tracks might be contained within the small cone making an algorithm optimised for much larger jets less effective.

Furthermore, the calibration of the MV2 b -tagging algorithm was also performed using fixed radius $R = 0.2$ jets at the time these studies were performed, which could lead to discrepancies between data and MC at high momentum when using VR track jets. Such behaviour was not observed in the earlier iterations of the calibration where fixed radius $R = 0.2$ track jets were used, supporting the hypothesis that the discrepancy could possibly be coming from the VR nature of the jets. The equivalent plots with fixed radius sub-jets are shown in figure A.1 in appendix A.

The preliminary double b -tagging scale factors are shown in figure 4.8. All scale factors were seen to be within 2σ of 1. It is notable that the modelling uncertainties from an alternative generator were not included, as explained in section 4.2.5. The

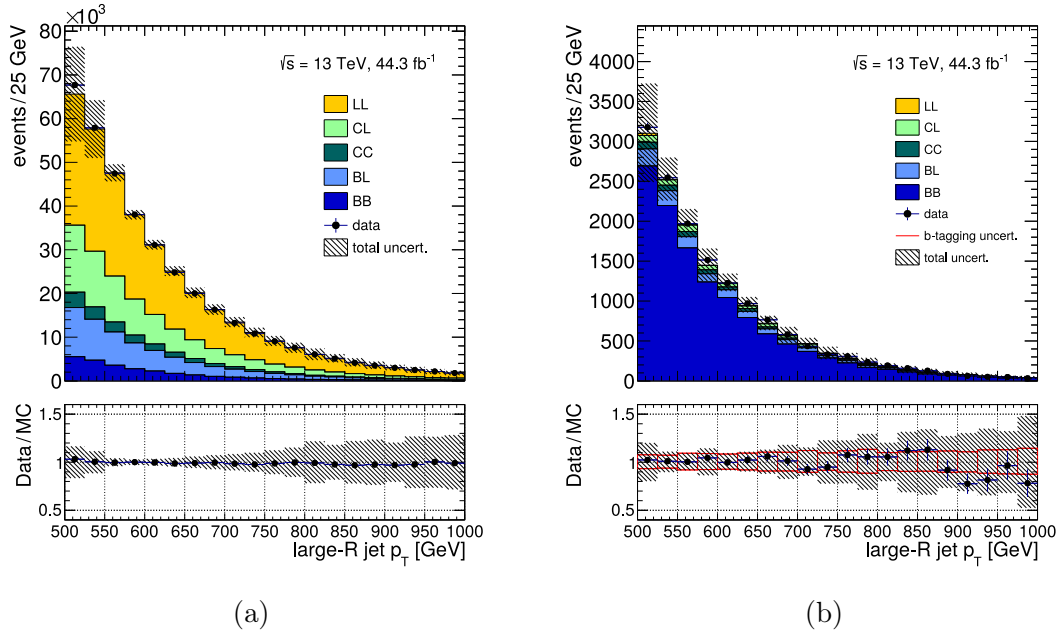


Figure 4.6: Large-R jet p_T distributions (a) before and (b) after double b -tagging ($2 \times \text{MV2}$ tags at 70% WP). The MC flavour composition was corrected (as described in 4.2.6) in both cases.

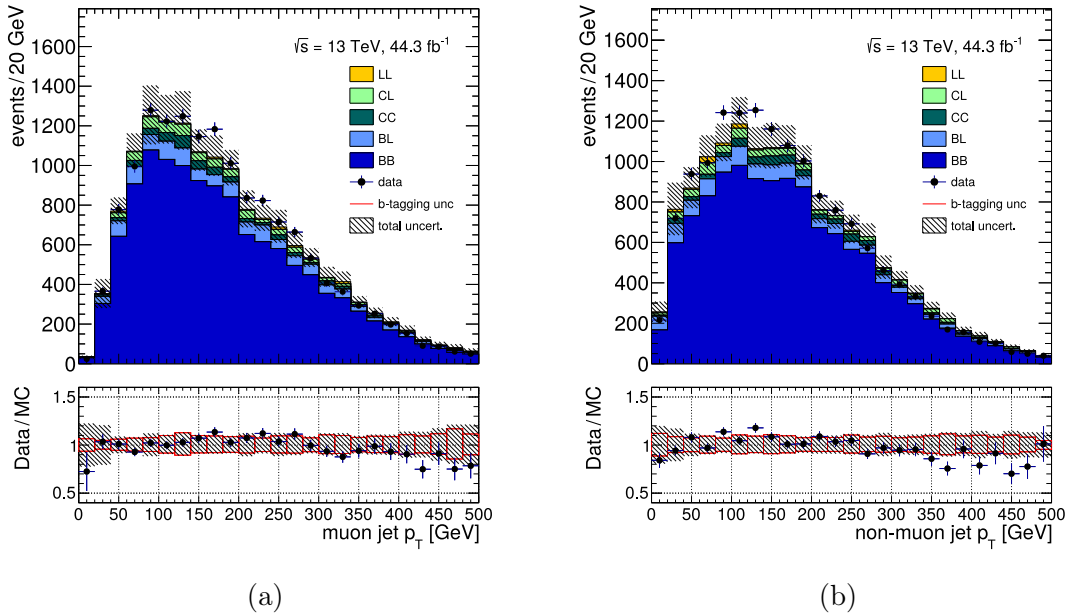


Figure 4.7: Transverse momentum distributions for (a) j_μ^{trk} and (b) $j_{\text{non-}\mu}^{\text{trk}}$ after double b -tagging ($2 \times \text{MV2}$ tags at 70% WP). In both cases the MC flavour composition was corrected before tagging (as described in 4.2.6).

$\sqrt{s} = 13 \text{ TeV}, 44.3 \text{ fb}^{-1}$ $g \rightarrow b\bar{b}$ calibration			
$p_T(\text{non-}\mu\text{-jet}) > 300 \text{ GeV}$	0.09 0.82 0.12	0.08 0.86 0.10	0.20 0.81 0.20
$p_T(\text{non-}\mu\text{-jet}) > 200 \text{ GeV}$ $< 300 \text{ GeV}$	0.10 1.00 0.09	0.09 1.09 0.08	0.07 0.88 0.07
$p_T(\text{non-}\mu\text{-jet}) > 100 \text{ GeV}$ $< 200 \text{ GeV}$	0.16 1.16 0.15	0.08 1.06 0.07	0.09 1.07 0.07
$p_T(\text{non-}\mu\text{-jet}) < 100 \text{ GeV}$	0.67 1.05 0.31	0.15 1.19 0.17	0.09 0.98 0.09
	$p_T(\mu\text{-jet}) < 100 \text{ GeV}$	$p_T(\mu\text{-jet}) > 100 \text{ GeV}$ $< 200 \text{ GeV}$	$p_T(\mu\text{-jet}) > 200 \text{ GeV}$

Figure 4.8: Preliminary double b -tagging calibration scale factors and uncertainties in bins of j_μ^{trk} and $j_{\text{non-}\mu}^{\text{trk}}$ transverse momentum.

validation study with 2015-2016 data saw (shown in table 2 of [63]) that the MC generator modelling uncertainties had a 23% effect on the total yield of the $b\bar{b}$ component, and a 13% effect on the total yield of all background components, making it the largest uncertainty for $b\bar{b}$ flavour jets, and second largest for background jets.

4.2.9 New Developments

The results shown in this chapter have been produced in late 2019. Since then the calibration team had studied and improved the procedure. This section gives a brief summary of the most important developments made in between late 2019 and the time of writing.

Prescaled Triggers: previously the calibration used the lowest available un-prescaled single jet trigger which, for data gathered in 2017, had a 420 GeV p_T threshold. To ensure that data was collected with a fully efficient trigger, this limited the large- R jet momentum to 500 GeV. Following equation 3.2 in chapter 3,

a Higgs boson decaying within a $R = 1.0$ cone, has $p_T \geq 250$ GeV. This means that a calibration starting at $p_T = 500$ GeV is not fully efficient for all possible Higgs bosons decaying within a large- R jet, which is the primary target of such a tagging algorithm. Using prescaled triggers with lower p_T thresholds has allowed the calibration to reduce the minimum large- R jet momentum to 250 GeV.

ML-based Tagger: as mentioned previously ATLAS has developed a ML-based double b -tagging algorithm, D_{Xbb} , shown to have better performance than using two single b -tags in this topology [81]. The tagger can only be calibrated using boosted $b\bar{b}$ events. Responding to the shown potential, the calibration effort has moved to calibrating the D_{Xbb} tagger.

Three Sub-jet Flavour Definition: the D_{Xbb} algorithm considers up to three highest p_T VR track jets associated to the large- R jet to make a decision. The two flavour definition currently used in the analysis is not compatible with the choices of the tagger. The calibration team is currently investigating a move to a three-flavour definition, flavour component merging schemes, and event selection changes.

New Fitting Software: the calibration is now using a more sophisticated ATLAS likelihood fitting software. It allows inclusion of systematic uncertainties in the fit, resulting in better treatment.

Fit Setup: a concern about the initial calibration setup derived directly from the validation study, was that the scale factor derivation is using a subset of data used for the flavour correction, which could possibly bias the results. Therefore the fit setup has been changed significantly.

Two mutually exclusive regions were defined: the **pass** region containing events passing double b -tagging requirements, and the **fail** region containing events which do not. The flavour correction factors are fit simultaneously in j_μ^{trk} and $j_{\text{non-}\mu}^{\text{trk}}$ $\langle s_{d_0} \rangle$ distributions in both **pass** and **fail** regions (i.e. 4 simultaneous fits per p_T bin). The double b -tagging scale factor ($\kappa_{b\bar{b}}$) is no longer derived analytically, but instead fit simultaneously with the flavour correction factors in the **pass** region fits. An

additional constraint on $\kappa_{b\bar{b}}$ is set by fitting and *anti-tag* scale factor, $\kappa_{\text{anti-}b\bar{b}}$, in the **fail** region, which is related to $\kappa_{b\bar{b}}$ as

$$\kappa_{\text{anti-}b\bar{b}} = \frac{1 - \epsilon_{b\bar{b}}^{\text{data}}}{1 - \epsilon_{b\bar{b}}^{\text{MC}}} = \frac{1 - \kappa_{b\bar{b}} \epsilon_{b\bar{b}}^{\text{MC}}}{1 - \epsilon_{b\bar{b}}^{\text{MC}}} . \quad (4.11)$$

As tagged data is now used in the fit, separation into j_{μ}^{trk} and $j_{\text{non-}\mu}^{\text{trk}}$ p_T bins would lead to regions with very low statistics. Fitting is now done in large- R jet p_T bins, which simplifies the procedure and allows for sufficient statistics to perform the fits.

4.2.10 Future Outlook

During the writing of this chapter, many studies were still ongoing. The systematic uncertainty treatment was being finalised. Candidate flavour definition studies were in progress concerning the inclusion of a third sub-jet. In the near future alternative generator modelling uncertainties will be added and their effect studied.

Boosted $b\bar{b}$ decays are a unique portal to Higgs physics at high energy scales. Advancing the ability to identify such decays accurately and efficiently is crucial to take advantage of the accessibility we have to the Higgs boson. As of October 2021, as this thesis is finalised, analyses focusing on boosted $b\bar{b}$ decays still have to rely on single b -tagging calibration scale factors which do not take into account possible intercorrelations between b -jets in a boosted topology, and are derived using track jets with $p_T < 400$ GeV, requiring scale factors for higher p_T jets to be extrapolated which has associated uncertainties. A dedicated double b -tagging calibration using boosted $b\bar{b}$ decays would provide more accurate estimates of double b -tagging performance differences in data and simulation at high p_T .

Furthermore, a new boosted double b -tagging algorithm has been developed by ATLAS, which can only be calibrated using boosted $b\bar{b}$ decays. Having access to this tool would greatly improve the capabilities of ATLAS analyses to efficiently identify $b\bar{b}$ decays. The boosted $H(\rightarrow b\bar{b}) + j$ decay measurement, which is the focus of this thesis, will also take advantage of this tool once it is fully calibrated.

Chapter 5

Building the Boosted $H(\rightarrow b\bar{b}) + j$ Analysis

5.1 Introduction

This chapter presents the analysis studying Higgs boson production through $H \rightarrow b\bar{b}$ decays with an additional jet in the final state: $H(\rightarrow b\bar{b}) + j$. An illustration of this topology is shown in figure 5.1, and a brief introduction and motivation for this study was given in section 1.3. This chapter gives an overview of the $H(\rightarrow b\bar{b}) + j$ analysis, describes the data and event selections used, presents the analysis strategy and the fits used in the studies and measurements¹ presented in this thesis.

This thesis was written while the analysis was still in its final stages. Some changes to the final measurement set-up were made after the completion of the studies presented in this thesis. The changes are summarised in section 9.1.1, and did not impact the outcomes of the presented studies.

The $H(\rightarrow b\bar{b}) + j$ analysis is the first dedicated Higgs boson analysis in this final state at the ATLAS experiment. It was developed from a low mass BSM resonance search with the same event signature ($X(\rightarrow b\bar{b}) + j$), which was released as a conference note in 2018 [4]. Aside from a BSM resonance, it explored a Higgs boson

¹ Note, the analysis presented in this thesis did not have high enough sensitivity to make Higgs boson cross-section measurements, and set confidence limits instead. Regardless, the word “measurement” will be used to refer to the attempted measurements for descriptive reasons.

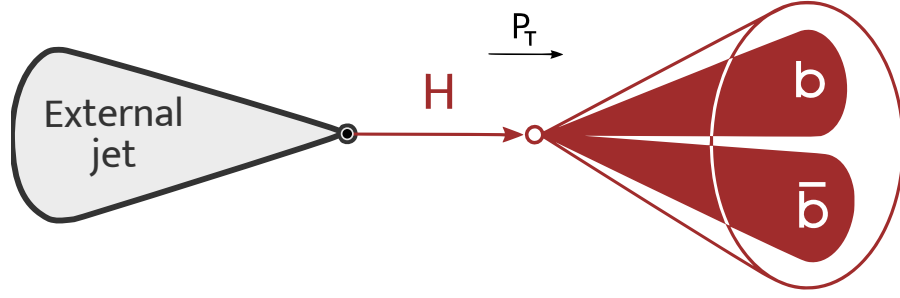


Figure 5.1: A diagram showing the $H(\rightarrow b\bar{b}) + j$ topology targeted by this analysis – a Higgs boson decaying to two b -quarks with a transverse momentum boost provided by an external jet in the event. The two b -jets collimate forming a single Higgs jet, and the event can be triggered on either the Higgs jet or the external jet.

hypothesis, measuring a small 1.6σ excess above the background-only hypothesis, compared to an expected sensitivity of 0.28σ . These results were also compatible with a 1.5σ excess (0.7σ expected) measured by a parallel study published by the CMS experiment [103] in early 2018.

Since then the CMS experiment has published a study in the same final state in 2020 [104], measuring a 2.5σ excess above the background-only hypothesis (0.7σ expected), and probing the Higgs boson production cross-section for $p_T^H > 650$ GeV. The $H(\rightarrow b\bar{b}) + j$ analysis presented in this thesis is the first ATLAS analysis to target Higgs bosons with $p_T^H > 650$ GeV [28] and set limits for inclusive Higgs boson cross-section in this high p_T^H domain [105].

Motivation

The most common decay of the Higgs boson is to two b -quarks ($\approx 58\%$), however it is difficult to observe due to a large QCD background in proton-proton collisions. Despite the challenges, developing the expertise to access the most prolific Higgs boson decay is of vital importance to further the knowledge of the Higgs boson.

One immediate challenge to studying $H \rightarrow b\bar{b}$ decays is posed by the ATLAS trigger system. To combat the immense QCD background, jet triggers have high p_T

thresholds, which sets a high minimum mass limit on any resonances producing two jets. For example, a 2016 ATLAS study of BSM resonances decaying to two b -jets ($X \rightarrow b\bar{b}$) triggering on two single b -jets was limited to a minimum resonance mass of 0.7 TeV [106], much larger than the 125 GeV mass of the Higgs boson.

This analysis overcame the triggering issue by looking for Higgs bosons produced with a large momentum boost. In this case the constituent b -jets collimate producing a high energy *Higgs jet* (described in section 3.2.1). The momentum boost to the Higgs boson is provided by an additional jet in the event ($H(\rightarrow b\bar{b}) + j$), and the event can be triggered on either the Higgs jet or the additional jet.

At the time of writing, $H \rightarrow b\bar{b}$ decays had only been observed in two types of ATLAS analyses, each focusing on a particular production mode: the VH production mode (5.3σ significance), which relied on triggering using muons and missing energy [107, 8]; and the VBF production mode (2.9σ significance), triggering on two additional jets in the event [108]. In the former case, the leptonic signature excluded the ggF production mode entirely, whereas in the latter case the ggF events behaved too similarly to the backgrounds the analysis aimed to remove.

The $H(\rightarrow b\bar{b}) + j$ analysis is the only $H \rightarrow b\bar{b}$ analysis at ATLAS which does not impose restrictions on production mode [28], and has the potential to develop into a future measurement of the Higgs boson production through ggF using $H \rightarrow b\bar{b}$ decays. As the Higgs boson production cross-section drops with Higgs boson p_T , reducing the restrictions on Higgs boson production modes provides an avenue to study regions of previously inaccessible regions of Higgs boson momentum.

Goals

The $H(\rightarrow b\bar{b}) + j$ analysis attempted three types of measurements. The **inclusive measurement** probed the Higgs boson signal strength μ_H (the ratio of measured and SM predicted signal yield, given in equation 1.8) over the entire accessible range of Higgs candidate jet p_T ($p_T^{\text{jet}} > 250$ GeV). The **fiducial measurement** probed

the inclusive Higgs boson production cross-section within a single fiducial volume of Higgs boson $p_T^H > 450$ GeV and $|y_H| < 2$. The **differential measurement** probed the inclusive Higgs boson production cross-sections in fiducial bins of Higgs boson $p_T^H \in 250 - 450$ GeV; $450 - 650$ GeV; $650 - 1000$ GeV; > 1 TeV, as defined by the STXS framework [109] introduced later, in section 5.5. All measurements were inclusive in Higgs boson production mode.

The highest momentum bin in the differential measurement, $p_T > 1$ TeV, was added late in the analysis, so the studies presented in this thesis (excluding the results in chapter 9), do not include this momentum bin. More information on analysis updates during the writing of this thesis can be found in section 9.1.1.

The expertise and machinery developed for this analysis is a necessary precursor for future studies of Higgs boson production separated by production mode in this final state. The details of the measurement strategies are given later in this chapter, in section 5.5.

5.2 Analysis Overview

This section gives a brief overview of the analysis. The measurement was performed by fitting Higgs boson candidate jet mass spectra with the Higgs, W and Z boson, $t\bar{t}$, and QCD background estimates in order to extract the Higgs boson signal strength (μ_H), which was then reinterpreted as a cross-section measurement.

The events containing the topology of interest in which the Higgs boson measurements were performed were collectively called the *signal region* (SR). Two signal regions were defined for this measurement, depending on whether the Higgs boson candidate jet was the leading or subleading p_T large- R jet in the event, denoted **SRL** (*Signal Region Leading jet*) and **SRS** (*Signal Region Subleading jet*), respectively. In all measurements the mass spectra of the two signal regions were fit simultaneously.

All resonant backgrounds were estimated by mass templates from Monte Carlo

(MC) simulations, whereas the QCD background was described by a parametric function derived using a data-driven method, using an independent *validation region*. The validation region was subdivided in the same way as the signal region - according to the Higgs boson candidate jet ranking in p_T - into **VRL** and **VRS**. The form of the QCD parametric description was determined using the validation regions, but the parameters of the function were set as free parameters in the signal region fits. The QCD background studies using validation regions are discussed in section 6.4.

A kinematically similar $t\bar{t}$ enriched *control region* (**CR_{t $\bar{t}$}**) was used to get a more precise estimate of the $t\bar{t}$ background normalisation, and provide additional constraints on related systematic uncertainties. This was achieved by fitting the $t\bar{t}$ template in **CR_{t $\bar{t}$}** and signal regions simultaneously. Chapter 8 discusses **CR_{t $\bar{t}$}** fits in detail. Another control region was used separately to derive more precise constraints on W and Z jet mass resolution, utilising hadronic W boson decays isolated from $t\bar{t}$ enriched events (**CR_W**). The procedure is discussed in section 7.7.

To summarise, the measurements were performed by fitting the signal regions and **CR_{t $\bar{t}$}** simultaneously. All resonant processes were modelled using simulations and the QCD background was modelled using a parametric function determined from studies in complementary validation regions. The measurements were performed by performing binned likelihood fits (described in section 5.7) to estimate the yields of all processes in data.

5.3 Data and Simulated Samples

5.3.1 Data

This analysis used 13 TeV pp collision data gathered by the ATLAS experiment throughout the entire *Run 2* period (2015-2018) and passing all data quality requirements [40]. Single large- R jet triggers were used to collect signal and validation region data. The trigger requirements consisted of minimum p_T^{jet} and in some cases

Table 5.1: The list of jet triggers used in the analysis to collect signal and validation region data for each data taking year. The last two triggers listed for 2018 (*) have the same requirements but are from different trigger chains and are not required to be active at the same time. Int. Lumi. – integrated luminosity.

Year	Thresholds		Int. Lumi.
2015	$p_T^{\text{jet}} > 360 \text{ GeV}$		3.2 fb^{-1}
2016	$p_T^{\text{jet}} > 420 \text{ GeV}$		33.0 fb^{-1}
2017	$p_T^{\text{jet}} > 440 \text{ GeV}$		41.2 fb^{-1}
	$p_T^{\text{jet}} > 390 \text{ GeV}$	$m_{\text{jet}} > 30 \text{ GeV}$	41.0 fb^{-1}
	$p_T^{\text{jet}} > 460 \text{ GeV}$		58.5 fb^{-1}
2018	$p_T^{\text{jet}} > 420 \text{ GeV}$	$m_{\text{jet}} > 35 \text{ GeV}$	58.5 fb^{-1*}
	$p_T^{\text{jet}} > 420 \text{ GeV}$	$m_{\text{jet}} > 35 \text{ GeV}$	55.4 fb^{-1*}

minimum jet mass (m_{jet}) thresholds, given in table 5.1.

The analysis used the lowest possible trigger thresholds, which were subject to changing pileup conditions², and therefore were different for each year. If more than one trigger is listed for a given year, all listed triggers were required to be active during data gathering, and at least one of the triggers had to be passed. In total the data used amounts to 136 fb^{-1} .

Muons from semileptonic top decays ($t \rightarrow Wb \rightarrow \mu\nu_\mu b$) were used to trigger data collection for $\text{CR}_{t\bar{t}}$ and CR_W which focus on $t\bar{t}$ decays. Table 5.2 lists the triggers used in the two control regions. If multiple triggers are listed for the same year (CR_W), at least one of the triggers had to be passed.

² Shown in figure 2.3 in section 2.1.

Table 5.2: The list of muon triggers used for $\text{CR}_{t\bar{t}}$ and CR_W data collection. The CR_W online trigger requirements also include `iloose` (for 2015) `ivarmedium` (for 2016-2018) isolation criteria described in section 4.2 of [110]. Int. Lumi. – integrated luminosity.

Region	Year	Threshold	Int. Lumi.
$\text{CR}_{t\bar{t}}$	All Years	$p_T^\mu > 50 \text{ GeV}$	136.0 fb ⁻¹
	All Years	$p_T^\mu > 50 \text{ GeV}$	
CR_W	2015	$p_T^\mu > 20 \text{ GeV}$	139.0 fb ⁻¹
	2016-2018	$p_T^\mu > 26 \text{ GeV}$	

5.3.2 Simulated Samples

Simulated Signal Samples

Four main Higgs boson production modes contributed significantly in the signal region: gluon-gluon fusion (ggF), vector boson fusion (VBF), Higgs-strahlung with an associated W or Z boson (VH), and Higgs boson production in association with a pair of top quarks ($t\bar{t}H$). The Higgs boson MC samples used in the analysis were produced separately for each production mode.

Matrix Element (ME) generation for all production modes was done with the Powheg-Box 2 [111–113] framework. The ggF event generation also used the HJ+MiNLO [114–116] prescription for finite mass effects, and the VH event generation used the MiNLO [117] prescription and the GoSAM package [118] for additional ME corrections. All Higgs boson production modes were generated using the NNPDF3.0 parton distribution function (PDF) set [119] derived at next-to-leading order (NLO) accuracy in QCD. Higgs boson production in association with W and Z bosons also included $gg \rightarrow ZH$ contributions calculated at leading order precision.

The parton showering for all production modes was done using the PYTHIA 8 [94] generator with the AZNLO parameter tune [120] and the CTEQ6L1 par-

ton distribution function [121]. Corrections for NLO electro-weak effects calculated using the HAWK program [122, 123] were applied to the VBF VH and $t\bar{t}H$ production modes. The Higgs boson production cross-sections of all generated samples were compared to the most recent recommendations of the LHC Higgs Cross-section Working Group [124, 30] and rescaled accordingly.

The $t\bar{t}H$ samples include all Higgs boson decay channels to model the occurrences where a hadronic top decay in the event is selected as the Higgs boson candidate. All other production mode samples only include $H \rightarrow b\bar{b}$ decays, as fake contributions were less relevant and would not compete with the other overwhelming backgrounds.

Simulated Background Samples

Simulated di-jet events used in the QCD background estimation were generated using the PYTHIA 8 generator with a leading order NNPDF2.3 PDF set [95] and the A14 underlying event parameter tune [62].

Events of hadronically decaying W and Z bosons with an additional jet in the event (V +jets events) were generated using the SHERPA 2.2.8 [125] generator to NLO accuracy in QCD for one additional parton and LO accuracy in QCD for up to four additional partons. The next-to-next-to-leading order NNPDF3.0 PDF set [119] was used. Approximate NLO electro-weak cross-section corrections [126, 127], as well as NNLO QCD [128–131] cross-section corrections were also applied.

The dedicated CR_W control region used to constrain W and Z boson jet mass resolution uncertainty, was built by isolating W boson candidates from $t\bar{t}$ events. As the constraint was to be derived for weak bosons, the most similar sample of $t\bar{t}$ events available at the time was used. The $t\bar{t}$ events were produced using the same generators and settings as those used to produce V +jets events, but with an older version of the SHERPA generator [125] – SHERPA 2.2.1. The compatibility of these samples to the V +jets samples in the investigated regime was tested and no significant differences were found. The $W(\ell\nu)$ samples used in the $\text{CR}_{t\bar{t}}$ region were

generated in the same way.

Single top-quark t -channel and s -channel production, and production in association with a W boson (Wt), collectively *single-top* events³, and $t\bar{t}$ events were generated at NLO in QCD using POWHEG-BOX 2 generator and the NNPDF3.0 next-to-leading order PDF set, using the diagram subtraction scheme [132] to take into account interference effects between single-top and $t\bar{t}$ events. The hadronisation was performed using PYTHIA 8 with the leading-order NNPDF2.3 PDF set and the A14 tune.

All simulations were using the EvtGen [96] package to accurately model b -quark decays. Pileup effects were included in all simulated samples by overlaying them with simulated minimum bias events. These events were simulated using the PYTHIA8 generator with a leading order NNPDF2.3 PDF set and the A3 [97] tune, and reweighted to match the observed pileup profile of each year of *Run 2*. All detector simulation was done using GEANT4 software [59, 60]. Further details on simulated samples, and a table summarising all MC generators used can be found in [5].

5.4 Event Selection

The $H(\rightarrow b\bar{b}) + j$ event topology was made up of two large- R calorimeter jets: the *Higgs jet*, and the recoil jet. The Higgs jet topology had two b -tagged variable-radius track jets within it, as described previously in section 3.2.1. The object reconstruction processes and criteria were as described in chapter 3. A diagram of the objects in the event is shown in figure 5.2.

All considered events were required to have at least one reconstructed vertex, and the vertex with the largest $\sum p_T^2$ was considered to be the primary vertex. Further selections were tailored for each region, which involved b -tagging requirements. For

³ The t -channel and s -channel samples were included late in the analysis, hence, the studies presented in this thesis, except for the final results presented in chapter 9, did not include their contributions. This did not have a significant impact on the presented work. More information can be found in section 9.1.1 and appendix H.2.

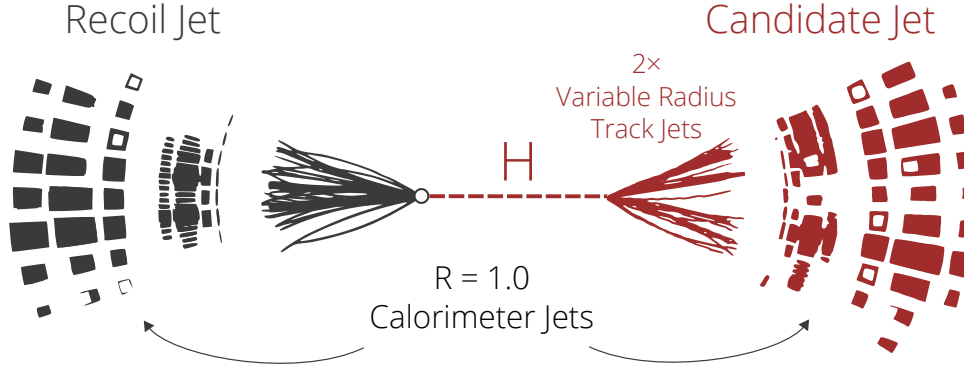


Figure 5.2: A stylised diagram showing the structure of an event of interest. Calorimeter deposits are depicted by rectangular shapes, and tracks are represented by curved lines near the interaction point.

a track jet to be considered *b*-tagged, it had to pass the 77% efficiency working point of the MV2 *b*-tagging algorithm.

5.4.1 Signal and Validation Regions

The trigger jet in the event was required to have $p_T^{\text{jet}} > 450$ GeV and $m_{\text{jet}} > 60$ GeV to ensure that all triggers used throughout all years were fully efficient. A second large- R jet with $p_T^{\text{jet}} > 200$ GeV was required, such that two jets made up the event: one for the Higgs boson candidate, and one for the recoil jet. The large- R jets were ordered in p_T , and the two leading p_T jets were considered for further selection.

Higgs Boson Candidate Jet

One of the two considered large- R jets in the event had to be a Higgs boson *candidate jet* (shown in red in figure 5.2). A candidate jet had to have $p_T^{\text{jet}} > 250$ and $2m_{\text{jet}}/p_T^{\text{jet}} < 1$ to ensure a boosted Higgs topology (discussed in section 3.2.1). To simplify the treatment, $m_{\text{jet}} > 60$ GeV was imposed, in line with the offline threshold imposed on the trigger jet. Large- R jet calibrations were produced for $|\eta_{\text{jet}}| < 2$, which was maintained in this analysis.

The candidate jet also had to have at least two ghost-associated variable-radius

(VR) track jets (described in section 3.2.5), representing the two quarks in the $H \rightarrow b\bar{b}$ decay. The two highest p_T associated track jets were considered for b -tagging and had to pass the overlap removal criteria described in section 3.2.5. The events were then divided into signal and validation regions using b -tagging. A candidate jet was said to "have one (or two) b -tag(s)" if one (or both) of the two highest p_T track jets passed the b -tagging requirements.

Region Definition

The events constituting the **signal region** were required to have a Higgs candidate jet with two b -tags. As introduced previously, the signal region was subdivided according to candidate jet p_T ordering:

SRL – leading p_T large- R jet is a **candidate jet** with **two b -tags**;

SRS – subleading p_T large- R jet is a **candidate jet** with **two b -tags**.

If both of the considered large- R jets passed these criteria, the leading jet was considered to be the candidate, and the event was classified as an SRL event.

The **validation region** was used for the studies of the functional form of the QCD background estimate. Events with candidates with strictly no b -tags were chosen to serve as kinematically equivalent (regarding QCD) independent proxies to the signal region. The validation region was similarly subdivided to:

VRL – leading p_T large- R jet is a **candidate jet** with **zero b -tags**;

VRS – subleading p_T large- R jet is a **candidate jet** with **zero b -tags**.

In the case where both candidates had zero b -tags, the event entered both VRL and VRS, so as not to introduce kinematic bias. The classification of signal and validation regions is shown in figure 5.3

Once the events were separated into regions a *muon-in-jet* correction for jet mass and p_T was applied. It accounted for some of the jet energy loss in the case of semileptonic decay in decay chain of the candidate (e.g. $b \rightarrow Wq \rightarrow l\nu q$). This

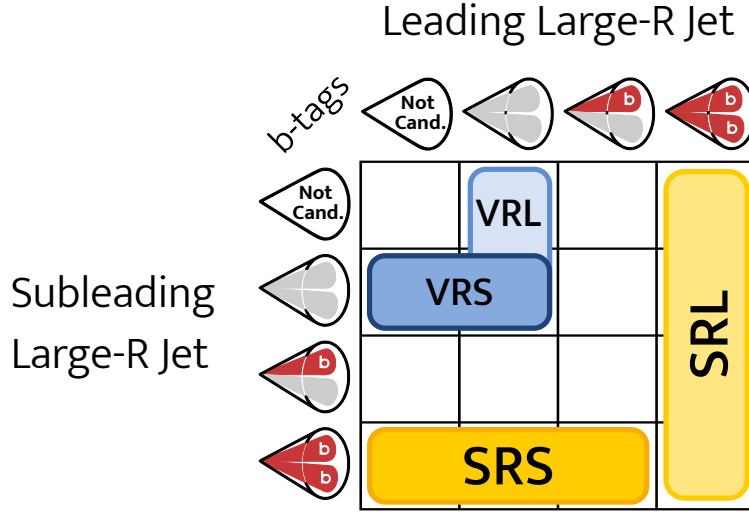


Figure 5.3: A diagram of the definitions of the *signal* and *validation* regions, as determined by the b -tagging of and p_T ordering of the Higgs boson *candidate jets* in the event. “Not cand.” – the large- R jet does not pass the criteria of a Higgs boson candidate.

phenomena mostly affected the candidate jets with subleading p_T , as the energy loss could have been the cause for the candidate to become the subleading jet. As neutrino energy losses could not be corrected, the resolution of the subleading events is worse. This will be shown later in figure 5.4. More information on the muon-in-jet correction can be found in appendix B.1.

Plots showing simulated events which passed the selection criteria of the signal and validation regions are shown in the top and bottom of figure 5.4, respectively. Data is also shown in the validation region plots. The components of the signal regions, in order of prominence, were: QCD, $t\bar{t}$, and Z and W boson; the components of the validation region, in the same order, were: QCD, W boson, $t\bar{t}$, and Z boson. The lower boundaries of the mass ranges were between 70 GeV and 75 GeV depending on the region. This is discussed in more detail in appendix B.3, and boundaries for all regions are shown in table B.1. They were determined by several experimental *turn-on* effects creating regions of reduced efficiency at low masses.

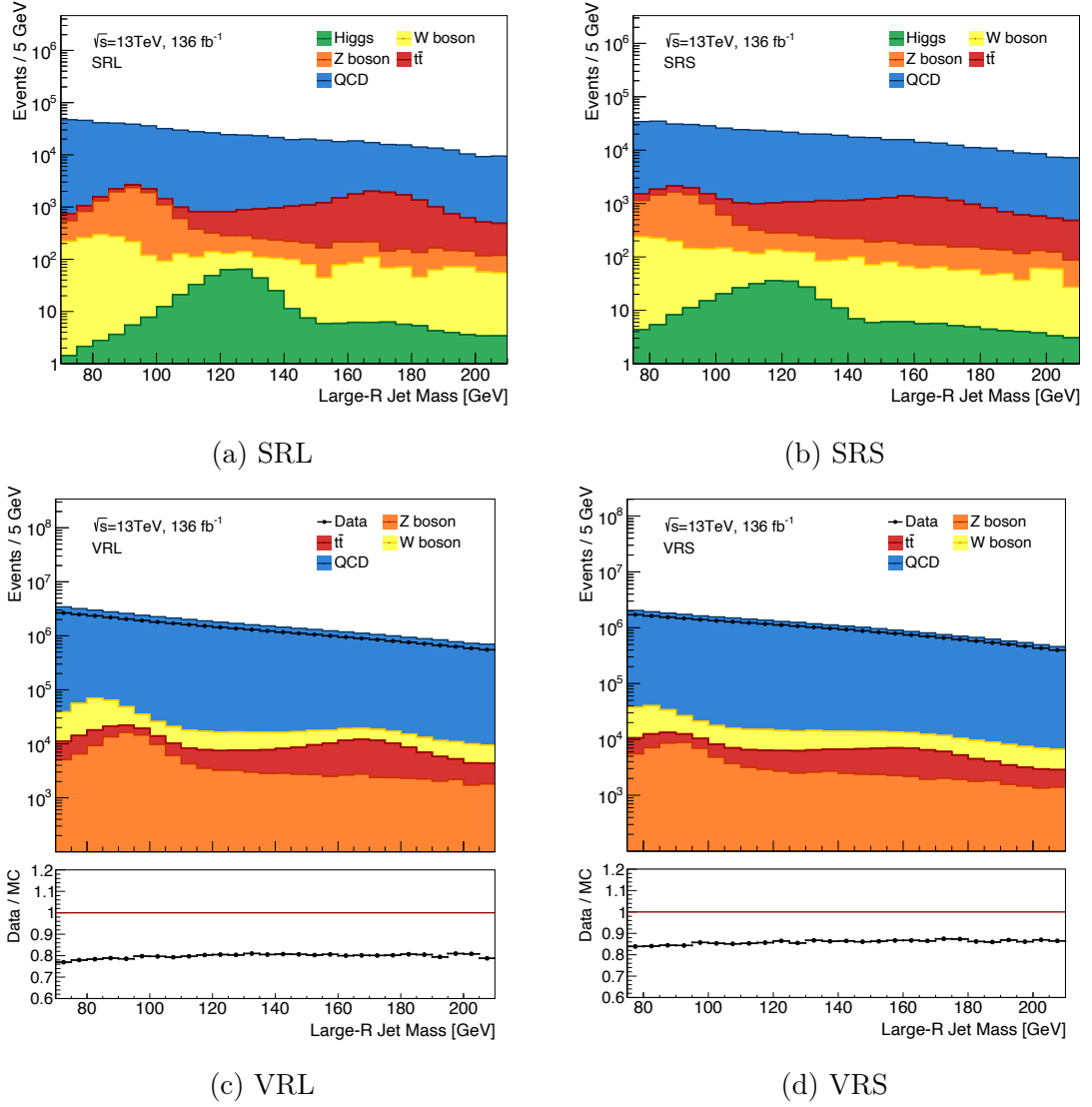


Figure 5.4: Stacked histograms of the simulated events passing the selection criteria of the signal regions: (a) SRL (b) SRS; and validation regions: (c) VRL (d) VRS. The ordering in the stack is based on contribution, such that components with larger yields are stacked on top of components with smaller yields. Validation region data is also shown.

The upper boundary was chosen to be 210 GeV to encompass the full $t\bar{t}$ resonance.

The resolution of the resonances was generally seen to be worse in the subleading candidate regions (SRS, VRS), as processes which lead to particle energy to not be registered in the jet and deteriorate jet resolution, such as final state radiation, energy deposits outside of the jet cone, and semi-leptonic decays, can also lead to

Table 5.3: Yields of SM expectations of various processes in terms of percentages of the total *data yield* – the total number of events in data passing the event selection, over the entire investigated mass ranges (total), and around the Higgs boson mass resonance ($m \in [105 - 140]$ GeV). The QCD background is excluded as it was modelled by a parametric function, but is expected (by subtraction) to make up around 95% of the yield in all cases

Process	Total		$m \in [105 - 140]$ GeV	
	SRL	SRS	SRL	SRS
$t\bar{t}$	3.3%	3.5%	2.3%	3.3%
Z +jets	1.8%	1.5%	0.9%	0.7%
W +jets	0.5%	0.4%	0.3%	0.4%
H	0.1%	0.1%	0.2%	0.1%
Data Yield	626532	560083	168762	168592

the candidate becoming the sub-leading jet in the event.

The agreement between data and simulation in the validation region, shown in figures 5.4c and 5.4d, was notably poor, with MC overestimating the data by 20-30%, illustrating the need for a data driven QCD background estimate. The expected percentage yields of all resonant processes are given in table 5.3. The event composition illustrates the complexity of this study. The Higgs boson signal was exceptionally small relative to other processes, making up around 0.1% of the events in the entire mass spectra, whereas the QCD background, which did not have a precise MC prediction, was remarkably dominant, making up around 95% of the events.

5.4.2 $t\bar{t}$ Control Region ($\text{CR}_{t\bar{t}}$)

The $\text{CR}_{t\bar{t}}$ event selection was focused on isolating boosted $t\bar{t}$ decays to constrain the $t\bar{t}$ background. The event topology was based on a back-to-back $t\bar{t}$ decay, where one top quark decays semileptonically ($t \rightarrow b\ell\nu$) and the other decays fully

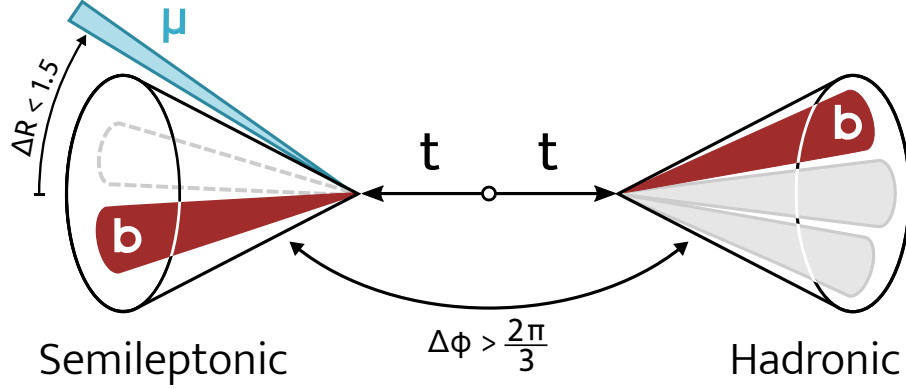


Figure 5.5: A diagram describing the topology of a $\text{CR}_{t\bar{t}}$ event.

hadronically ($t \rightarrow qq'b$). A diagram of an event is given in figure 5.5. Events with at least two large- R calorimeter jets with $p_T^{\text{jet}} > 250$ GeV and $|\eta_{\text{jet}}| < 2$ were selected. The two large- R jets with the largest p_T were considered for further selection.

The semileptonically decaying top quark was used to identify an event of interest. The events were triggered using a $p_T^\mu > 50$ GeV muon trigger. The muon with the highest p_T in the event had to pass the isolation criteria discussed in section 3.4, be matched to a trigger muon, and pass a $p_T^\mu > 52.5$ GeV cut to ensure full trigger efficiency. One of the two considered large- R jets had to be within $0.04 + 10 \text{ GeV}/p_T^\mu < \Delta R < 1.5$ of the muon, where the lower boundary was set such that the muon is isolated. The large- R jet also had to have ≥ 1 associated VR track jet, and exactly one of the associated track jets had to be b -tagged (only the two highest p_T track jets were considered). The muon and b -tagged jet together formed the leptonic top-quark decay topology.

The hadronically decaying top quark, represented by the other considered large- R jet in the event, was used as the candidate jet. It had to have at least 3 associated VR track jets, exactly one of which was b -tagged. The two large- R jets had to be separated by $\Delta\phi > 2\pi/3$ to ensure a back-to-back topology, reducing contamination from QCD and weak boson decays with associated jets (V +jets).

Table 5.4: Data and simulated process yields in the $\text{CR}_{t\bar{t}}$ regions, within the $\text{CR}_{t\bar{t}}$ fit range, $m_{\text{jet}} \in [140, 200]$ GeV. All yields are also shown as a percentage of all MC events passing the event selection, to illustrate sample composition and highlight the differences between MC and data. Differential measurement binning: $\text{CR}_{t\bar{t}}0$: $p_T^{\text{jet}} \in [250, 450]$ GeV; $\text{CR}_{t\bar{t}}1$: $p_T^{\text{jet}} \in [450, 650]$ GeV; $\text{CR}_{t\bar{t}}2$: $p_T^{\text{jet}} \in [650, 1000]$ GeV.

Process	Inclusive		Differential Bins					
	Yield	%	$\text{CR}_{t\bar{t}}0$		$\text{CR}_{t\bar{t}}1$		$\text{CR}_{t\bar{t}}2$	
			Yield	%	Yield	%	Yield	%
$t\bar{t}$	4579	97.3%	1926	98.4%	2051	97.1%	552	95.5%
single-top	74	1.6%	20	1.0%	39	1.8%	12	2.1%
$W(\ell\nu)$	53	1.1%	12	0.6%	22	1.1%	14	2.4%
Data	3791	80.6%	1687	86.2%	1628	79.1%	442	76.5%

The event yields of data and simulated processes in the $\text{CR}_{t\bar{t}}$ inclusive and differential regions are given in table 5.4. Both the MC and data yields are also shown as a percentage of all MC events passing the event selection, to provide a better insight into sample composition, and highlight the differences between MC and data. The $\text{CR}_{t\bar{t}}$ region was seen to be highly pure in $t\bar{t}$ events, which made up 97% of events in the region. The remaining 3% were contributed by single-top and $W \rightarrow \ell\nu$ (later referred to as $W(\ell\nu)$) processes. Both of these processes were included in the $\text{CR}_{t\bar{t}}$ fits. As their small contributions to $\text{CR}_{t\bar{t}}$ were not influential to the fit they were fixed to the SM predicted yields. Events from the multi-jet QCD background were also considered, but were seen to make up $< 0.1\%$ of the events in the inclusive region, and therefore were omitted from the $\text{CR}_{t\bar{t}}$ fits.

Figures 5.6a and 5.6b show the m_{jet} and p_T^{jet} distributions of candidate jets in the $\text{CR}_{t\bar{t}}$ region. The MC simulation was seen to generally overshoot the data, with the discrepancy increasing with p_T^{jet} . The same trend was seen looking at the data-to-MC fractions in the differential measurement p_T^{jet} bins in table 5.4. The observed discrepancies (around 20%) between data and the MC were in line with

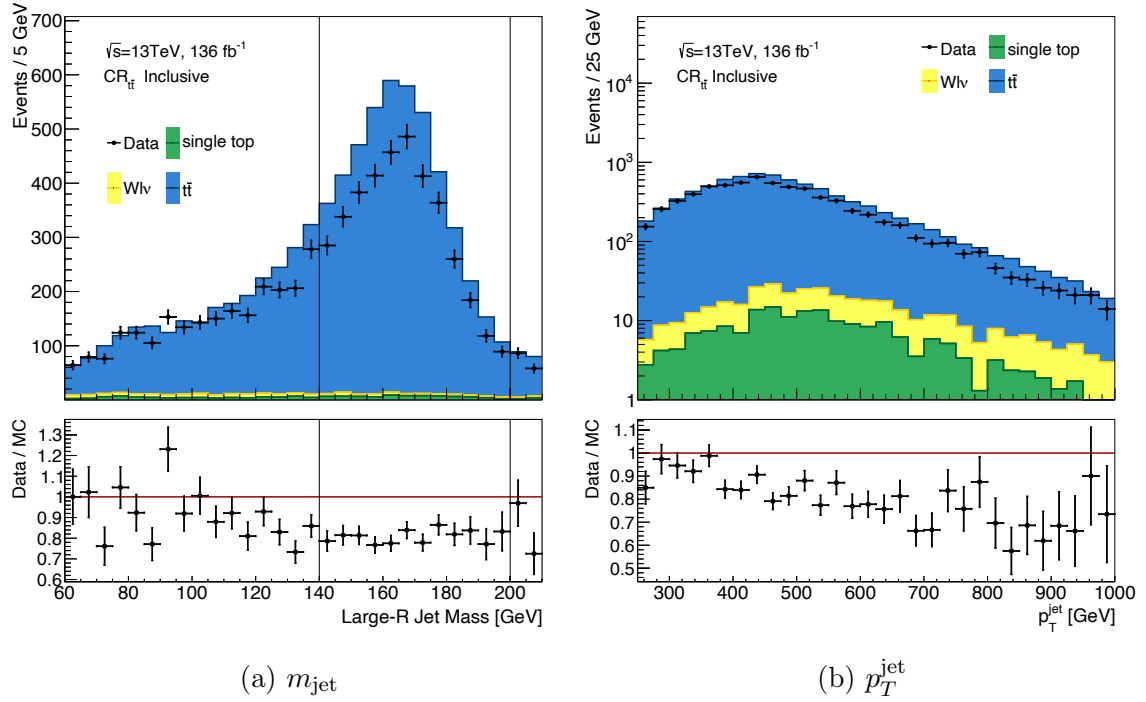


Figure 5.6: Stacked CR_{t $\bar{t}$} candidate jet (a) m_{jet} and (b) p_T^{jet} distributions of data and simulations of component processes. The vertical lines indicate the CR_{t $\bar{t}$} fit range, chosen such as to exclude contributions from W boson resonance. The p_T^{jet} distribution is shown for all events passing the selection criteria without imposed mass range restrictions.

the findings of the top-quark differential cross-section measurements by the ATLAS experiment [133] (figure 54).

As CR_{t $\bar{t}$} was used to constrain the $t\bar{t}$ background and related systematic uncertainties, it was undesirable to have W boson contamination in this region. Therefore the CR_{t $\bar{t}$} fits were performed in a shorter, $m_{\text{jet}} \in [140, 200]$ GeV range, indicated by vertical lines in figure 5.6a.

5.5 The Measurements

This section will provide more detail on the three types of measurements: inclusive, fiducial and differential measurements, the $H(\rightarrow b\bar{b}) + j$ analysis aims to make. In

all cases the measurements were made by performing a binned likelihood fit to data, to extract the Higgs boson signal strength (μ_H) from the signal regions. In the case of the fiducial and differential measurements the extracted signal strengths were reinterpreted as cross-section measurements (described in section 9.2).

In all cases the measurement fits were performed simultaneously in SRL, SRS and $\text{CR}_{t\bar{t}}$ regions, and the Higgs boson signal strength was 100% correlated between SRS and SRL (i.e. μ_H is set to be the same in both signal regions). This treatment was the same for all resonant backgrounds as well. Unless stated otherwise, the maximum p_T^{jet} in all cases, was set to 3 TeV, beyond which no sensitivity was expected.

Inclusive Measurement

The inclusive measurement was performed over the entire accessible candidate jet momentum spectrum. For SRL this was $p_T^{\text{jet}} > 450$ GeV, and for SRS and $\text{CR}_{t\bar{t}}$ it was $p_T^{\text{jet}} > 250$ GeV.

Fiducial Measurement

Fiducial cross-sections are cross-sections within a phase-space defined by the acceptance cuts of the analysis. The fiducial Higgs boson cross-section measurement within the entire fully accessible Higgs boson phase-space for this analysis, defined by $p_T^{\text{jet}} > 450$ GeV and $|\eta_{\text{jet}}| < 2$ is called the *fiducial measurement*⁴. The measurement was performed simultaneously in SRL, SRS and $\text{CR}_{t\bar{t}}$, and the p_T^{jet} ranges of all regions were set to $p_T^{\text{jet}} > 450$ GeV.

The cross-section within the fiducial volume was measured by splitting the Higgs boson sample into two truth-level p_T^H bins: one within the fiducial volume ($p_T^H > 450$ GeV, $|\eta_H| < 2$), and one outside of the fiducial volume ($p_T^H < 450$ GeV). The signal strength outside of the fiducial volume was fixed to the SM expectation

⁴ In late stages of the analysis, after the studies presented in this thesis were made, the definition was redefined from $|\eta| < 2$ (pseudorapidity) to $|y| < 2$ (rapidity) which is more compatible with massive particles. The same was done for the differential measurement as well.

value, with all uncertainty descriptions (given in section 7.2) on the mass template included in the fit. The signal strength within the fiducial volume was measured in the fit, and reinterpreted as a cross-section.

Differential Measurement

The differential measurement targeted the Higgs boson production cross-sections in fiducial phase-space regions, defined by the *Simplified Template Cross Sections (STXS) framework* [109]. The STXS framework is a common framework for differential Higgs boson production cross-section measurements utilised by the LHC experiments.

The STXS framework defines mutually exclusive regions of phase-space (*bins*) in which the differential measurements are made. These regions are defined by Higgs boson p_T and rapidity y , reflecting typical experimental kinematic selections, simplifying the combination of results from different analyses.

The $H(\rightarrow b\bar{b}) + j$ differential measurement simultaneously fit three Higgs boson signal strengths (as parameters of interest), defined by truth Higgs boson quantities: $|\eta_H| < 2$, and Higgs boson p_T :

$$\begin{aligned}\mu_{H,0}: \quad p_T^H &\in [300, 450] \text{ GeV}, \\ \mu_{H,1}: \quad p_T^H &\in [450, 650] \text{ GeV}, \\ \mu_{H,2}: \quad p_T^H &\in [650, 1000] \text{ GeV}.\end{aligned}$$

The measurement was made by fitting the SRL, SRS, and $\text{CR}_{t\bar{t}}$ regions simultaneously, which in this case were separated into bins based on corresponding candidate jet quantities: $|\eta_{\text{jet}}| < 2$ and⁵:

$$\begin{aligned}\textbf{bin 0: } p_T^{\text{jet}} &\in [250, 450] \text{ GeV}, \\ \textbf{bin 1: } p_T^{\text{jet}} &\in [450, 650] \text{ GeV}, \\ \textbf{bin 2: } p_T^{\text{jet}} &\in [650, 1000] \text{ GeV}.\end{aligned}$$

⁵ The lowest p_T^{jet} bin starts at 250 GeV to include candidates with $p_T^H \gtrsim 300$ GeV which could have lost energy due to resolution effects.

In the SRL, where the candidate was the leading p_T jet in the event, the minimum p_T^{jet} was determined by the trigger jet momentum cut: $p_T^{\text{jet}} > 450$ GeV, making the lowest momentum bin (bin 0) inaccessible. This produced five signal regions used for the differential measurement: SRL1, SRL2, SRS0, SRS1, and SRS2. Equivalent divisions were imposed for VRL and VRS (in studies), and $\text{CR}_{t\bar{t}}$ ⁶. The candidate jet mass distributions in differential measurement $\text{CR}_{t\bar{t}}$ and SR bins are given in figures B.5 and B.6 in appendix B.2.

The data yields in SRL1 and SRL2 were around 86% and 12% of the inclusive SRL data yield. Likewise, the data yields in SRS0/1/2 were approximately 30%, 64% and 9% of the inclusive SRS data yield⁷. In both cases the highest fraction of events resided in bin 1 ($p_T^{\text{jet}} \in [450, 650]$ GeV). Overall, event production rates tend to drop with jet p_T . However, there is also a *turn-on* effect (a region of reduced efficiency) below $p_T^{\text{jet}} = 450$ GeV, resulting from the trigger jet requirement of $p_T^{\text{jet}} > 450$ GeV in the event selection.

Within each of the signal regions the Higgs boson mass templates were separated into four components with different p_T^H ranges: three corresponding to the μ_H measurement bins, and one outside of the fiducial volume ($p_T^H < 300$ GeV). The signal strengths within the fiducial volumes were measured in the fit, and the signal strength outside the fiducial volume ($\mu_{H,\text{out}}$) was set to its SM expectation, and the uncertainty descriptions on its mass template included in the fit (as in the fiducial measurement). A summary of all measurement configurations⁸ is given in table 5.5.

Another feature of the STXS framework, is that the cross-sections are defined for different production modes. This reduces theoretical uncertainties on the fractional

⁶ The $\text{CR}_{t\bar{t}}$ had three regions, as it is not separated into leading / subleading candidate. Hence, the differential measurement fit was a simultaneous fit over 8 regions (5 SR + 3 $\text{CR}_{t\bar{t}}$).

⁷ Note, SRS1 region has a 5 GeV wider mass range than the SRS inclusive region, which leads to $\sum \text{SRS0/1/2} > 100\%$ of SRS inclusive yield.

⁸ In the $H(\rightarrow b\bar{b}) + j$ paper [5] and internal documentation [73] the differential signal strengths $\mu_{H,i}$ are offset by $i + 1$, such that $\mu_{H,\text{out}} \mapsto \mu_{H,0}$; $\mu_{H,0} \mapsto \mu_{H,1}$, etc.. The author chose to change the indexes, such that the corresponding indexes of the signal regions (SRL*i*, SRS*i*) and $\mu_{H,i}$ used in the thesis would refer to the same p_T ranges.

Table 5.5: (Left) the signal region definitions in terms of p_T^{jet} used for each measurement in the analysis, and (right) the Higgs boson signal strengths (μ_H) extracted in each measurement, defined by truth-record Higgs boson momentum (p_T^H) and pseudorapidity (η). Each SR had corresponding $\text{CR}_{t\bar{t}}$ and VR regions. The maximum jet p_T in all regions was 3 TeV. “bin 0/1/2” – differential p_T^{jet} -binned signal region labels. “PoI” – the parameter(s) of interest in the measurement. Adapted from [5].

Region		SRL	SRS	Measurement		
		Cand.	jet p_T [GeV]	PoI	p_T^H [GeV]	$ \eta_H $
Inclusive		> 450	> 250	μ_H	inclusive	inclusive
Fiducial		> 450	> 450	μ_H	> 450	< 2
Diff.	bin 0	–	250 – 450,	$\mu_{H,0}$	300 – 450,	
	bin 1	450 – 650,	450 – 650,	$\mu_{H,1}$	450 – 650,	< 2
	bin 2	650 – 1000	650 – 1000	$\mu_{H,2}$	650 – 1000	

contributions of production modes. Considering that the $H(\rightarrow b\bar{b}) + j$ analysis was new, and faced large QCD backgrounds with no precise modelling, the differential measurement was performed inclusively for all Higgs boson production modes to maximise the sensitivity. However, production mode separation is expected to be implemented in the next stages of the analysis. Henceforth, regions will be referred to regarding the measurement they are intended for, e.g. *inclusive signal regions* will refer to SRL and SRS as defined for the inclusive measurement.

Z Boson Measurement

Before the Higgs boson measurements were made, equivalent inclusive and differential measurements were performed for the Z boson. The inclusive Z boson measurement was used for method validation, and the differential measurement was considered as an additional deliverable of the analysis. Measurements of Z boson production in $Z \rightarrow b\bar{b}$ decays at high p_T are an area of active research in the physics community, as a probe of the validity of theoretical predictions and MC modelling for weak boson decays to two b quarks, prevalent in $H \rightarrow b\bar{b}$ measurements [134,135].

5.6 Blinding Strategy

The analysis was first designed and validated without looking at the signal region data, so as not to bias the results. This is called *blinding the analysis*, and is common practice in particle physics analyses. Once the analysis was validated, the signal region restrictions could be removed in order to make the measurement. This procedure is called *unblinding*.

This analysis took the approach of a staged unblinding. First, the analysis was built and validated without looking at the data in the signal regions. Then, parts of the inclusive signal region mass spectra were unblinded for QCD modelling validation, as discussed in section 6.4. Once the QCD model was determined to be well behaved, the full signal region unblinding was staged in 4 parts, each focusing on a measurement:

1. Z boson inclusive measurement;
2. Z boson differential measurement;
3. Higgs boson inclusive and fiducial measurement;
4. Higgs boson differential measurement.

The Z boson measurements were performed using the full signal region data, fixing the Higgs boson events to SM expectations within uncertainties. Also, the data within the ± 20 GeV window around the Higgs boson mass was kept blinded in any signal region plots.

The staged unblinding process was necessary to ensure a robust treatment of the QCD background, and systematic uncertainties in the fit. As the QCD background was modelled by a flexible function, it was important to observe the QCD modelling and interaction with a resonance similar to the Higgs boson in the signal region, before making the “high stakes” Higgs boson measurement. A thorough review process was held by the ATLAS Higgs boson physics community before and after each unblinding stage. The analysis group only proceeded with an unblinding once

comprehensive approval was received.

5.7 The Likelihood Fit Definition

Statistical analyses based on likelihood fits were used extensively throughout this work: in modelling and validation studies, and in the final measurements. In all cases, binned likelihood functions were used:

$$\mathcal{L} = \prod_{i=1}^n p(y_i | x_i(\boldsymbol{\mu}, \mathbf{k}, \boldsymbol{\theta})) , \quad (5.1)$$

where n is the number of bins in the mass spectrum, p is the probability distribution of events in a bin, y_i is the number of data events in each bin, and x_i is the number of predicted events in each bin subject to the signal and background model. The number of expected events in a bin, x_i , depended on three sets of parameters: the set of the signal strengths $\boldsymbol{\mu}$ for all signals considered in the fit, the set of the scale factors $\mathbf{k}$ of all the backgrounds (equivalent to $\boldsymbol{\mu}$ for signals), and the set of all considered nuisance parameters (NP) $\boldsymbol{\theta}$. It was expressed as the sum of all the expected signal ($x_{i,s}$) and background ($x_{i,b}$) events in the bin, each scaled by the corresponding signal strength (μ_s) or scale factor (k_b):

$$x_i(\boldsymbol{\mu}, \mathbf{k}, \boldsymbol{\theta}) = \sum_{s=1}^{n_s} \mu_s x_{i,s}(\boldsymbol{\theta}) + \sum_{b=1}^{n_b} k_b x_{i,b}(\boldsymbol{\theta}) , \quad (5.2)$$

where n_s and n_b are the number of considered signals and backgrounds, respectively. The numbers of signal or background events in the bin $x_{i,s/b}$ were fixed, taken from the signal or background expectations from MC mass templates of the resonances, or the initial QCD parametric description. Whereas, the signal strengths (μ_s) and background scale factors k_b are free parameters estimated by the fit. In the signal regions the scale factors of all relevant processes were:

- μ_H – Higgs boson signal strength;
- μ_Z – Z boson signal strength (scale factor);
- $SF_{t\bar{t}}$ – $t\bar{t}$ scale factor;
- $yield_{QCD} (srl/srs)$ – QCD background yield.

The systematic uncertainties entered the likelihood fit as free nuisance parameters $\boldsymbol{\theta}$. They were described as separate mass templates with a Gaussian prior centred at 0 (preferring the nominal distribution), and a standard deviation of 1 (corresponding to the systematic uncertainty).

The probability distribution of data events in a bin, given the signal and background model is assumed to follow a Poisson distribution:

$$p(y_i|\boldsymbol{\mu}, \boldsymbol{k}, \boldsymbol{\theta}) = \frac{e^{-x_i(\boldsymbol{\mu}, \boldsymbol{k}, \boldsymbol{\theta})} (x_i(\boldsymbol{\mu}, \boldsymbol{k}, \boldsymbol{\theta}))^{y_i}}{y_i!}. \quad (5.3)$$

The best-fit values of μ and the uncertainty σ_μ , were obtained by maximising the likelihood $\mathcal{L}$.

5.7.1 Likelihood Fit Binning

The likelihood fits were done in bins of candidate jet mass (m_{jet}) with a 5 GeV binning. However, this binning choice was not used throughout the entire analysis development. Initially, an issue in the fitting software (*RooFit*⁹), introduced a bias [136] in fits which included both binned templates and parametric functions (i.e. the QCD description). The nature of the bias was such that it reduced with bin size, and was found to be negligible when very fine binning was used [137] (internal). Therefore, studies involving signal and validation region fits (where parametric QCD estimates are used) were performed using 0.5 GeV binning until the issue was fixed in September 2020¹⁰.

⁹ The choice for this software is motivated in section 5.8.

¹⁰ For reference, the analysis efforts began in January 2019.

The very fine 0.5 GeV binning used introduced many challenges, so once a fix was available it was decided to use 5 GeV binning instead. The author performed the initial comparison studies validating the consistency between the results found with 0.5 GeV and 5 GeV SR binning, presented in appendix H.1. The validation studies showed no significant differences which would indicate the need to review analysis methodology developed using a 0.5 GeV binning.

5.7.2 Asimov Data

The $H(\rightarrow b\bar{b}) + j$ analysis made extensive use of *Asimov datasets* (or *Asimov data*) [138] – “ideal” artificial datasets formed by combining the expected distributions in a given region. For example, the Asimov data of a signal region would have been formed by combining the simulated mass templates of the resonances, and the initial expectation of the QCD parametric function in that region (obtained from studies in the validation region).

A likelihood fit to an Asimov dataset, where the fit model (expectations) correspond to the model used to build the Asimov dataset (i.e. fitting the model to itself), will return the expected values of the parameters, and uncertainties on them. In other words, fitting a model with an expectation of $\mu_H = 1$ to a dataset in which $\mu_H = 1$, will return a fit result of $\hat{\mu}_H = 1 \pm \hat{\sigma}(\mu_H)$, where $\hat{\sigma}(\mu_H)$ are the expected uncertainties of the μ_H measurement. In this thesis, all *expected results* were obtained through fits to Asimov data. Fits to Asimov data were also performed to observe expected uncertainty effects, and study the sensitivity of the fit.

5.8 The Fitting Framework

An important challenge for this analysis was to build a new analysis framework, capable of constructing a wide range of complex fit models, used in studies and measurements. This analysis was developed from a BSM search, and the software

was written using tools common to BSM searches. The $H(\rightarrow b\bar{b}) + j$ analysis moved to use common Higgs boson measurement tools, to enable future combination of results with other Higgs boson analyses. The new software enabled a significantly improved treatment of the QCD background estimate, which was studied in-depth by the author, and is discussed in appendix C

The new framework used fitting tools from the *XML Analytic Workspace Builder*, *QuickFit* and *StatisticsTools* packages, all of which are based on *RooFit* [139] fitting software, and are widely used in ATLAS Higgs boson analyses. The author of the thesis was the main contributor to the implementation, validation and maintenance of the framework. It was an extensive piece of work and a major contribution to the analysis.

The author built much of the machinery which prepared data, simulated samples and systematic uncertainties, and encoded the fit model information to be parsed to the fitting software. She wrote a large part of the core software allowing the universal creation of fits from the event-by-event inputs, used in all complex fit studies; she implemented the inclusion and smoothing of systematic uncertainties (section 7.5); the parametric smoothing of resonances (appendix F), used early in the analysis; the final smoothing procedure for V +jets templates (discussed in section 6.5 and detailed in appendix E) and many other contributions. The author also supported other members of the analysis with studies and software implementation.

The framework was thoroughly validated by the author, using the Higgs boson hypothesis results from the previous iteration of the analysis (BSM search [4]). The extensive studies validating the framework and highlighting its advantages over the previously used framework are discussed in appendix C.

The framework was built to have an efficient and user-friendly pipeline to accommodate the large number of fits required in some studies. It was also repurposed by the double b -tagging calibrations in $Z(\rightarrow b\bar{b}) + \gamma$ and $Z(\rightarrow b\bar{b}) + j$ events (described in [3]), which attests the utility of this framework.

5.9 Chapter Overview

This chapter gave a broad overview of the $H(\rightarrow b\bar{b}) + j$ analysis, which targets exceptionally high regions of Higgs boson momentum, through a boosted Higgs jet topology, to contextualise the work presented in the following chapters.

Two types of signal region were defined, SRL – where the Higgs boson candidate jet is the leading p_T jet in the event, and SRS – where the Higgs boson candidate jet is the subleading p_T jet in the event. All measurements were performed by fitting SRL, SRS and a $t\bar{t}$ control region $\text{CR}_{t\bar{t}}$ simultaneously. Dedicated leading and subleading candidate jet validation regions (VRL and VRS) were used for studies of the parametric QCD background estimates presented in the following chapter. This chapter also discussed the data and simulated samples used, and presented the event selections for the discussed regions.

Three types of measurement attempted by the $H(\rightarrow b\bar{b}) + j$ analysis were introduced: the **inclusive measurement**, measuring the inclusive Higgs boson signal strength (μ_H) over the entire accessible jet p_T range; and **fiducial** and **differential measurements** of Higgs boson inclusive production cross-sections. The fiducial measurement was performed over the entire fully accessible Higgs boson phase-space ($p_T^H > 450$ GeV), and the differential measurement made cross-section measurements in Higgs boson p_T^H bins. To make the differential measurement the signal regions and $\text{CR}_{t\bar{t}}$ were separated into p_T^{jet} bins, forming 8 separate regions (5 SR + 3 $\text{CR}_{t\bar{t}}$) fit simultaneously to make the differential measurement.

The chapter also presented the binned likelihood fits used to make the measurements and the studies presented in this thesis, and gave an overview of the fitting framework, as well as the extensive contributions the author had made towards building the framework and the analysis.

Chapter 6

Signal And Backgrounds

In simple terms, the principle of this, and many other particle physics analyses, could be reduced to a few main steps: choosing an interesting final state; developing an event selection; understanding the expectations and related uncertainties for said final state; building a model based on the expectations; and fitting the model to data. This chapter explores two of these analysis cornerstones - the study of signal and background expectations, and their modelling in the measurement.

6.1 Author's Contributions

This chapter contains general knowledge about the analysis, as well as studies from the author, and other members of the analysis group. The following explicitly lists the contributions of the author presented in this chapter. All figures shown in this chapter have been produced by the author unless cited or stated otherwise.

Higgs Boson Modelling: (section 6.3) the author produced the Higgs boson treatment studies for the differential measurement, presented in section 6.3.3.

QCD Background Modelling: (section 6.4) the author implemented validation region data slicing, and model building machinery (excluding hybrid VR slice building) in the fitting framework. She was involved in some very early likelihood ratio test studies, however all studies presented in the section were produced by other

members of the analysis team.

Vector Boson Modelling: (section 6.5) the V +jets smoothing procedure introduced in section 6.5 (and discussed in detail in appendix E) was designed, and tested using the validation region data by other members of the group, using stand-alone code. The thesis author integrated this procedure into the analysis workflow, and performed validation studies on the effects on the m_{jet} and p_T^{jet} distributions of the candidate jets, discussed in appendix E.2, which helped refine the procedure.

$t\bar{t}$ Modelling: (section 6.6) all presented work was produced by the author.

Parametric Treatment of Resonances: (appendix F) the author also studied the parametric treatment of resonant processes, which could have mitigated software issues encountered by the analysis. These studies were beyond the scope of the thesis, and are presented in appendix F. The studies found that the mass template shapes of the processes had complex features, which could not be described by the function used to empirically model them.

Mass template smoothing using parametric fitting was also used by the BSM resonance search [4] from which this analysis was developed. Replicating the parametric smoothing of resonances was crucial to validate the new fitting framework. This was successfully done by the author and is also presented in appendix F.

6.2 Signals and Backgrounds

Five main processes were considered in the signal regions:

- $H(\rightarrow b\bar{b}) + j$ (*Higgs boson or the signal*);
- $Z(\rightarrow b\bar{b}) + j$ and $W(\rightarrow qq') + j$ (Z +jets, W +jets or collectively V +jets);
- $t\bar{t}$;
- QCD events with multiple jets (QCD).

Figure 6.1 shows the SM predictions of these components in the inclusive SRL and

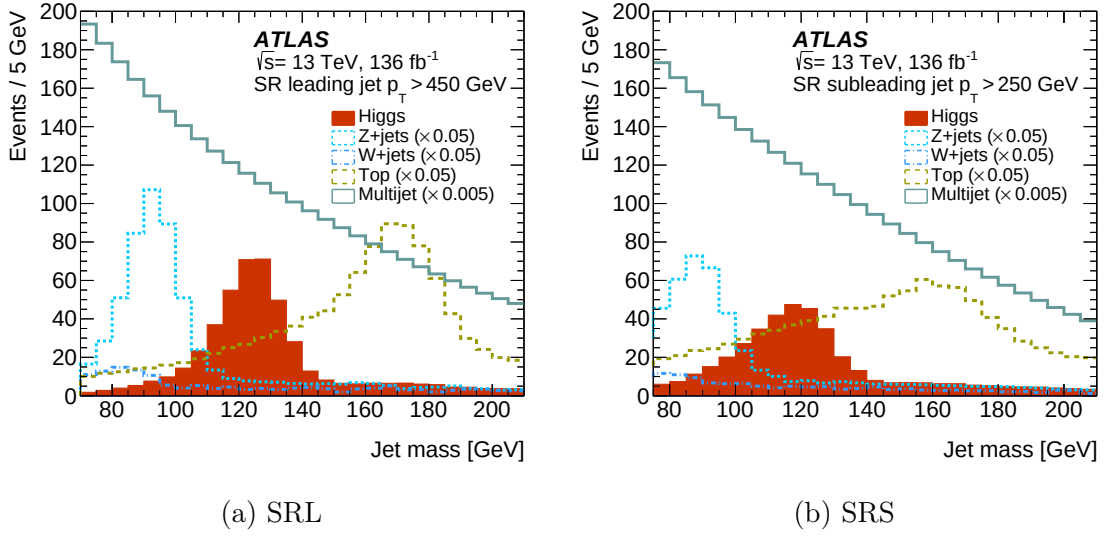


Figure 6.1: Candidate jet mass (m_{jet}) distributions of the processes in (a) SRL and (b) SRS (leading and subleading candidate jet signal regions). The Higgs, Z +jets, W +jets, top-quark¹, contributions are Standard Model expectations, and QCD multi-jet distribution was taken from fits to SR data [5]. For visibility the Z +jets, W +jets and $t\bar{t}$ contributions were scaled down by a factor of 20, and QCD – by a factor of 200.

SRS (leading and subleading candidate jet signal regions). Notably, all resonances had considerably poorer resolution in the SRS region due to various energy loss effects, which caused the candidate to become the subleading jet. Such effects include jet resolution, final state radiation, failure to contain the full decay within the jet cone, and semileptonic decays of heavy quarks in the candidate decay chain.

The main signal in this analysis was the Higgs boson. The analysis also aimed to measure the Z +jets process in the signal region, which was taken into account when designing the analysis. The QCD background was by far the largest contributor to the signal regions as the final state investigated in this analysis was fully hadronic (all objects of interest are jets).

The Higgs boson resonance lies between the V +jets and $t\bar{t}$ backgrounds, over-

¹ The $t\bar{t}$ process with a single-top contribution ($\sim 5\%$ of $t\bar{t}$) added late in the analysis, which was not included in the presented studies. See section 9.1.1 for more details.

lapping with the tails of the two resonances. The yields of these backgrounds within the Higgs boson resonance region ($m_{\text{jet}} \in [105, 140]$ GeV) were much larger than that of the Higgs boson, the V +jets background was 6 and 7.5 times larger in SRL and SRS, respectively, and the $t\bar{t}$ background was 11.5 and 23 times larger in the same two regions. Therefore, robust modelling of these backgrounds, as well as the overwhelming QCD background, was crucial.

6.3 Higgs Boson Modelling

6.3.1 Composition

The analysis event selection did not intrinsically restrict Higgs boson production modes. The four main production modes were considered: ggF , VH , VBF , and $t\bar{t}H$. The ggF production mode was the dominant contributor to the resonance region, defined as $m_{\text{jet}} \in [105, 140]$ GeV, making up 55% and 40% of the yield within this range in SRL and SRS, respectively. All other production modes contributed similar smaller amounts to the resonance, between 14% and 25%. Inclusive, the Higgs resonance yield in the SRS was around 30% smaller than in the SRL.

The simulated candidate jet mass distributions (m_{jet}) for different Higgs boson production modes in the inclusive signal regions are shown in figure 6.2, illustrating the contributions. It was notable that a sizeable portion of candidate jets in $t\bar{t}H$ events were top decays, as was evident from the events seen around the top quark mass (173 GeV). Summaries of yields and fractional yield contributions in the resonance region are given in tables D.1 and D.2 in appendix D.1.

Figure 6.3 shows the contributions of events from different Higgs boson production modes to the Higgs boson resonance region as a function of candidate jet p_T in the inclusive signal regions. ggF was generally the dominant production mode, except in the lowest p_T^{jet} region of the SRS, which was dominated by $t\bar{t}H$ events due to its topology. In a two body final state, such as VH , the trigger jet significantly

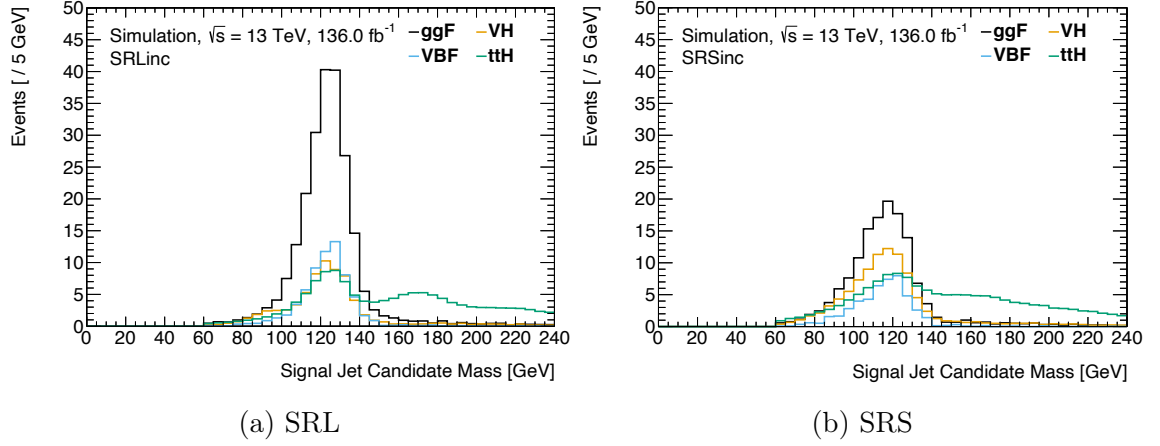


Figure 6.2: Candidate jet mass (m_{jet}) spectra of simulated Higgs boson events passing the inclusive (a) SRL and (b) SRS event selection requirements [73] (internal), illustrating the contributions of different Higgs boson production modes to said signal regions. Note, the contributions are not stacked. The fractional contributions as a function of jet p_T are shown in figure 6.3.

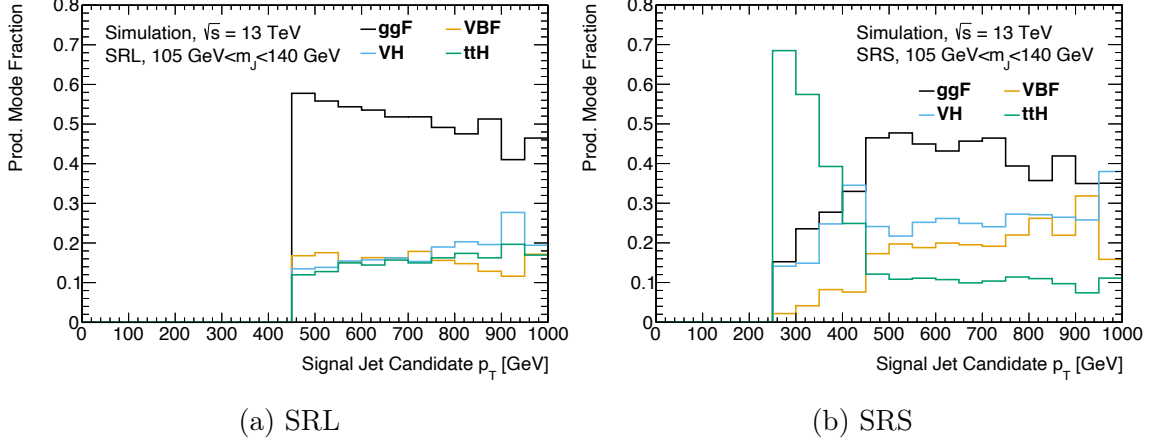


Figure 6.3: The fractional contributions of candidate jets from different Higgs boson production modes to the Higgs boson resonance ($m_{\text{jet}} \in [105, 140] \text{ GeV}$) as a function of candidate jet p_T passing the (a) SRL and (b) SRS requirements [73] (internal).

boosts the other jet in the event, however, in a three body system, such as $t\bar{t}H$, the boost from the high energy trigger jet is shared by the two remaining bodies, which can result in a subleading candidate jet with a lower p_T boost, particularly if the candidate is a top quark, which is more massive than the Higgs boson.

6.3.2 Mass and Momentum Resolution

The mass and p_T resolution of Higgs boson jets was assessed using ggF events, in which the candidate jet was associated to a truth-record Higgs boson. Table 6.1 lists the Higgs candidate jet mass (m_{jet}) and p_T^{jet} resolution estimates in bins of truth-record Higgs boson p_T (p_T^H). The resolution estimates were derived by fitting the distributions of the differences between “true” and reconstructed values, i.e.: $\Delta(125 \text{ GeV}, m_{\text{jet}})$, and $\Delta(p_T^H, p_T^{\text{jet}})$, with Gaussian functions. The resolution estimates were the widths of the curves (σ_{gauss}) derived from the fits.

Both m_{jet} and p_T^{jet} resolutions were generally worse when the candidate was the subleading jet in the event. As mentioned in section 5.4.1, processes which can lead the candidate jet to become the subleading jet in the event, such as final state radiation, out-of-jet energy deposits, or semi-leptonic decays within the jet, also deteriorate the jet resolution.

The trends displayed by the mass resolution agreed with the expected behaviour of the combined jet mass definition (m^{comb}) shown previously in figure 3.8. The absolute p_T^{jet} resolution was seen to deteriorate with increasing momentum, but the relative p_T resolution was seen to improve, which was consistent with the expected behaviour².

Table 6.1: Jet mass, m_{jet} , and p_T^{jet} resolutions for candidate jets associated to truth-record Higgs bosons in bins of truth Higgs boson p_T^H , in simulated ggF events. The resolutions are the σ_{gauss} values from Gaussian distribution fits to $\Delta(125 \text{ GeV}, m_{\text{jet}})$, and $\Delta(p_T^H, p_T^{\text{jet}})$ [73] (internal).

p_T^{jet} Range [GeV]	m_{jet} Resolution [GeV]		p_T^{jet} Resolution [GeV]	
	Leading	Subleading	Leading	Subleading
$250 < p_T^H < 450$	–	17.7 ± 0.7	–	38.3 ± 1.2
$450 < p_T^H < 650$	11.3 ± 0.1	13.4 ± 0.2	29.3 ± 0.3	39.9 ± 1.2
$650 < p_T^H < 1000$	10.8 ± 0.3	13.5 ± 0.4	38.3 ± 0.9	56.1 ± 2.1

6.3.3 Higgs Boson in the Differential Measurement

The differential Higgs boson measurement was performed in bins of candidate jet p_T (p_T^{jet}), within which the Higgs boson mass templates were divided into truth-level p_T^H bins. The signal strengths (μ_H) of each truth p_T^H template were measured separately in the fit. More details can be found in the overview of measurements made by the $H(\rightarrow b\bar{b}) + j$ analysis in section 5.5.

Figures 6.4a and 6.4b show the fractional distributions of Higgs boson events across p_T^H and p_T^{jet} bins in the signal regions. The distributions illustrate the extent of resolution effects causing events to migrate from a p_T^H bin to a non-corresponding p_T^{jet} bin. The templates of such events ($p_{T,i}^H \rightarrow p_{T,j}^{\text{jet}}$, where $i \neq j$) are referred to as *off-diagonal* templates. The smaller the fractions of events are in the off-diagonal elements, i.e. the better the resolution, the less correlated the measurements of the signal strengths $\mu_{H,i}$ will be. The distributions of Higgs boson events in Figure 6.4, show that in most cases the off-diagonal templates made up relatively small fractions of the total number of Higgs boson events.

Simplifying the Differential Measurement Fit

Systematic uncertainty descriptions were in most cases correlated across all Higgs boson contributions in the fit and enter the model as a single nuisance parameter with descriptions for each template³. Due to the low rates of event migration, it was thought to be unlikely that the constraints on systematic uncertainties would be significantly affected by off-diagonal templates, as most of the constraints were expected to come from diagonal contributions. This was exploited to reduce the number of uncertainty descriptions in the differential measurement fit. This section describes the strategy and validation of the reduction of uncertainty descriptions for off-diagonal mass templates of the Higgs boson signal.

² The momentum of the large- R jet objects used was calculated from calorimeter information, and relative energy resolution at high energies generally follows $\sigma(E)/E \propto 1/\sqrt{E}$.

³ A discussion on the treatment of systematic uncertainties will be presented in chapter 7.

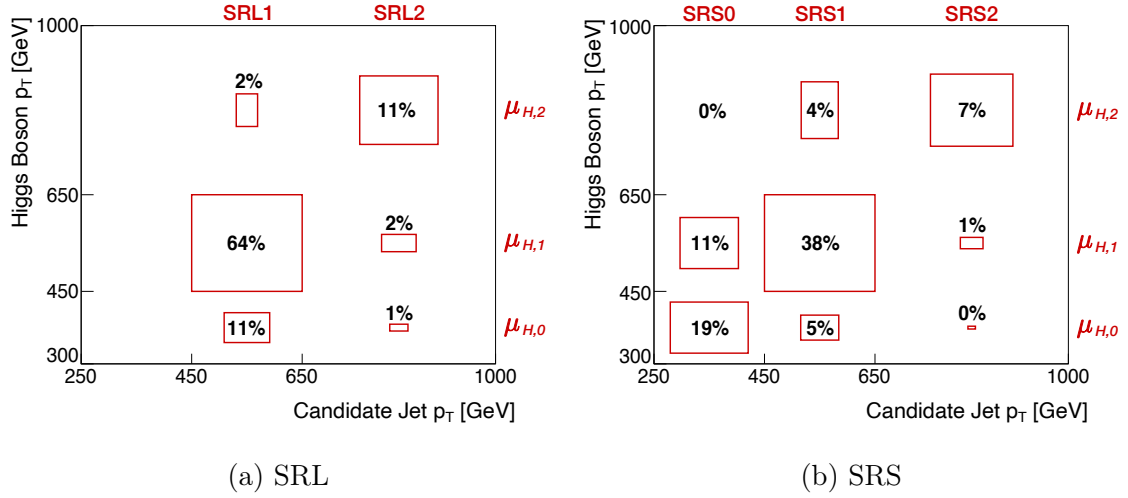


Figure 6.4: Fractional distributions of simulated Higgs boson events in differential measurement p_T^{jet} bins, which define the signal regions, and truth-level p_T^H bins, which were used in the measurement. The fractions are in terms of the total Higgs boson events in the differential signal regions (i.e. $\sum \text{SRL } 1/2$ and $\sum \text{SRL } 0/1/2$). The contributions with $p_T^H < 300$ were fixed to SM expectations in the differential measurement fit, and are not shown in the plot, but were included in the total event calculation. SRL was limited to $p_T^{\text{jet}} > 450$ GeV by the event selection.

Stacked histograms of p_T^H -binned Higgs boson templates in differential measurement signal regions are shown in figure 6.5, presenting a clear view of the contributions from different p_T^H bins. The fractional contributions of all templates within $m_{\text{jet}} \in [105, 140]$ GeV are given in the legends of figure 6.5. The systematic uncertainty descriptions were removed (i.e. not included in the final measurement fit) for all off-diagonal templates except for $p_{T,1}^H$ ($p_T^H \in [450, 650]$ GeV) in the SRS0 region ($p_T^H \in [250, 450]$ GeV), which made up 23% of events within the Higgs boson resonance ($m_{\text{jet}} \in [105, 140]$ GeV) of SRS0. All other off-diagonal templates had contributions $\leq 11\%$ in the Higgs boson resonance region.

In total this strategy removed 201 systematic uncertainty descriptions⁴ from the Higgs boson differential measurement fit. This significantly simplified the fit model,

⁴ Note that the number of systematic uncertainty descriptions is different to the number of nuisance parameters in the fit, as explained at the start of this section. The quoted reduction in uncertainty descriptions was calculated after the uncertainty pruning, discussed in section 7.6.

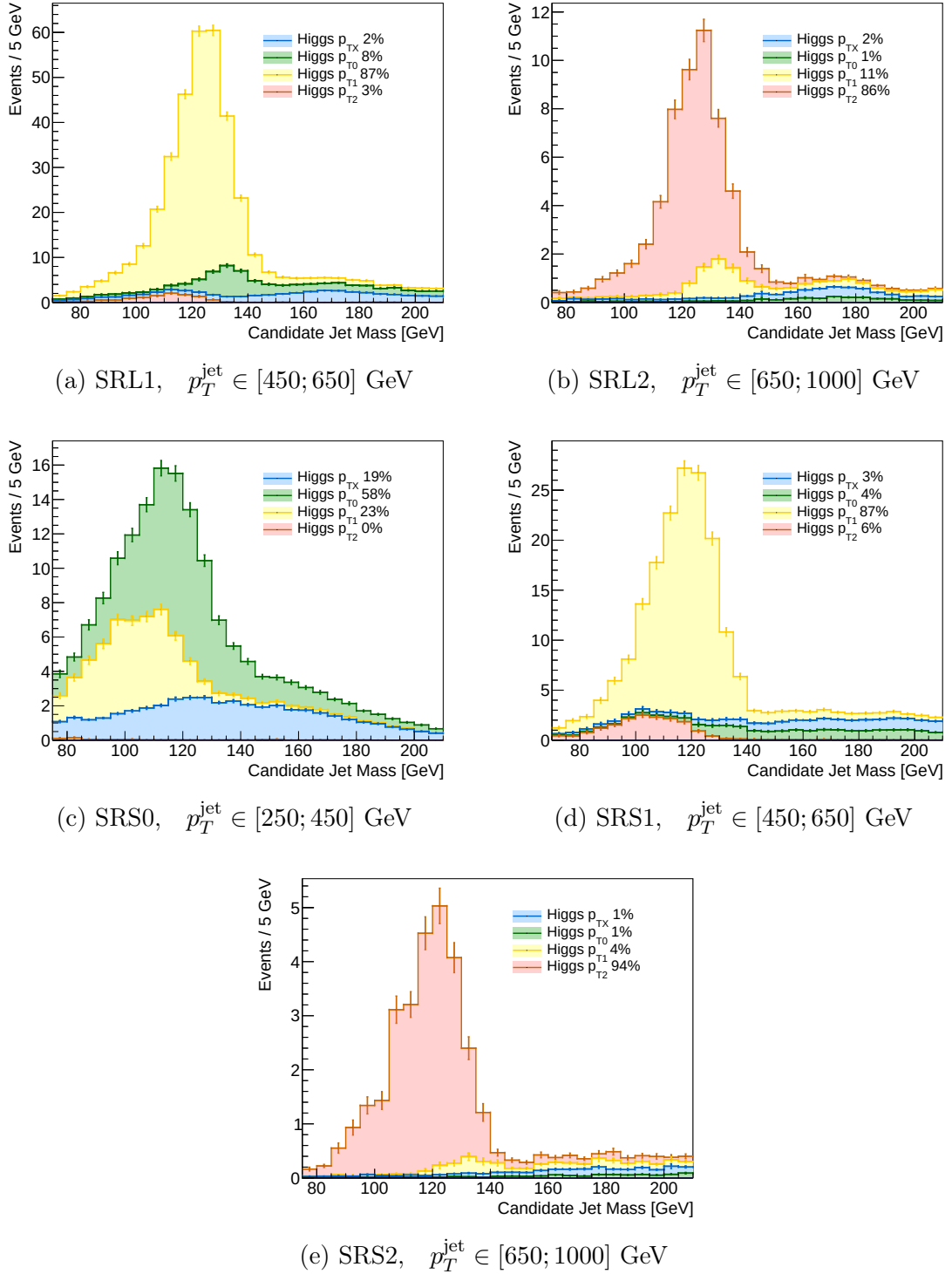


Figure 6.5: Stacked histograms of simulated Higgs boson events in truth p_T^H bins (used in the signal strength $\mu_{H,i}$ measurements) in differential measurement signal regions. The percentage of yield each template contributes within $m_{\text{jet}} \in [105, 145]$ GeV is shown in the legend. The p_T^H momentum bins are: $250 \text{ GeV} < p_{T,X}^H < 300 \text{ GeV} < p_{T,0}^H < 450 \text{ GeV} < p_{T,1}^H < 650 \text{ GeV} < p_{T,2}^H$.

without relevant loss of precision. The impact of the uncertainty model reduction was tested by performing differential measurement fits to Asimov datasets⁵ with the full and reduced systematic descriptions and comparing the uncertainties on the measured μ_H values.

The comparison fits were performed using a 0.5 GeV binning in the signal regions, as was used throughout a large part of the analysis development⁶. Overall the impact of the removal of the uncertainties was shown to be minor. The only effect was a relatively small 1.3% reduction in total uncertainties, for the $\mu_{H,0}$ measurement in the lowest p_T^H bin, which had very poor sensitivity, with an expected significance of 0.06σ . The effects on the signal strengths in higher momentum bins were compatible with zero. Given the negligible impact, it was decided to neglect these uncertainty descriptions and significantly simplify the fit models.

The studies described in this section informed the analysis on which Higgs boson templates in the differential measurement set-up did not require systematic uncertainty descriptions, and studied the impact of this model simplification. The same approach was taken with Z +jets templates in the Z boson differential fit. The determined uncertainty configuration is given in table D.3 and plots equivalent to 6.5 for Z +jets templates are given in figure D.1.

6.4 QCD Modelling

All objects of interest in the final state of this analysis were jets. As the data was gathered in proton-proton collisions, the overwhelming background for this signature was from QCD interactions producing multiple jets in the final state. As the event selection of the signal region required candidate jets to have two b -tags, the QCD background candidates were mostly made up of boosted heavy quark pairs.

⁵ Asimov data is an idealised dataset, built from the model itself, providing the expected results and sensitivity of the measurement. Described in section 5.7.2.

⁶ See section 5.7.1 for more details on the binning.

QCD processes were by far the most prominent background in the signal regions. In the full mass ranges of the signal regions the QCD yield was 25 – 30 times larger than the yield of the second-largest background – $t\bar{t}$, and around 1500 times larger than that of the Higgs boson. Therefore, a good understanding and robust modelling of this background was paramount to this analysis.

The QCD background is known to be poorly modelled by MC simulations. MC-to-data comparisons of the validation region events given in the previous chapter (figure 5.4) showed significant discrepancies of around 20% between data and simulation. Because of this a data-driven QCD background estimation method was used, which is the main subject of this section.

The QCD background was empirically modelled using a parametric function. The functional form was determined using data from external data regions – validation regions (VR) – which were complimentary proxies to the signal regions. The values of the function parameters were not predetermined, and entered the signal region fits as nuisance parameters.

The Parametric Description

The QCD background was continuously smoothly falling, and therefore could be approximated using a parametric function. The functional form used for the estimation was a family of exponential polynomial functions:

$$f_N(x | \boldsymbol{\theta}) = \theta_0 \exp \left(\sum_{i=1}^N \theta_i x^i \right), \quad (6.1)$$

where $\boldsymbol{\theta}$ are the parameters in the fit, and

$$x = \frac{m_{\text{jet}} - 140\text{GeV}}{70\text{GeV}}, \quad (6.2)$$

such that the values of x over the entire m_{jet} range of the signal regions were limited to ± 1 , providing numerical stability to the function. Each signal region had an independent QCD parametric function. The number of parameters⁷ (N) in each function were determined using the corresponding validation regions. The parameters of each

QCD estimate function entered the signal region fits as free nuisance parameters. The parameters of QCD functions in different signal regions were treated independently, i.e. were described by separate nuisance parameters.

This functional form was used to describe the QCD background in the BSM resonance search ($X \rightarrow b\bar{b} + j$) [4] from which this analysis was derived. An alternative Laurent series description was tested, following the same procedures described in this section. The difference between the two descriptions was found to be negligible in the context of the statistical uncertainties of the data and expected Higgs boson sensitivity.

6.4.1 The Validation Region

The validation regions were used to determine the optimal number of parameters in the QCD estimate function, and validate the modelling performance. To do so, the shapes of the QCD backgrounds in the validation regions had to be as similar as possible to the QCD shapes in the corresponding signal region (SR). This was particularly important, as the Higgs boson signal was very small compared to the QCD background, and therefore slight differences in the modelling could have affected the measurement.

The validation regions (VRL and VRS) were defined in the same way as signal regions (SRL and SRS), but rather than requiring both sub-jets within the candidate large- R jet to be b -tagged, i.e. have 2 b -tags, both sub-jets within the candidate large- R jet were required not to be b -tagged, i.e. have exactly zero b -tags. The validation region event selection and definitions were described in detail in section 5.4.

⁷ Note, the zeroth parameter, θ_0 is not included in N , as shown in equation 6.1. Henceforth, the *number of parameters* refers to N unless stated otherwise.

Slicing

The event yields in the validation regions were much larger – approximately 58 and 51 times⁸ for QCD events in SRL and SRS, respectively. It was expected that the number of parameters N needed to describe the backgrounds would scale with luminosity, as greater precision in the data would require a more flexible parametric model. Therefore, the validation region data was divided into *slices* using random assignment of events. This provided an ensemble of datasets with similar shape and precision to that expected in the signal region, which was used to validate the performance of the QCD estimate functions.

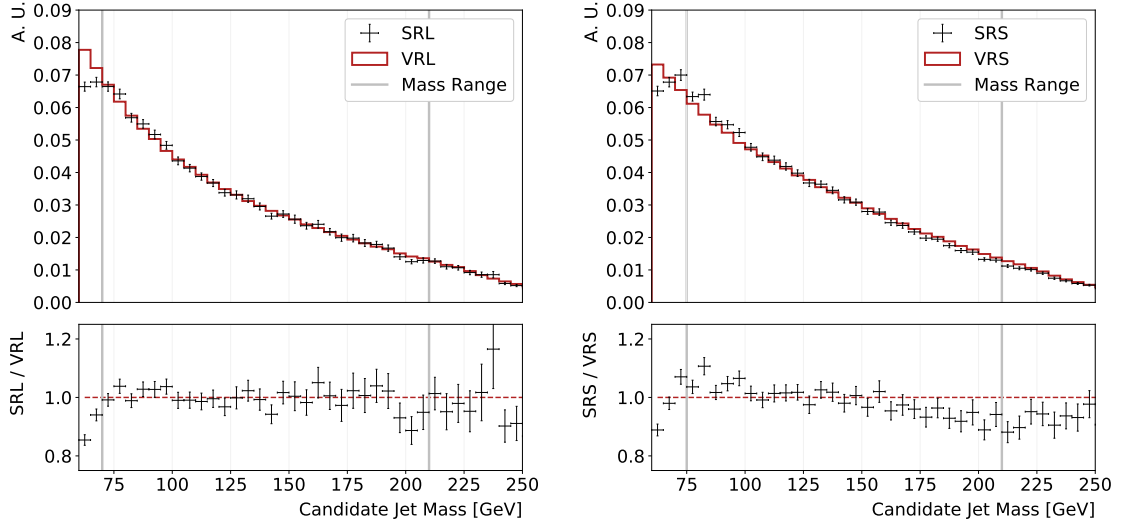
Validation Region Correction Using Signal Region Data

The event selection provided a mostly flat ratio between the simulated QCD m_{jet} distributions in the corresponding signal and validation regions, shown in figure 6.6. At low masses, an efficiency turn-on effect was seen in both signal regions. This was due to a reduced double b -tagging efficiency at low masses, as candidate jets become highly collimated and the track matching between sub-jets becomes ambiguous. A slight downward slope could be observed towards high m_{jet} values (around $m_{\text{jet}} \approx 230$ GeV) in the SRS/VRS ratio (figure 6.6b), which returned to a ratio of around 1 at higher mass values. This was an indication that the validation region description could be improved.

While encouraging, the agreement between the signal and validation regions in MC does not ensure that the agreement will be the same in data, as mismodelling could affect the two regions differently. To account for possible discrepancies in data, a “correction” procedure was developed.

Correction factors for the QCD shape were derived for each validation region by taking the ratios of the QCD shapes (f) estimated from fits⁹ to blind SR data, and validation region data¹⁰, $f_{\text{SR}}/f_{\text{VR}}$. The correction factors were used in the creation

⁸ The numbers of slices were calculated by subtracting the estimated yields of the resonances as predicted by MC simulations from data.



(a) Leading Candidate

(b) Subleading Candidate

Figure 6.6: Simulated QCD events in signal and validation regions, normalised within the mass ranges of the measurement fit indicated by the vertical lines.

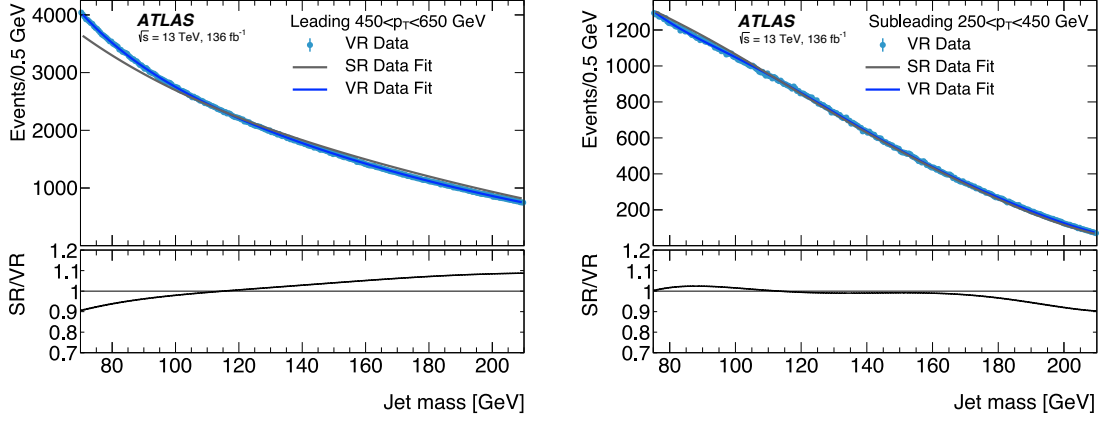
of *hybrid VR slices* (VR_{hyb}). The SR fits used to derive f_{SR} were performed fully blind, such that only the shapes of QCD estimate functions were extracted, and no other post-fit distributions were observed.

The hybrid VR slices (VR_{hyb}) were created by:

1. taking a VR slice (VR^i), and subtracting the expected V +jets and $t\bar{t}$ contributions in the VR slice (V_{VR} and $t\bar{t}_{VR}$). The expected resonance scale factors (μ_V and $SF_{t\bar{t}}$) were measured in VR fits used to extract f_{VR} . The VR slice after subtraction was seen as a proxy for QCD in the validation region;
2. scaling the said slice by a correction factor derived from fits to data (f_{SR}/f_{VR}) to make the slice a good proxy for QCD in the signal region;

⁹ The fits included systematic uncertainties, and used functions with $N = 5$ parameters. The procedure was repeated with $N = 4$ and $N = 6$ parameters, which did not show significant differences.

¹⁰ The validation region was sliced into 10 slices, to maximise statistical precision without needing to use larger values of N for accurate description, and 10 fits were performed. The t_θ values from the fits were averaged to derive f_{VR} .



(a) lead. candidate, $p_T^{\text{jet}} \in [450, 650]$ GeV (b) sublead. candidate, $p_T^{\text{jet}} \in [250, 450]$ GeV

Figure 6.7: Comparisons of QCD shapes found from fits to validation region data (f_{VR}), and partial signal region data (f_{SR}), as well as data points from VR slices after the subtraction of VR resonances, for two differential measurement regions: (a) SRL1 and VRL1 (leading candidate, $p_T^{\text{jet}} \in [450, 650]$), and (b) SRS0 and VRS0 (subleading candidate, $p_T^{\text{jet}} \in [250, 450]$) [5]. Both figures show differences in the estimated QCD shapes, illustrating the need for the shape correction procedure.

3. adding the expected contributions of V +jets, $t\bar{t}$, and the Higgs boson in the signal regions (as extracted from MC predictions¹¹, V_{SR} , $t\bar{t}_{\text{SR}}$ and H_{SR}) to make the slice into a signal region proxy.

The procedure can be written down as:

$$\text{VR}_{hyb}^i = (\text{VR}^i - V_{\text{VR}} - t\bar{t}_{\text{VR}}) \times \left(\frac{f_{\text{SR}}}{f_{\text{VR}}} \right) + V_{\text{SR}} + t\bar{t}_{\text{SR}} + H_{\text{SR}}, \quad (6.3)$$

The same procedure was used for VRS and VRL (leading and subleading candidate jet validation regions) and differential momentum bins.

A comparison of QCD estimates obtained from fits to partial signal region data and validation region data in two of the differential measurement bins (SRL1/VRL1, $p_T^{\text{jet}} \in [450, 650]$ GeV, and SRS0/VRS0, $p_T^{\text{jet}} \in [250, 450]$ GeV) is shown in figure 6.7. Clear differences between the shapes in the SR and VR regions were seen, which

¹¹ The $t\bar{t}$ component was scaled by $\text{SF}_{t\bar{t}} = 0.85$, compatible with the expected yield from the studies of the $\text{CR}_{t\bar{t}}$ region in section 6.6.1.

demonstrated the need for the hybrid method. The same observations were made in the inclusive regions, and other differential measurement bins. The following studies used VR_{hyb} slices unless specified otherwise.

6.4.2 Statistical Tests and The Minimum Parameter Number

The determination of the optimal number of parameters, N , in the QCD background estimate required striking a delicate balance. The QCD background estimate was a flexible smoothly falling function. Each additional parameter would provide the function with a further degree of flexibility. All of the resonances, particularly the Higgs boson resonance, were quite small in comparison to the QCD background. If the QCD estimate was too flexible, parts of the resonance could have been absorbed.

Conversely, if the estimate had too few parameters, it would not be flexible enough to describe the background shape, resulting in a bias. Figure 6.8 shows examples of the residuals $((\text{data} - \text{fit})/\sigma_{\text{data}})$ from fits to a random VR_{hyb} slice with $N = 2$, $N = 3$ and $N = 4$ parameters. It was clear that a function with $N = 2$ parameters was not flexible enough to fit the background, with distinct regions where the fit overestimated or underestimated the data, whereas with $N = 3$ parameters, such behaviour was not observed. Moving to an even higher number of parameters, i.e. from $N = 3$ to $N = 4$ did not show significant differences, giving some indication that $N = 3$ parameters could be sufficient to describe the data globally, however a more precise method of parameter number determination was needed.

A Likelihood Ratio test was used to determine the minimum number of parameters needed to describe the background. According to Wilks' theorem [140], for two nested functions $f(x, \theta_a)$ and $f(x, \theta_b)$, where θ_n is a vector of parameters of length n , $a < b$, and the former function is fully contained in the latter, the likelihood (L) ratio test statistic

$$t_{\theta} = -2 \log \frac{L(\theta_a)}{L(\theta_b)}, \quad (6.4)$$

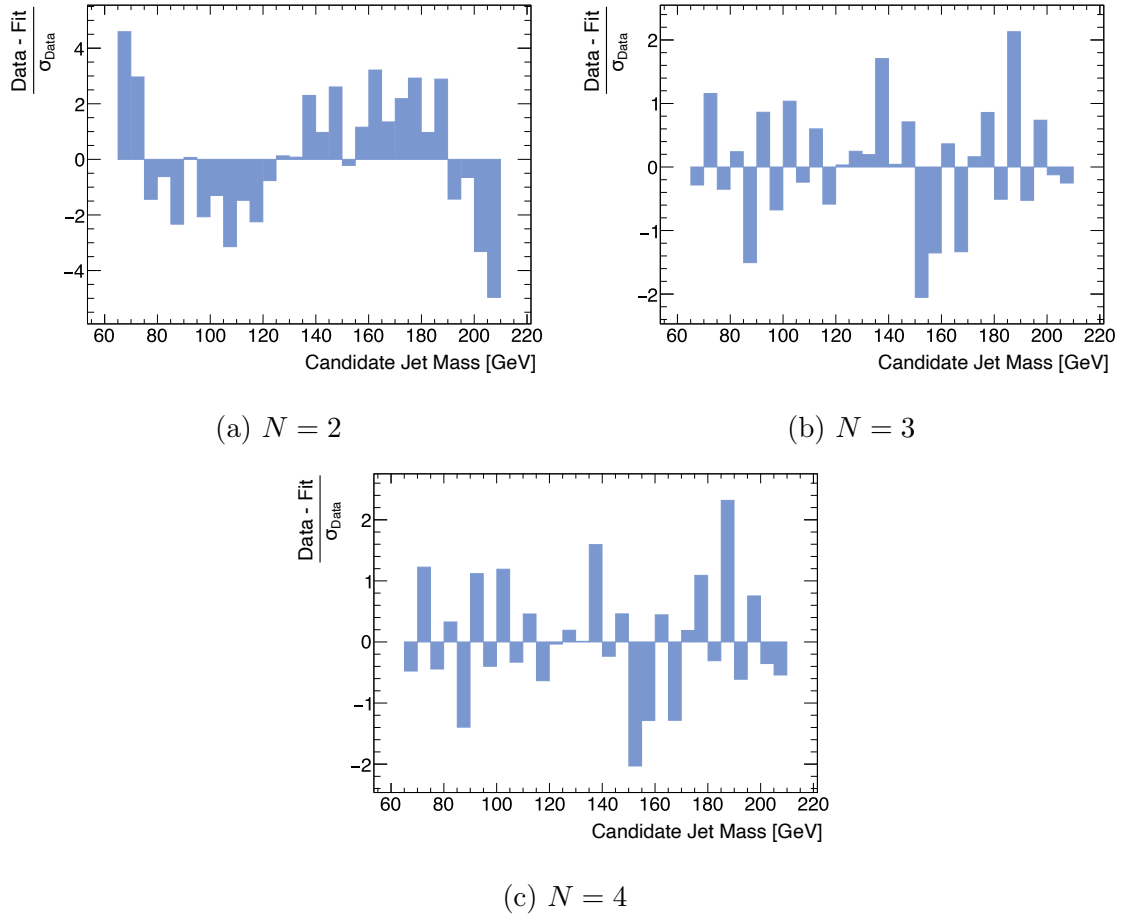


Figure 6.8: Distributions of residuals $((\text{data} - \text{fit})/\sigma_{\text{data}})$ of fits to a random VR_{hyb} slice using models with QCD estimates with (a) $N = 2$, (b) $N = 3$ and (c) $N = 4$ parameters [73] (internal). When $N = 2$ parameters were used in the QCD description, a clear bias in the residuals was seen, indicating that the function was not flexible enough to give a global description of the data. In the cases of $N = 3$ and $N = 4$ no clear bias was observed.

will asymptotically follow a χ_d^2 distribution ($f(t_{\theta}|\theta) \rightarrow \chi_d^2$) with $d = b - a$ degrees of freedom, given sufficiently large sample sizes.

The null hypothesis (H_0) described by this test statistic implies that $f(x, \theta_a)$ describes the data as well as $f(x, \theta_b)$, giving similar values of $L(\theta_a)$ and $L(\theta_b)$, and resulting in a small t_{θ} . Conversely, if there is a significant difference between the two models, the more complex model is preferred, $L(\theta_b)$ is larger than $L(\theta_a)$, resulting in large t_{θ} .

The p -value for this hypothesis is defined as the value of the complimentary cumulative distribution function of the χ_d^2 distribution, evaluated at the observed t_θ (i.e. the integral of the normalised χ_d^2 distribution for $x \geq t_\theta$). It describes the probability to observe a t_θ which is greater or equal to the currently observed value if H_0 is true. Small t_θ values result in large p -values, indicating that H_0 is likely, and vice versa.

A single p -value measurement is subject to statistical fluctuations, therefore, a more robust approach is to look at the distributions of p -values. Generally, if H_0 can be rejected, the distribution of p -values will be weighed towards small p -values, whereas if H_0 is true, the p -values will tend towards a uniform distribution due to their random nature [141].

Ensemble tests were conducted for QCD descriptions in each signal region (inclusive and differential) using corresponding VR_{hyb} slices as proxies¹². Pairs of QCD estimate functions with $a = n$ and $b = n + 1$ variables were compared. In this case H_0 implied that n parameters describe the data as well as $n + 1$ parameters. As the minimum possible number of parameters was sought for, the smallest n giving a uniform p -value distribution was selected ($N = n_{\min}$). The cumulative distributions of the p -values for the inclusive regions are shown in figure 6.9. A uniform p -value would result in a linear cumulative distribution, which was seen with a $n_{\min} = 3$ for VRL_{hyb} , and a $n_{\min} = 4$ for VRS_{hyb} . The results for all signal regions, inclusive and differential, are shown in table 6.2. The results were verified by performing F-tests, which compared the reduced χ^2 values of fits, rather than the obtained likelihoods. The tests returned similar results.

¹² For example, VRL_{hyb} was used as a proxy for SRL , etc. for both inclusive and differential (binned in jet p_T) signal regions, described in section 5.5.

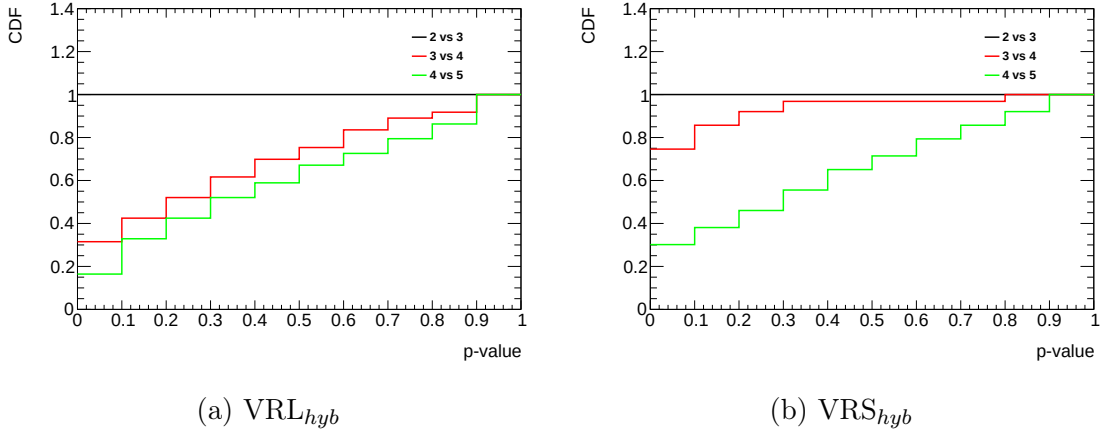


Figure 6.9: Cumulative distribution functions (CDF) of p -values obtained from likelihood ratio (LR) tests comparing fits to (a) VRL_{hyb} and (b) VRS_{hyb} slices with n and $n + 1$ parameters [73] (internal). If a function with $n + 1$ parameters describes the data better than a function with n parameters, the p -values of the LR test will tend towards low values, whereas if the functions are equally good at describing the data, the p -values will be uniformly distributed, appearing as linear distributions in a CDF plot. It was desirable to choose the lowest n which returns a linear CDF distribution (3 in VRL_{hyb} and 4 in VRS_{hyb}).

Table 6.2: The minimum number of parameters needed to describe the QCD background in the inclusive and differential measurement signal regions, as found by performing likelihood ratio tests to corresponding VR_{hyb} slices. * – indicates the candidate jet (leading, L, or subleading, S), and the differential bins are defined in terms of jet p_T : $250 \text{ GeV} < \text{SR}^*0 < 450 \text{ GeV} < \text{SR}^*1 < 650 \text{ GeV} < \text{SR}^*2 < 1000 \text{ GeV}$, $\text{SRL}0$ is unpopulated due to the event selection. From [73] (internal).

Candidate	Inclusive	Differential Bins		
	SR*	SR*0	SR*1	SR*2
Leading Jet (*=L)	3	–	3	3
Subleading Jet (*=S)	4	5	4	3

6.4.3 Signal Injection and Spurious Signal Tests

The statistical tests provide global information on the performance of models over the entire fit range, which might overlook local effects arising from the QCD model interaction with the resonances of interest (Higgs and Z bosons). Such effects were investigated by performing fits to VR_{hyb} slices and observing various features of the fit results, related to the obtained signal strengths ($\mu_{H/Z}^{\text{VR}}$) of the resonances and the associated statistical uncertainties ($\sigma_{\text{stat}}^{\text{VR}}$) as functions of QCD estimated parameter numbers (N).

Two types of tests were used to assess fit performance: a **linearity test**, which considered the compatibility between the “true” signal strength of a resonance and the value extracted from the fit; and **spurious signal tests** which tested the ability of the model to fit a greater signal strength than the “true” one, or fit a signal where there was none.

The linearity test compared average fit results extracted from fits to VR_{hyb} slices, constructed with artificial Higgs or Z boson resonances with signal strengths of $\mu_{H/Z} = 0, 1, 2$ (using SR simulated samples), from fits with different numbers of parameters in the QCD estimate function. Such artificial addition of signal to a dataset is called *signal injection*. The results for Higgs boson test in the inclusive VRL_{hyb} is shown in figure 6.10. It was seen that with a QCD description with $N = 3$ parameters, the Higgs boson signal was inflated in all injected signal cases. This indicated that a QCD description with $N = 3$ parameters lacked needed flexibility, biasing the fit.

The spurious signal tests considered two figures of merit to evaluate the optimal number of parameters. The first indicator was $F_{2\sigma}$ – the fraction of fits to VR_{hyb} created with $\mu_{H/Z} = 1$, which return a measured signal deviation larger than $2\sigma_{\text{stat}}^{\text{VR}}$, i.e. $|\mu^{\text{VR}} - 1| > 2\sigma_{\text{stat}}^{\text{VR}}$. It informed of the tendency of a model to significantly amplify or diminish a signal.

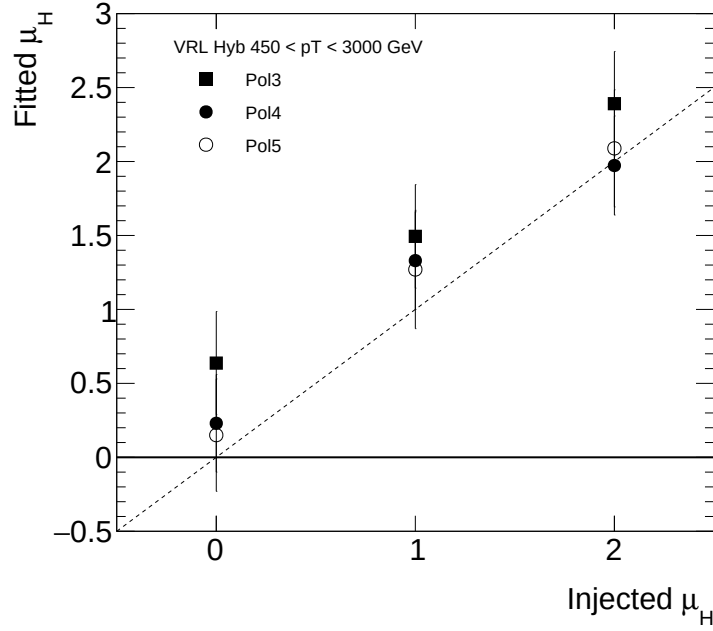


Figure 6.10: Average fit results from fits to VR_{hyb} slices injected with Higgs boson signal at $\mu_H = 0, 1, 2$, with different parameter numbers N in the QCD estimate functions [73] (internal).

The second figure of merit was $\langle \mu_H^{VR} / \sigma_{stat,H}^{VR} \rangle$ – the average measured Higgs boson signal significance when no signal was present in the data (the VR_{hyb} slices were created with $\mu_H = 0$). It described the ability of the model to misinterpret statistical fluctuations as signal. A QCD estimate function with the optimal number of parameters had to satisfy $F_{2\sigma} < 5\%$ and $\langle \mu_H^{VR} / \sigma_{stat,H}^{VR} \rangle < 20\%$ conditions, which are standard within the collaboration.

The tests were performed for the QCD estimate functions for each signal region (inclusive and differential) individually, using corresponding VR_{hyb} proxies. The optimal number of parameters for QCD estimate functions in each signal region determined after these tests are given in table 6.3. The same number of parameters ($N = 5$) was determined to be optimal for both inclusive signal regions (SRL and SRS), whereas in the differential measurement signal region bins $N = 4$ and $N = 5$ was used depending on the bin. The parameter numbers N given in table 6.3 were used in the QCD descriptions of all fits involving signal or validation regions.

Table 6.3: The number of parameters used to describe the QCD background in the inclusive and differential measurement signal regions, as found by performing statistical, and Higgs and Z boson resonance fitting tests, using corresponding VR_{hyb} slices. * – indicate the candidate jet (leading, L, or subleading, S), and the differential bins are defined in terms of jet p_T : $250 \text{ GeV} < SR^*0 < 450 \text{ GeV} < SR^*1 < 650 \text{ GeV} < SR^*2 < 1000 \text{ GeV}$, SRL0 is unpopulated due to the event selection. From [73] (internal).

Candidate	Inclusive	Differential Bins		
	SR*	SR*0	SR*1	SR*2
Leading Jet (*=L)	5	–	5	4
Subleading Jet (*=S)	5	5	4	5

6.5 Vector Boson Modelling

Vector boson backgrounds populate the signal regions in the m_{jet} range between 60 and 140 GeV, with resonance tails overlapping with the Higgs boson signal. The Z +jets and W +jets components are treated separately in the fits, with fully correlated uncertainties.

Around 93% of the Z +jets contribution comes from candidate jets with an associated truth-level Z boson, resulting in a clearly resonant signature, whereas a majority of the W +jets contribution (53% – 68%) does not have an associated truth-level boson, and likely comes from a QCD recoil jet. Plots of the V +jets contributions to the inclusive signal regions, and the truth-level boson components, are given in figure 6.11.

V +jets Nominal Template Smoothing

It was found that MC statistical limitations of the available V +jets MC samples introduced biases in the measurement of the Z boson resonance, in particular when a 0.5 GeV binning was used in the signal regions. This was remedied by developing

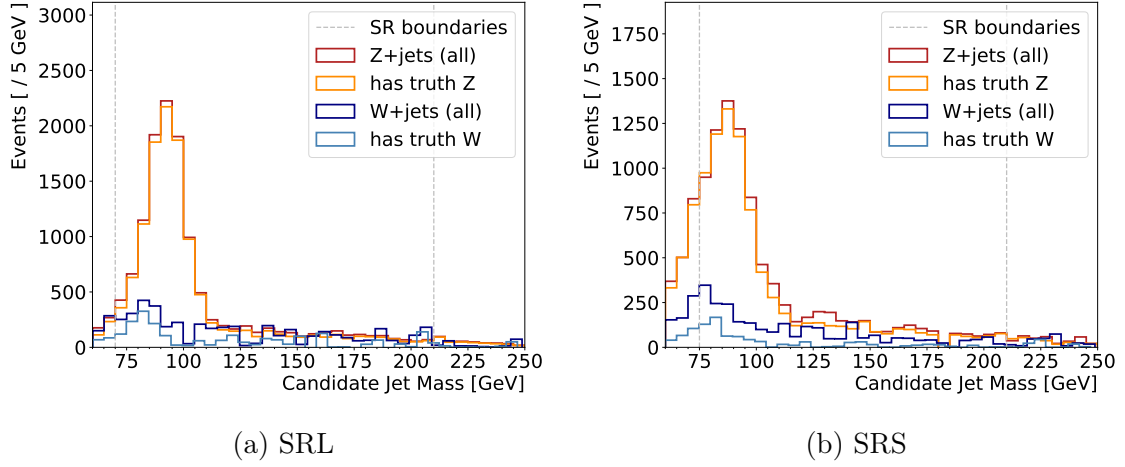


Figure 6.11: Candidate jet mass (m_{jet}) spectra of simulated Z +jets and W +jets events in inclusive (a) SRL and (b) SRS regions. The vertical lines indicate the jet mass ranges within which the signal region fits are made. Also shown are the components of candidate jets with truth boson association.

a custom smoothing procedure for these samples, which considered their physical composition of a mixture of V boson and QCD events. This procedure was kept after the move to 5 GeV bins, as the differential measurement templates with particularly small statistics could still suffer from such issues.

The measurement bias, the smoothing procedure, and validation studies performed by the author are discussed in detail in appendix E. A comparison of Z +jets and W +jets mass templates in the inclusive SRL region (with 0.5 GeV binning) before and after smoothing are shown in figure 6.12. After smoothing, the templates were significantly smoother, and the shapes of the original and smoothed templates agreed well.

The validation studies performed by the author highlighted sculpting effects on m_{jet} and p_T^{jet} distributions by an initial version of the procedure, and lead to its refinement. As well as performing validation tests, the author implemented the smoothing procedure in to the fitting framework for use in fit studies and measurements.

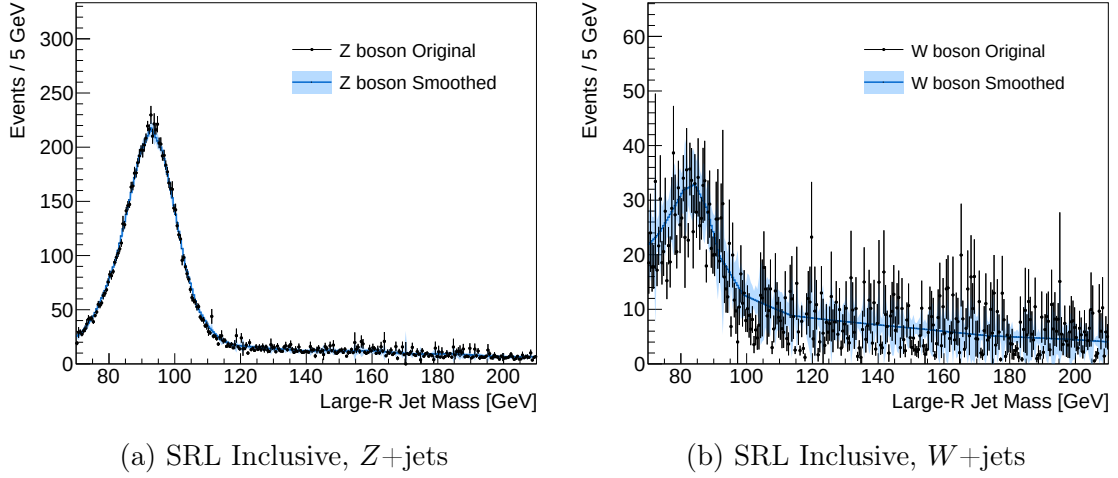


Figure 6.12: Comparisons of original and smoothed templates of (a) Z +jets and (b) W +jets processes in inclusive SRL regions, using the smoothing procedure described in appendix E, with a former fit setup using 0.5 GeV binning and smaller MC samples used throughout a large part of analysis development.

6.6 $t\bar{t}$ Modelling

The $t\bar{t}$ background candidates primarily come from top-quark decays, and therefore result in a resonant contribution in the high end of the SR mass spectra ($m_{\text{jet}} > 140$ GeV). An external, kinematically similar data region – $\text{CR}_{t\bar{t}}$ – was used to gain stronger constraints on the $t\bar{t}$ background scale factor ($\text{SF}_{t\bar{t}}$) and $t\bar{t}$ systematic uncertainties. The $\text{CR}_{t\bar{t}}$ region was enriched with $t\bar{t}$ events by looking for a muon associated to the recoil jet, indicative of a semileptonic top decay. The full event selection is given in section 5.4.2.

This section discusses the $t\bar{t}$ background modelling, and gives a brief overview of the constraints on $t\bar{t}$ processes provided by the $\text{CR}_{t\bar{t}}$ region, including the standalone fit results. In the final measurement set-up, the fit to the $\text{CR}_{t\bar{t}}$ region¹³ used to constrain the $t\bar{t}$ background was performed simultaneously with the signal region fits. In depth studies of the $\text{CR}_{t\bar{t}}$ standalone fits, and the simultaneous fit with the

¹³ In the differential measurement fits three $\text{CR}_{t\bar{t}}$ regions were used, binned in equivalent p_T^{jet} bins as the signal regions, constraining the $t\bar{t}$ scale factor $\text{SF}_{t\bar{t}}$ separately in each bin.

signal regions, will be presented in chapter 8.

The p_T^{jet} Composition of $t\bar{t}$ Events

This thesis presents several studies of the $t\bar{t}$ background, both inclusively and in p_T^{jet} bins. A look at the p_T^{jet} composition of this background is important to contextualise the following discussions.

The simulated templates of the $t\bar{t}$ process in inclusive and p_T^{jet} -binned SRL, SRS and $\text{CR}_{t\bar{t}}$ regions are shown in figures 6.13a, 6.13b, and 6.13c. In all cases the high p_T^{jet} components had significantly smaller statistics, making up between 7%–15% of events. The low and medium p_T^{jet} bins had similar prominence, making up 40%–47% of the total yields in SR and $\text{CR}_{t\bar{t}}$ (where the low p_T^{jet} bin is present).

Notably, the low p_T^{jet} components in the SRS and $\text{CR}_{t\bar{t}}$ regions (figures 6.13b, and 6.13c) were seen to be wider and shifted towards lower masses. This is because most of the top quarks in this momentum range were not boosted enough¹⁴ to deposit all their energy within a large-R jet with a size parameter of $R = 1.0$. To a smaller extent, due to resolution effects, this also affected the medium momentum bin, causing it to peak slightly below the true top mass.

Another important feature was a small relative increase of events in the $\text{CR}_{t\bar{t}}$ templates (figure 6.13c) between 70 GeV and 100 GeV, which was not as prominently seen in the signal regions. The cause of this were W bosons from top-quark decays, passing the ≥ 1 b -tagged sub-jet requirement in the $\text{CR}_{t\bar{t}}$ selection (as opposed to a 2 b -tagged sub-jet requirement for candidates in the signal regions). This motivated the choice to perform $\text{CR}_{t\bar{t}}$ fits in a shorter mass range of $m_{\text{jet}} \in [140, 200]$ GeV.

6.6.1 The $\text{CR}_{t\bar{t}}$ Fit

In the measurement fits the $t\bar{t}$ background was controlled by performing simultaneous likelihood fits of the m_{jet} spectra in the $\text{CR}_{t\bar{t}}$ and signal regions. The $t\bar{t}$ scale

¹⁴ $\Delta R \approx p_T^{\text{jet}}/2m$, see section 3.2.1 for more details.

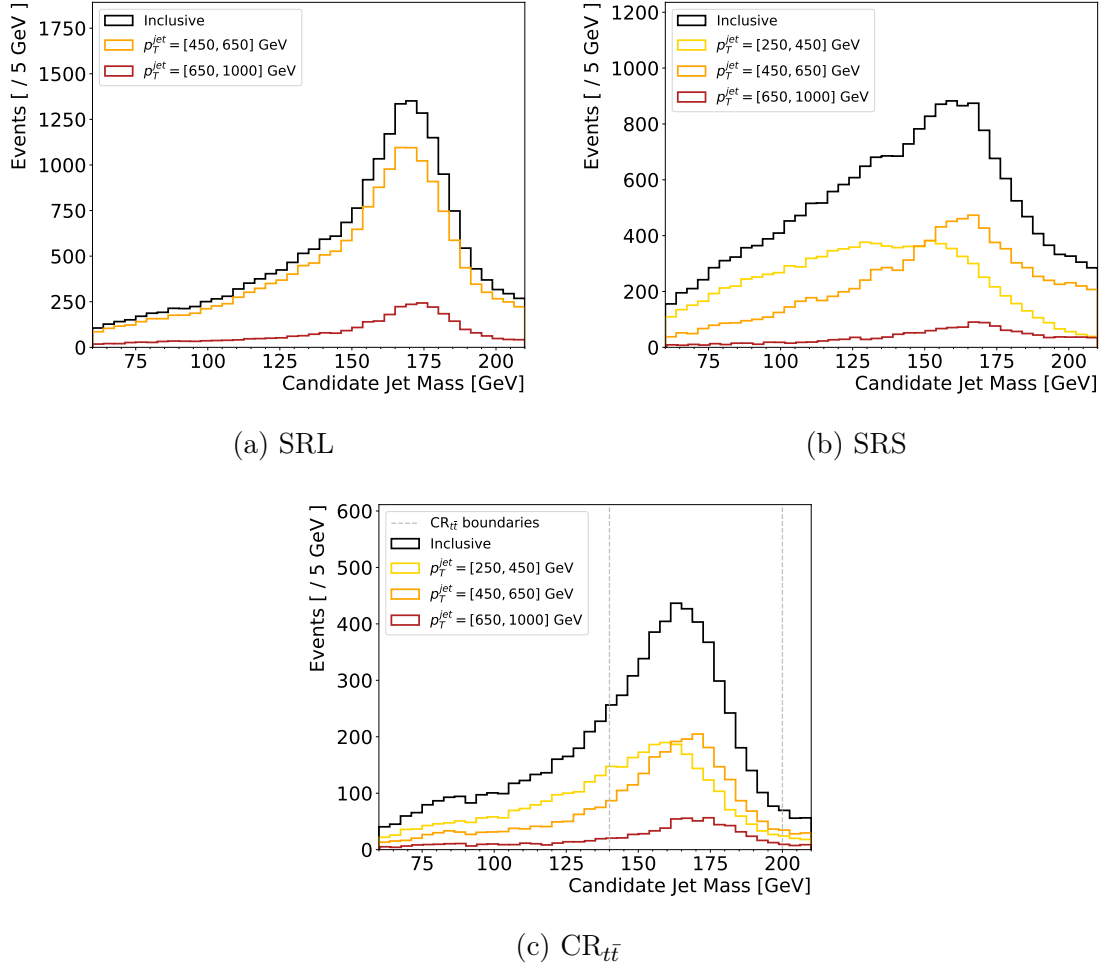


Figure 6.13: The inclusive and p_T^{jet} -binned components of simulated $t\bar{t}$ template shapes in (a) SRL, (b) SRS, and (c) $\text{CR}_{t\bar{t}}$ regions.

factor ($\text{SF}_{t\bar{t}}$) and systematic uncertainties were fully correlated (100%) between the $\text{CR}_{t\bar{t}}$ and signal regions. As $\text{CR}_{t\bar{t}}$ was highly pure in $t\bar{t}$ decays it provided most of the constraints for this background. The simultaneous fitting of the $\text{CR}_{t\bar{t}}$ and SR regions is discussed in detail in chapter 8.2. Both standalone $\text{CR}_{t\bar{t}}$ fits, and simultaneous $\text{CR}_{t\bar{t}}$ and SR fits followed the likelihood fitting procedure described in section 5.7.

Unlike the QCD background, known to lack modelling accuracy, the $t\bar{t}$ process is modelled with high precision in MC simulations. However, this analysis targets extremely high momentum regions, where the predictions were less certain. The

ability to construct and use an external data region with a highly pure $t\bar{t}$ signal was exploited to get targeted constraints on the $t\bar{t}$ background in this topology, and constrain the uncertainties on this process.

The expected standalone $\text{CR}_{t\bar{t}}$ fit results in the inclusive and differential regions found by fitting corresponding Asimov data¹⁵ are given in table 6.4. The measurement precision was dominated by systematic uncertainties, and was worse in the high p_T^{jet} region where the statistics were significantly lower. The expected signal significances ($\text{SF}_{t\bar{t}}/\sigma_{\text{total}}$) ranged between 14σ and 9σ , indicating highly precise fits.

The fit results from standalone fits to $\text{CR}_{t\bar{t}}$ data are shown in table 6.5. The measured scale factor of ~ 0.8 between data and the MC prediction agreed with the findings from top quark differential cross-section measurements by the ATLAS experiment [133] (figure 54). The measurement accuracy also agreed well with the expected values in table 6.4. The systematic uncertainties were slightly reduced compared to the Asimov fits, which was studied and understood to be due to scaling effects. The study is presented in section 8.1. A validation study observing systematic uncertainties and their correlations is also presented in section 8.1.

The inclusive $\text{CR}_{t\bar{t}}$ data and model before and after the fit are shown in figures 6.14a and 6.14b, respectively. Before the fit the $\sim 20\%$ discrepancy between data and simulation can be clearly seen. Regardless, the shape of the distribution was seen to be modelled well, presenting a flat ratio between data and MC. After the fit, the model was seen to describe the data well. The data-to-model ratio was shown to closely agree with 1, and any differences between the data and model were seen to be within 1σ of the total fit uncertainties. The same distributions for fits in differential measurement bins are shown in figures D.2 and D.3 in appendix D.3.

¹⁵ Asimov data is an idealised dataset, built from the model itself, providing the expected results and sensitivity of the measurement. Described in section 5.7.2.

Table 6.4: The expected measurement results of $t\bar{t}$ scale factors ($\text{SF}_{t\bar{t}}$), statistical and systematic uncertainties (σ) and signal significances ($\text{SF}_{t\bar{t}}/\sigma_{\text{total}}$) in standalone fits to inclusive and differential $\text{CR}_{t\bar{t}}$ regions, found from fits to corresponding Asimov datasets with $\text{SF}_{t\bar{t}} = 1$.

Range		$\text{SF}_{t\bar{t}}$	σ_{stat}	σ_{syst}	$\text{SF}_{t\bar{t}} / \sigma_{\text{total}}$
Inclusive		1	0.02	0.07	13.8
$\text{CR}_{t\bar{t}}0$	$p_T^{\text{jet}} \in [250, 450] \text{ GeV}$	1	0.02	0.07	14.1
$\text{CR}_{t\bar{t}}1$	$p_T^{\text{jet}} \in [450, 650] \text{ GeV}$	1	0.02	$^{+0.09}_{-0.08}$	11.7
$\text{CR}_{t\bar{t}}2$	$p_T^{\text{jet}} \in [650, 1000] \text{ GeV}$	1	0.04	$^{+0.11}_{-0.09}$	9.2

Table 6.5: Measurement results of $t\bar{t}$ scale factors ($\text{SF}_{t\bar{t}}$), statistical and systematic uncertainties (σ) and signal significances ($\text{SF}_{t\bar{t}}/\sigma_{\text{total}}$) from standalone fits to inclusive and differential $\text{CR}_{t\bar{t}}$ region data.

Range		$\text{SF}_{t\bar{t}}$	σ_{stat}	σ_{syst}	$\text{SF}_{t\bar{t}} / \sigma_{\text{total}}$
Inclusive		0.79	0.01	0.06	13.4
$\text{CR}_{t\bar{t}}0$	$p_T^{\text{jet}} \in [250, 450] \text{ GeV}$	0.86	0.02	0.06	13.6
$\text{CR}_{t\bar{t}}1$	$p_T^{\text{jet}} \in [450, 650] \text{ GeV}$	0.76	0.02	0.07	11.6
$\text{CR}_{t\bar{t}}2$	$p_T^{\text{jet}} \in [650, 1000] \text{ GeV}$	0.73	0.04	$^{+0.08}_{-0.07}$	8.9

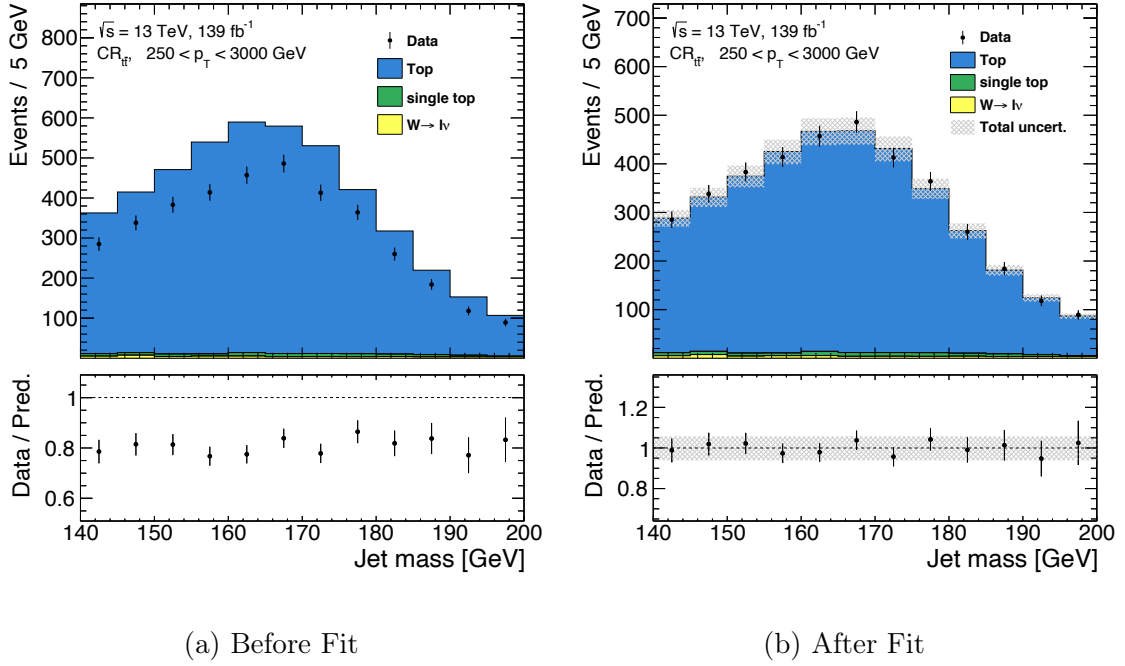


Figure 6.14: The $\text{CR}_{t\bar{t}}$ data and model m_{jet} distributions before and after the likelihood fit of the inclusive $\text{CR}_{t\bar{t}}$ region, performed standalone, without inclusion of the signal regions. The measured $t\bar{t}$ scale factor was found to be $\text{SF}_{t\bar{t}} = 0.79 \pm 0.01$ (stat) $^{+0.06}_{-0.06}$ (syst). The single-top and $W(\ell\nu)$ backgrounds were fixed to the SM predictions in the fit.

6.7 Chapter Overview

This chapter has explored important features of the signals and backgrounds in this analysis, and various considerations taken in their modelling in the statistical fits.

The composition of Higgs boson production processes, and m_{jet} and p_T^{jet} experimental resolution was discussed. A study of Higgs boson event distribution in p_T^H and p_T^{jet} bins was presented, which led to a simplification of the Higgs boson uncertainty model in the differential measurement fits.

The QCD modelling using a data driven method was presented. The QCD background function was shown to be described well by an exponential function of a polynomial, and studies used to determine the optimal number of parameters in the description were presented.

The vector boson background composition was described, and the smoothing of V +jets mass templates used to combat shape fluctuations due to the low MC statistics was introduced. The smoothing procedure and validation studies performed by the author, which led to improvements of the smoothing procedure are presented in appendix E.

The features in the $t\bar{t}$ background shape were explored, and the $\text{CR}_{t\bar{t}}$ region – an independent $t\bar{t}$ enriched control region, used to constrain the $t\bar{t}$ background – was introduced. The fit results from standalone $\text{CR}_{t\bar{t}}$ fits were presented and briefly discussed, which agreed to the expectations from other ATLAS analyses.

This chapter presented comprehensive signal and background modelling studies, which were crucial to produce a robust measurement framework, and allow a correct interpretation of results.

Chapter 7

Systematic Uncertainties

Any measurement is only as good as the confidence in its uncertainty estimate. Statistical uncertainties depend only on the amount of data available, but the sources of systematic uncertainties are many, and a robust understanding and treatment of them is vital to achieve a reliable result.

The Higgs boson signal was very small compared to the immense backgrounds in a fully hadronic decay channel. Hence, most of the Higgs boson measurements made were statistically limited¹. To a lesser degree, this also applied to the differential Z boson measurement as well.

However the expected systematic uncertainties on the Higgs boson measurements were comparable in the inclusive and fiducial measurements, and the more sensitive regions of the differential measurement. Furthermore, the estimates of the Z boson background in the inclusive measurement, and the $t\bar{t}$ background in all regimes were dominated by systematic uncertainties. The estimations of these backgrounds served as “anchors” to the QCD background prediction which was highly correlated with the Higgs boson measurements. Hence, it was important to have a robust treatment of systematic uncertainties in the measurement fits.

This chapter provides an overview of the main sources of systematic uncertain-

¹ Except for a differential measurement in a p_T^H bin ($p_T^H \in [450, 650]$ GeV) determined by signal regions with the highest statistics.

ties and their treatment in the measurement, required to contextualise studies and results. Overviews of the sources of systematic uncertainties, and their treatment are given in sections 7.2 and 7.3, respectively. The following sections focus on the many studies performed to finalise the treatment of the systematic uncertainties in the fit models for the measurements.

Section 7.4 discusses the concepts of uncertainty *pulls* and *impact* used frequently through this chapter and further analysis. Section 7.5 presents a smoothing procedure used to mitigate the impact of MC statistical fluctuations. Section 7.6 presents studies, which enabled uncertainty reduction in the model. Section 7.7 gives an overview of the derivation of external jet mass resolution (JMR) constraints for $V+\text{jets}^2$ processes, and section 7.8 discusses uncertainty correlation scheme studies for the differential measurements.

7.1 Author's Contributions

The systematic uncertainties described in section 7.2 were derived by dedicated groups at ATLAS, and the treatment described in section 7.3 follows the recommendations of said groups unless stated otherwise. The following explicitly describes the contributions from the author presented in this chapter.

Systematic Uncertainty Smoothing: (section 7.5) all presented work, including the development of the smoothing technique, and validation studies were performed by the author.

Systematic Uncertainty Pruning: (section 7.6) the uncertainty pruning optimisation procedure was developed by the author, and used to optimise the pruning in $\text{CR}_{t\bar{t}}$ regions. The same procedures were later used by other analysis members to optimise the uncertainty pruning in the signal regions.

Systematic Uncertainty Decorrelation Studies: (section 7.8) the initial uncer-

² $V+\text{jets}$ collectively refers to $Z+\text{jets}$ and $W+\text{jets}$ processes.

tainty decorrelation studies were initially performed by the author, which were later repeated without significant change of methodology by other analysis members.

The external constraint derivation for V +jets JMR uncertainties, described in section 7.7, were the work of other analysis members. All figures shown in this chapter have been produced by the author unless cited or stated otherwise.

7.2 Sources of Systematic Uncertainties

Four categories of systematic uncertainties were considered:

- jet uncertainties;
- flavour tagging uncertainties;
- spurious signal uncertainties;
- theoretical (modelling) uncertainties.

Each uncertainty category contains multiple sources of uncertainties, some significant and some minor, which were treated separately in the measurement. This section will give a brief overview of the categories and prominent sources of systematic uncertainties. The descriptions of all sources and their labels are given in appendix G.1. Where uncertainties are discussed in the following studies, an overview of the uncertainties used in the section will be given at the start.

The uncertainties on the process estimates can be decomposed into two components: the *normalisation* component which describes the effect on the yield of the process, and the *shape* component, which describes the effect on the m_{jet} distribution shape of the process. Many uncertainties, such as jet uncertainties include both types of effect. The uncertainties and their propagation in the measurement followed the recommendations from dedicated working groups within ATLAS. The correlations scheme used in the analysis is described in section 7.3.

Most uncertainties were included in the fit, however some uncertainties, which only had normalisation components, and were not expected to be correlated with

other uncertainties, were included after the measurement. The treatment is stated explicitly in the description. All uncertainties shown or quoted in this section are of the initial extent, i.e. without constraints from the fit to data; and after the smoothing procedure described in 7.5. The sizes of the normalisation components of uncertainties acting in the inclusive signal regions (SRL and SRS) and $t\bar{t}$ control region ($\text{CR}_{t\bar{t}}$) are given in table G.1 in appendix G.2. Examples of the mass templates of higher importance uncertainties investigated throughout the thesis are given in appendix G.3.

7.2.1 Large- R Jet Uncertainties

Large- R Jet uncertainties can be subdivided into four categories:

- JES – jet energy scale;
- JMS – jet mass scale;
- JER – jet energy resolution;
- JMR – jet mass resolution.

All jet uncertainties were derived by the calibration procedures described in section 3.2.4. The jet mass uncertainties (JMR and JMS) were the some of the largest and most impactful uncertainties on the measurement. The JMR uncertainty was a relative 20% on the mass of the jet. The JMS modelling uncertainty, derived through comparison between MC generators, was also one of the most prominent uncertainties overall, generally affecting the position of the resonance.

The $\pm 1\sigma$ variations of JMR and JMS modelling uncertainties on the Higgs boson template in the inclusive SRL are shown in figures 7.1a and 7.1b. The jet energy scale (JES) uncertainties tend to be smaller and less significant than JMS, and the jet energy resolution (JER) uncertainty had negligible impact on the measurements and was not included.

At of time of writing, new recommendations for JER and JMR uncertainties

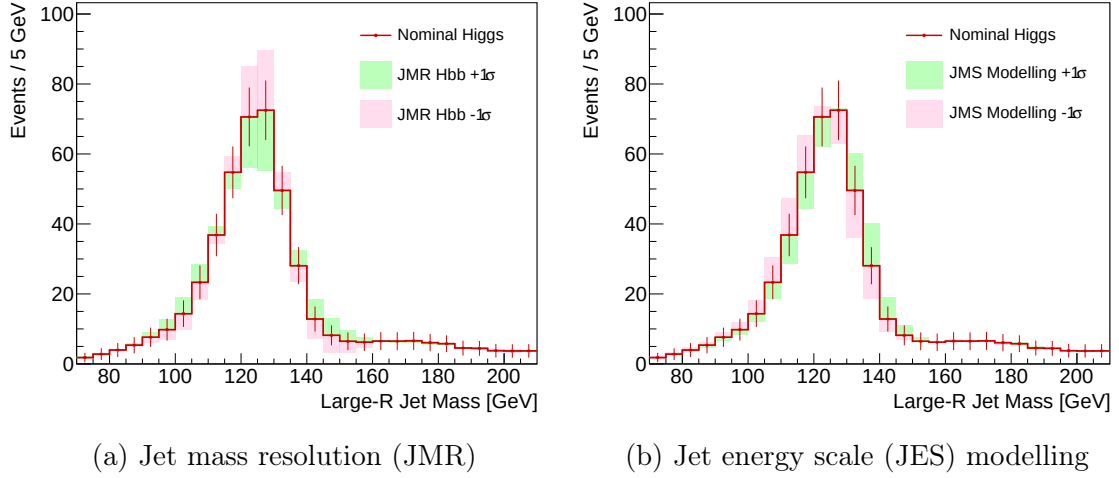


Figure 7.1: The nominal MC m_{jet} template of the Higgs boson estimate in MC, and $\pm 1\sigma$ variations of the (a) jet mass resolution (JMR) and (b) jet mass scale (JMS) modelling uncertainties in the inclusive SRL (leading candidate jet signal region). The uncertainties shown on the nominal template are Poisson distributed to provide a sense of scale.

were available, derived using a more-sophisticated *in-situ* method [78]. According to the new recommendations both the JER and JMR uncertainties are reduced, emphasising that the uncertainties used in the analysis were conservative estimates.

The large JMR uncertainties showed strong correlations with the Z +jets signal strength, so the analysis used validation region data and dedicated control region (CR_W) data to derive external constraints for JMR uncertainties of V +jets processes, described in section 7.7.

7.2.2 Flavour Tagging Uncertainties

Flavour Tagging Uncertainties are uncertainties derived from b -tagging efficiency, c -jet mistagging rate and light-jet mistagging rate calibrations, described in section 3.3.1. Several tagging efficiency uncertainties were assigned to each jet flavour type, which were derived using an eigenvector scheme described in section 8.3 of [91]. Each flavour tagging uncertainty group – b -tagging, c -jet and light jet mistagging,

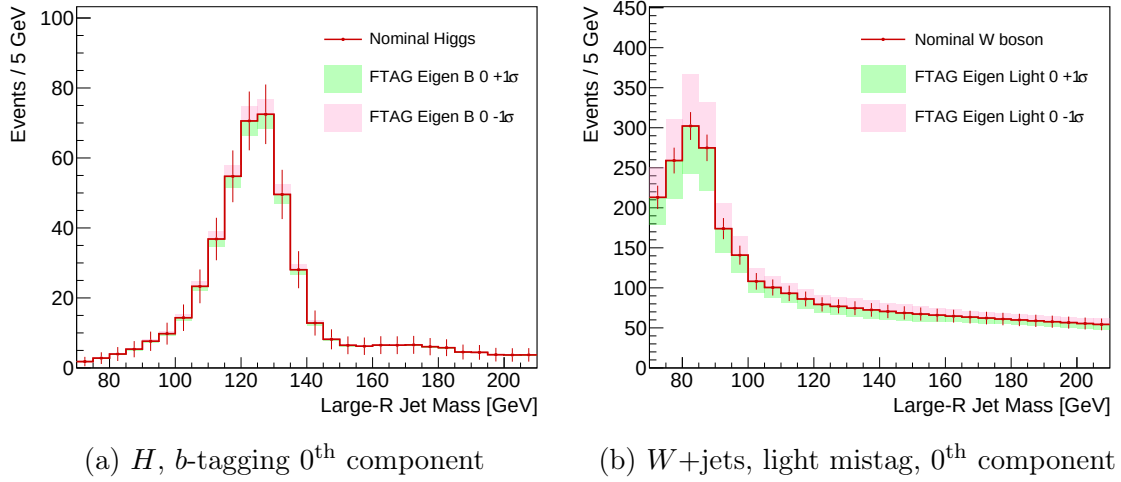


Figure 7.2: Examples of relevant flavour tagging uncertainties included in the inclusive measurement in the SRL region. Subfigure (a) shows a b -tagging uncertainty on the Higgs boson template ($\sim 5\%$ of the yield); (b) shows a light jet mistagging uncertainty on the W +jets template ($\sim 16\%$ of the yield). The uncertainties shown on the nominal template are Poisson distributed to provide a sense of scale.

are labelled by **B**, **C**, and **Light**, respectively, and has up to 5 components, indexed from 0 to 4.

Flavour tagging uncertainties can have both shape and normalisation components, but the shape components tended to be small and were mostly not included in the fits, as they failed to pass the threshold³ imposed by the uncertainty reduction procedure (*pruning*, described in section 7.6).

Examples of two flavour tagging uncertainties in the inclusive SRL region, with relatively large extent on their respective processes, are shown in figure 7.2. Figure 7.2a shows one of the b -tagging uncertainties (**B0**) on the Higgs boson template with an approximately 5% impact on the normalisation, and figure 7.2b shows one of the light jet mistagging uncertainties (**Light0**) on the W +jets template with an approximately 16% impact on the normalisation.

³ The condition is given in equation 7.9, the threshold is 2%.

7.2.3 Spurious Signal Uncertainties

Spurious signal uncertainties on the QCD estimate function were derived as part of the QCD background studies using validation region data performed by members of the $H(\rightarrow b\bar{b}) + j$ analysis group, described in section 6.4. The spurious signal uncertainty, σ_{SS} was defined as the product of the average spurious signal significance: $\langle \mu / \sigma_{\text{stat}}^{\text{VR}} \rangle$, derived from spurious signal tests⁴ using hybrid validation region slices⁵ (VR_{hyb}); and the expected statistical uncertainty on μ derived from fits to signal region (SR) Asimov data⁶, $\sigma_{\text{stat}}^{\text{A,SR}}$, i.e. the spurious signal uncertainty is:

$$\sigma_{SS} = \frac{\mu^{\text{VR}}}{\sigma_{\text{stat}}^{\text{VR}}} \times \sigma_{\text{stat}}^{\text{A,SR}}. \quad (7.1)$$

Spurious signal uncertainties were not included in the fit itself, but added in quadrature to the post-fit systematic uncertainty. The σ_{SS} uncertainty ranges, quoted in terms of expected statistical uncertainty $\sigma_{\text{stat}}^{\text{A,SR}}$ were between 1% and 0.33% of σ_{stat} for the Higgs boson signal, and between 15% and 65% of σ_{stat} for the Z +jets measurement. In both cases, the spurious signal uncertainties had minor effects on the total sensitivities of the measurements [5].

7.2.4 Theoretical and Modelling Uncertainties

Theoretical uncertainties enter the measurement through the use of simulated samples. Simulations are imperfect, and have associated modelling uncertainties, rising from theoretical predictions, and approximations made in the simulation process. More information on MC event simulation can be found in section 3.1.

⁴ Spurious signal tests were described in section 6.4.3 .

⁵ Hybrid validation region data slices (VR_{hyb}) were signal region proxies used for fit studies, described in section 6.4.1.

⁶ Asimov data is an idealised dataset, built from the model itself, providing the expected results and sensitivity of the measurement. Described in section 5.7.2.

Higgs Boson Modelling Uncertainties

Each Higgs boson production mode had an associated acceptance uncertainty derived through renormalisation and factorisation (QCD) scale variations [30]. The acceptance uncertainty on the ggF production mode also included parton distribution function (PDF) and parton shower (PS) uncertainties, found using alternative generators. Next-to-leading-order (NLO) electroweak (EW) corrections were also included for VBF, VH and $t\bar{t}H$ processes. All Higgs boson uncertainties were found to be flat in the investigated phase-spaces. They were not expected to be constrained by the fit and therefore were added in quadrature to the uncertainties on the measurements after the fits. The uncertainty sizes⁷ are given in table 7.1.

Table 7.1: List of relevant Higgs boson theoretical uncertainties. All uncertainty effects were seen to be flat in p_T^H and m_{jet} , and therefore were treated as normalisation-only uncertainties included after the measurement.

Uncertainty	Size
ggF acceptance	20%
VBF acceptance	0.5%
VH acceptance	5%
$t\bar{t}H$ acceptance	13%
NLO EW Correction	2 – 6%

V+jets Modelling Uncertainties

Factorisation and renormalisation scale uncertainties were derived using scale variations, and were some of the largest V +jets uncertainties (along with V boson JMR, $B0$ b -tagging uncertainty, and JMS modelling). An example of this uncertainty on the Z +jets template in the inclusive SRL region is given in figure 7.3a.

⁷ Note, the extent of most other uncertainties is not easily described as they act on both normalisation and shape of the process. The sizes of the normalisation components of systematic uncertainties on processes in the inclusive SRL, SRS and $CR_{t\bar{t}}$ regions are given in table G.1 in appendix G.2.

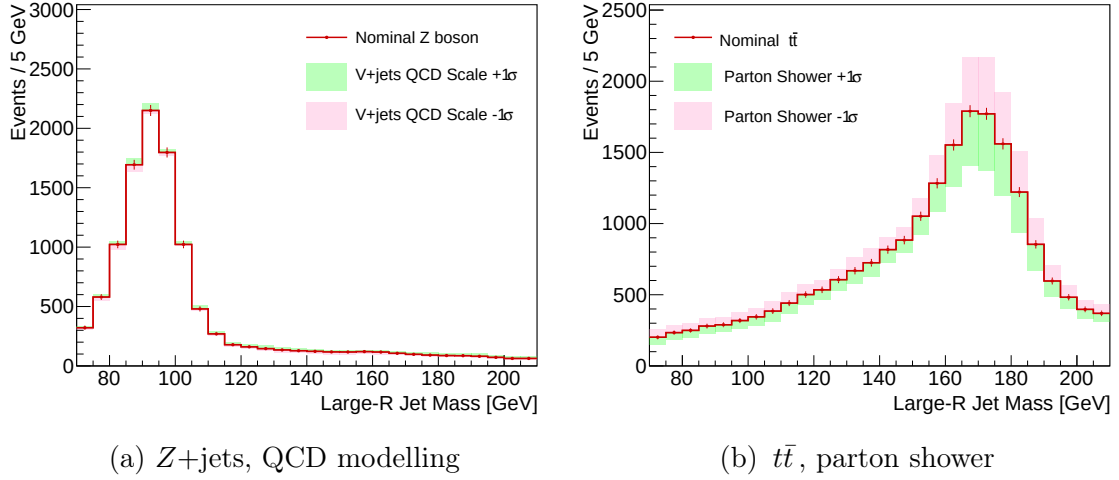


Figure 7.3: Examples of (a) Z +jets QCD modelling uncertainties and (b) $t\bar{t}$ parton shower uncertainties included in the inclusive measurement in the SRL region. The normalisation components of shown uncertainties were (on average) (a) 5% and (b) 18% of the yield. The uncertainties shown on the nominal template are Poisson distributed to provide a sense of scale.

Other investigated modelling uncertainties, such as comparisons to an alternative PDF or fragmentation model, etc. were found to be negligible. In the fit model, the W +jets process was constrained to the SM cross-section which had an associated 10% uncertainty [142]. It was included in the likelihood description as a Gaussian prior on the W +jets yield.

$t\bar{t}$ Modelling Uncertainties

Matrix element (ME) calculation, parton shower (PS) modelling uncertainties were derived using alternative generators, which (along with top-quark JMR, B0 b -tagging uncertainty, and JMS modelling) were the largest uncertainties on the $t\bar{t}$ process. The initial and final state radiation (ISR/FSR) rate uncertainties were derived by varying internal weights provided in the simulated sample, and were also included. The renormalisation and factorisation scale uncertainties derived using scale variations were found to be negligible. An example of the parton shower uncertainty on the $t\bar{t}$ process in the inclusive SRL region is given in figure 7.3b.

The V +jets and $t\bar{t}$ modelling uncertainty templates in the inclusive signal regions and $\text{CR}_{t\bar{t}}$, are given in figures G.3 and G.4 in appendix G.3.

7.3 Treatment of Systematic Uncertainties in The Fit

In the fit model, all resonant processes (H , Z , W , and $t\bar{t}$), were described by two components⁸: a m_{jet} histogram (*template*) normalised to an integral of 1, which described the shape of the process, and an expected yield, which is used as an initial scale factor for the template. All uncertainties included in the measurement fit were described by nuisance parameters and decomposed in the same way. The normalisation components of uncertainties were included in the model as Gaussian or log-normal priors on the yield of a process, and the shape components were added as two histograms (normalised to 1) representing $\pm 1\sigma$ variations of the process shape. If an uncertainty on a process had both a shape and a yield component, the normalisation and shape descriptions were described by a single nuisance parameter.

Some modelling uncertainties which are applied only on the normalisation were included after the fit (i.e. spurious signal and some theoretical uncertainties). This was done only for normalisation uncertainties which were not expected to be constrained by the fit. Henceforth this chapter will primarily focus on the treatment of uncertainties included in the fit.

In the following, if an uncertainty is *decorrelated*, for example, “decorrelated across processes”, it means that the uncertainty is described as a separate nuisance parameter for each process, whereas if an uncertainty was said to be “*correlated* across processes”, it means that the same uncertainty on multiple processes is described by a single nuisance parameter.

Systematic uncertainty propagation and correlation schemes follow the recommendations of the dedicated research groups at ATLAS, except for the cases where

⁸ The separate treatment was imposed by the fitting software used, but such decomposition of uncertainties also allowed to simplify the fit model as discussed in section 7.6.

dedicated studies, described in section 7.8, suggested a need for a different treatment. The correlation scheme is presented in the following, and a summary of all uncertainties and their treatment is given in table 7.2.

All flavour tagging uncertainties, and most jet uncertainties, with the exception of the jet mass resolution (JMR) were (individually) correlated across all processes, p_T bins, and leading / subleading candidate jet categories. Generally, there were no reasons to expect a significantly varied behaviour, and, as long as the uncertainties in question were not strongly constrained by the fits, the correlation would not have an impact on the fit.

Decorrelation studies of high-impact uncertainties, to which the fit could be sensitive, were conducted to mitigate possible biases introduced by the broad correlation approach. The studies are presented in section 7.8, and the changes made in light of studies were:

- JMR was decorrelated across p_T^{jet} bins for all processes;
- JMS Modelling was decorrelated across p_T^{jet} bins for all processes;
- JMS Modelling was decorrelated between V +jets and Higgs boson processes.

The JMR uncertainties were decorrelated across H , V +jets, and $t\bar{t}$ processes, as a secure approach, as the JMR uncertainties are particularly large and strongly constrained by the fits. The JMS uncertainties were decorrelated between $t\bar{t}$ and other processes, due to the different topologies between $t\bar{t}$ and $X \rightarrow b\bar{b}$ jets, as well as the use of the dedicated $t\bar{t}$ control region $\text{CR}_{t\bar{t}}$. As modelling uncertainties tend to be process dependent, they were applied separately on each corresponding process.

Uncertainty Symmetrisation

Jet mass resolution uncertainties, and $t\bar{t}$ modelling uncertainties derived from alternative generators ($t\bar{t}$ parton shower and matrix element generators) only had *one-sided* descriptions, i.e. only a $+1\sigma$ variation. The best or “most physical” treatment

Table 7.2: A summary of the systematic uncertainties included in H and Z boson measurements. The “Process” column indicates the processes for which uncertainties apply. Processes separated by “|” have independent (decorrelated) uncertainties. The “Category” column indicates the regions (p_T or candidate jet) with independent (decorrelated) uncertainties. The label “all” indicated the uncertainties are correlated over all processes or categories. The “Effect” column indicates whether the uncertainty acts on the normalisation (N) and/or the m_{jet} template shape (S) of the process. * – uncertainty added after the fit, as described in section 7.2; ** – only applied to Z +jets uncertainties in the Z +jets measurements. Adapted from table 8 of [143].

Description	Processes	Category	Effect
Experimental Systematic Uncertainties			
JMR	$t\bar{t}$ V +jets H	p_T^{jet} bins	N+S
JMS Modelling	$t\bar{t}$ V +jets H	p_T^{jet} bins	N+S
JMS (others)	$t\bar{t}$ V +jets + H	all	N+S
JES	all	all	N+S
b -tagging b -jets	all	all	N+S
b -tagging c -jets	all	all	N+S
b -tagging l -jets	all	all	N+S
Modelling Systematic Uncertainties			
Cross-section and acceptance	W +jets	all	N
QCD Modelling Scale	V +jets	all	N+S
Parton shower model	$t\bar{t}$	all	N+S
Matrix element calculation	$t\bar{t}$	all	N+S
ISR/FSR	$t\bar{t}$	all	N+S
Acceptance	ggF	all	N*
NLO EW corrections	VBF + VH + $t\bar{t}H$	all	N*
Spurious signal	H	p_T^H bins	N*
	Z +jets**	p_T^Z bins	N*

for such uncertainties is a common subject of debate between particle physicists, however the $H(\rightarrow b\bar{b}) + j$ analysis, as many others, choose to symmetrise these uncertainties to allow for a continuous likelihood description. The symmetrisation is done by creating a -1σ variation (σ^-), of the uncertainty template from the nominal process template N and the $+1\sigma$ variation (σ^+) using the following logic:

$$\begin{aligned}\sigma^+ &= N + \Delta \quad \text{and} \quad \sigma^- = N - \Delta, \\ &\text{which leads to} \\ \Delta &= N - \sigma^+ \quad \text{and} \quad \sigma^- = 2N - \sigma^+.\end{aligned}$$

The uncertainty-to-nominal ratios were smoothed using a custom algorithm to mitigate effects of low statistics in the MC samples, discussed in section 7.5. Small uncertainties, with $< 2\%$ differences between them and their nominal process have been removed following studies described in section 7.6. External constraints for V boson JMR uncertainties were derived and included in the likelihood description as described in section 7.7.

7.4 Tools to Study Uncertainties

Systematic uncertainty studies in this analysis often used a set of common “tools”. As well as the indicators described further, fit parameter correlations and various comparisons of fit results were utilised.

Nuisance Parameter Pulls and Widths:

One of the most commonly used indicators was a nuisance parameter (NP) *pull*:

$$\text{pull} = \frac{\hat{\theta} - \theta_0}{\sigma} \tag{7.2}$$

where $\hat{\theta}$ and θ_0 are the post-fit and pre-fit values of the NP, and σ is the size of the pre-fit uncertainty on the NP in the direction of the pull⁹. Most NPs in the analysis

⁹ In NP pull plots σ is referred to as $\Delta\theta$, which is a common notation.

described systematic uncertainties, where $\theta_0 = 0$, such that a nominal description of a process is initially preferred, and $\sigma = \pm 1$.

A NP pull quantifies how significantly the data prefers the systematic uncertainty description compared to the nominal description. For example, a $+1\sigma$ pull of the Higgs boson JMR uncertainty would mean that the data prefers the Higgs boson estimate to take the form of the $+1\sigma$ variation of the Higgs boson JMR uncertainty, as opposed to the nominal description.

The fits are also able to use data and the correlations between the fit parameters to change (usually constrain) the uncertainties on the NPs. This is called *profiling*. An analyst should be aware of exceptional features in the post-fit sizes (widths) of the NP uncertainties¹⁰, such as strong constraints, large asymmetry, or *under-constraints* - uncertainties determined to be larger than the estimate (post-fit width $> \pm 1\sigma$). Examples of plots showing uncertainty pulls and widths will be seen in the following section, e.g. figure 7.5.

Nuisance Parameter Impact Ranking:

The parameters in the fit naturally correlate - i.e. a change in one parameter induces a change in another. Quantifying how much a given uncertainty affects a parameter of interest, such as the Higgs boson signal strength μ_H can indicate which uncertainties are important and need to be investigated more thoroughly, or point to biases in the model. To do this, as well as observing parameter correlations, the studies quantified and observed nuisance parameter impact.

The impact of a nuisance parameter θ_i on a parameter of interest μ is quantified by fixing θ_i to its $\pm 1\sigma$ values, rerunning the fit, and observing the resulting changes in μ :

$$\text{impact} = \frac{\mu(\theta_i^{\text{fixed}}) - \hat{\mu}}{\hat{\mu}}, \quad (7.3)$$

¹⁰ As most NPs described systematic uncertainties, i.e. $\theta = \pm 1$ when $\sigma = \pm 1$, the widths of the NP uncertainties are commonly referred to as *NP widths* throughout this thesis.

where $\hat{\mu}$ is the best-fit value of μ from the full likelihood model, and $\mu(\theta_i^{\text{fixed}})$ is the best-fit value of μ in the model where the NP in question is fixed. An example of a nuisance parameter ranking plot can be seen in figure 8.2.

7.5 Smoothing of Systematic Uncertainty Templates

All studies shown in this section have been produced before a late-stage update to $t\bar{t}$ modelling uncertainties, and using 0.5 GeV binning in the signal regions. Neither of these changes altered the outcome of the discussed studies. The smoothing procedure, and effects before and after the procedure are shown using uncertainty variations as examples. Below are the most commonly described uncertainties in this section and their relative size:

<i>Label</i>	<i>Source</i>	<i>Size</i>
JMR	– jet mass resolution	large
JMS_	– jet mass scale:	
_Modelling	– nominal vs. alternative MC generators	large
Tracking[1-3]	– various tracking-related uncertainties	moderate
JES_	– jet energy scale:	
_EffectiveNP_R10_	– central region calibration, $ \eta < 0.8$	
_Modelling[1-4]	– Nominal vs. alternative MC generators	small
Flavor	– quark vs. gluon modelling	
_Response	– quark and gluon jet response modelling	small

The labels and descriptions of all uncertainties included in the fits are given in appendix G.1.

As discussed previously, the measurement fit was performed as a simultaneous fit across the candidate jet mass (m_{jet}) spectra in two signal regions (SRL and SRS) and a $t\bar{t}$ control region ($\text{CR}_{t\bar{t}}$)¹¹. The estimates describing the resonant processes and their associated uncertainties were included in the model as mass *templates* –

histograms of the m_{jet} spectra. Each uncertainty was described by two histograms representing the $+1\sigma$ and -1σ variations.

Like the nominal process estimates, the uncertainty templates were derived from MC simulations and have MC statistical fluctuations from the generation process. These MC statistical uncertainties (on uncertainties) were not included in the model, i.e. the fit assumed there were no statistical variations on the uncertainty descriptions. At best, this can add noise to the model, and at worst, as will be seen in this section, it can distort the uncertainty shape and induce biases in the fit model.

In this analysis, large MC statistical fluctuations were observed in all investigated regions. Example comparisons of Higgs boson and $t\bar{t}$ nominal templates and variations of their `JES_Tracking_1` uncertainties are shown in figure 7.4. Statistical fluctuations can be seen in both examples. The Higgs boson example (left), shows that the issue was pertinent when a 0.5 GeV binning was used in the signal regions¹². However, even for templates with relatively high statistics, such as $t\bar{t}$ in the inclusive $\text{CR}_{t\bar{t}}$ region, statistical fluctuations can be observed in the high mass regions where statistics were low.

Addressing this issue by adding the descriptions of the MC statistical uncertainties for each systematic uncertainty would immensely complicate the model and was not considered as a viable option. However the statistical effects can be mitigated by smoothing the ratio between the uncertainties and their nominal templates, in effect smoothing the statistical fluctuations between them. For simplicity this is called the *smoothing of systematic uncertainties*, and uncertainties derived from the

¹¹ The signal regions were: SRL and SRS, i.e. leading and subleading candidate signal regions, and a $t\bar{t}$ control region $\text{CR}_{t\bar{t}}$. The inclusive and fiducial measurements were made over the three regions, whereas in the differential measurement the regions were split into p_T^{jet} bins, resulting in 8 regions in total (5 SR + 3 $\text{CR}_{t\bar{t}}$), and the signal estimate was separated in p_T^{truth} bins. More information on the measurements can be found in section 5.5.

¹² The final measurements were made using 5 GeV binning in the signal regions, however, as the comparisons were made using the same 0.5 GeV binning in all cases, and the impact studied in inclusive signal regions was seen to be small, this did not invalidate the conclusions of the studies. See section 5.7.1 for more details on the binning, and appendix H.1 for the study on the impact of this change.

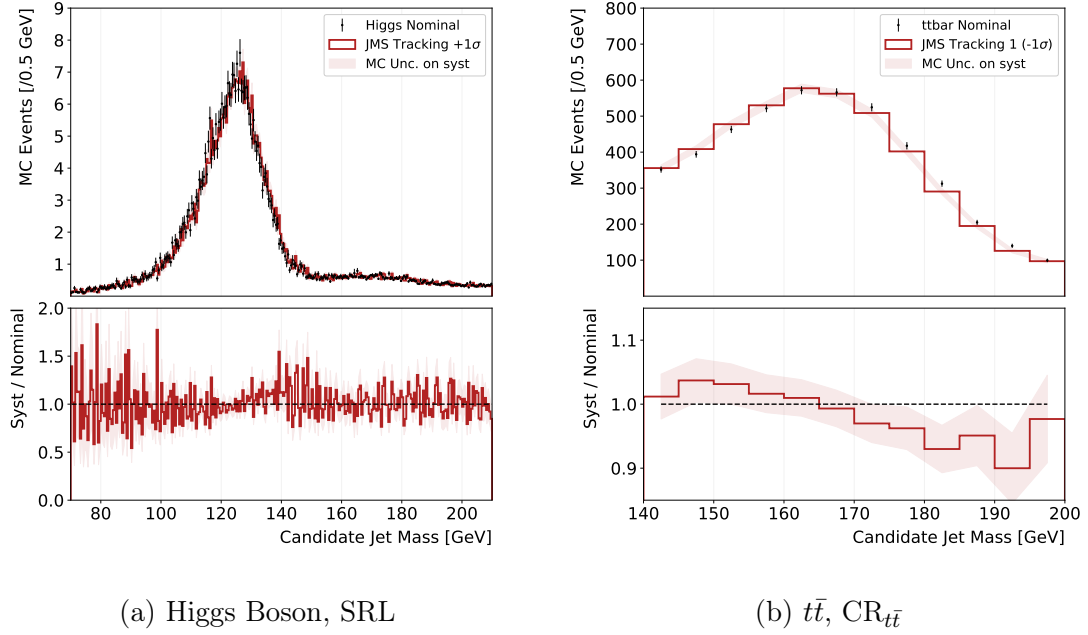


Figure 7.4: Comparisons of the nominal templates of (a) the Higgs boson in SRL, and (b) $t\bar{t}$ in $CR_{t\bar{t}}$, with corresponding `JMS_Tracking_1` uncertainty templates. (a) shows a $+1\sigma$ variation and (b) shows a -1σ variation of the uncertainty. The uncertainties on the templates in the plots are MC statistical uncertainties. Issues in the fit can arise, as the fit has no knowledge of the MC statistical uncertainties, and can interpret them as features.

smoothed ratios are called *smoothed uncertainties*.

Unaccounted statistical fluctuations can cause *false constraints* in the fits, if some statistical fluctuations are significant enough to be identified as relevant physical features by the fit. The fit then can pull and profile uncertainties and parameters describing the nominal processes to accommodate such features, making the measurement untrustworthy.

Indications of false constraints were observed both in the early signal region studies and $CR_{t\bar{t}}$ studies, and, over the course of these studies were shown to be due to MC statistical fluctuations. An example of such effects on systematic uncertainties in a standalone $CR_{t\bar{t}}$ 2 ($p_T^{\text{jet}} \in [650, 1000]$ GeV) fit¹³ are shown in figure 7.5.

¹³ The high p_T^{jet} bin is a good example due to low statistics, similar effects were seen in other bins as well.

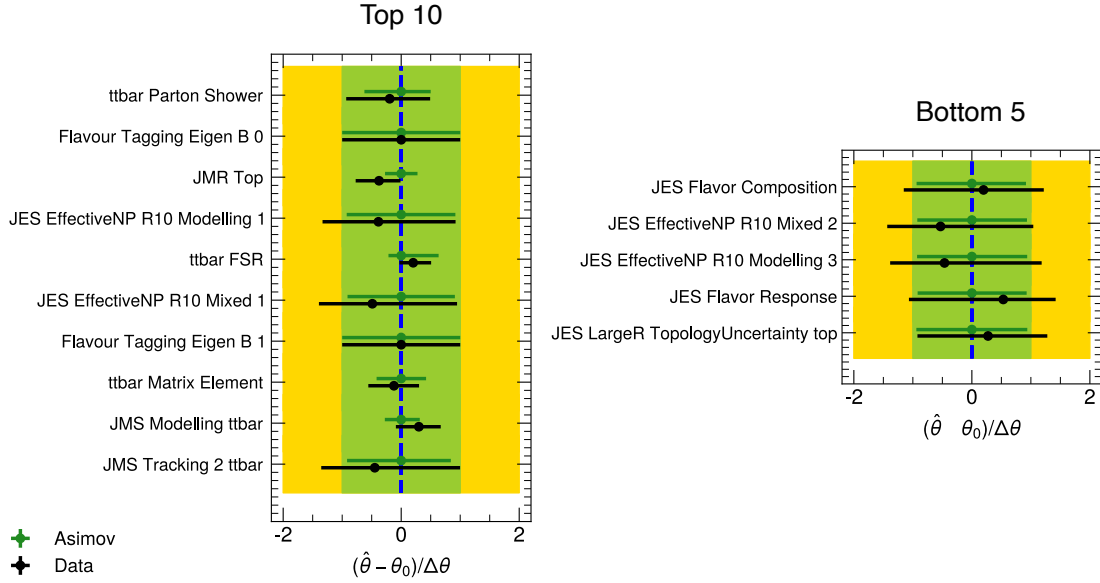


Figure 7.5: The post-fit pulls and width of the 10 highest ranking and 5 lowest ranking uncertainties from standalone $\text{CR}_{t\bar{t}} 2$ ($p_T^{\text{jet}} \in [650, 1000]$ GeV) fits to Asimov and real data, without systematic uncertainty smoothing. The uncertainties are shown in order of post-fit impact to $\text{SF}_{t\bar{t}, b2}$, highest-to-lowest shown top-to-bottom. The labels and descriptions of all uncertainties included in the fits are given in appendix G.1. The under-constraints and strong pulls of low impact uncertainties were indicative of possible bias in the fit.

The false constraints manifested in several ways. In both Asimov¹⁴ and data fits some uncertainties were *over-constrained*, i.e. the constraints were stronger than they would be in an unbiased fit. However, this was difficult to identify initially as the $\text{CR}_{t\bar{t}}$ region was expected to have the ability to strongly constrain large uncertainties, due to its purity. It will be shown later (in figure 7.9), when the fit results with and without the smoothing are compared, that several uncertainties shown in figure 7.5, such as $t\bar{t}$ final state radiation (FSR), or `Matrix_Element` and `Parton_Shower` modelling uncertainties were over-constrained.

A better initial indicator of false constraints was the presence of *under-constrained*

¹⁴ Asimov data is an idealised dataset, built from the model itself, providing the expected results and sensitivity of the measurement. Described in section 5.7.2.

uncertainties, i.e. uncertainties estimated to be larger than $\pm 1\sigma$. To a small extent, such effects can arise in complex models, however large and prominent under-constraints were a clear sign of issues, such as the fit attempting to compensate for over-constraints in some uncertainties by “extending” other ones. In figure 7.5, such features were seen in the sizes of `JES_R10_Modelling_1/3`, `JES_R10_Mixed_1/2`, `JES_Flavour_Composition`, and `JMS_Tracking_2` uncertainties.

Furthermore, low-impact uncertainties were not expected to display large pulls or profiling, as the data should not have had strong discriminating power over small uncertainties. Most uncertainties shown in the right panel of figure 7.5, display such features. All of the discussed behaviour was worrisome, and required investigation. It was understood that such effects could be caused by MC statistical fluctuations, so a smoothing procedure was implemented and applied.

7.5.1 The Smoothing Method

The smoothing procedure relied on re-binning the systematic-to-nominal template ratios to variable-size bins according to the MC statistical uncertainties, such that a coarse smooth ratio was achieved. The procedure was as follows:

1. if the bin width is < 5 GeV, re-bin all templates to 5 GeV bins;
2. take the ratio between the nominal template and the systematic uncertainty;
3. re-bin the ratio to variable-sized bins;
4. fit a spline to the variably-binned ratio;
5. return to the original binning by sampling the spline;
6. multiply a copy of the nominal template by the smooth ratio to get a new systematic uncertainty template.

The smoothing procedure was applied to templates with a wider mass range to ensure that spline effects on the boundaries did not impact the end result. As the splines were fit through the centres of the bins, a boundary condition was applied by setting values at the boundaries to the nearest bin centre values. Cubic splines

were used, quintic splines were also tested and made no visible differences to the shapes.

The variable binning proceeded by merging bins left-to-right until the relative statistical uncertainty in the bin passed a threshold (t),

$$\frac{\sigma_r}{r} < t, \quad (7.4)$$

where r and σ_r were the ratio value and statistical uncertainty in the bin. When bins were merged, the new ratio value in the bin was calculated as:

$$r_{\text{merged}} = \frac{\sum (r y_{\text{nom}})}{\sum y_{\text{nom}}}, \quad (7.5)$$

where y_{nom} is the value of the nominal process m_{jet} template in the corresponding bin. This retains the values of the original ratio, as $\sum (r y_{\text{nom}}) \equiv \sum y_{\text{syst}}$.

By performing the variable binning directly on the ratio, both MC statistical uncertainties on the nominal template and the systematic uncertainty variation were taken into account. Examples of variably-binned ratios, splines, and comparisons of the original and smoothed ratios, are given in figure 7.6. The variably-binned ratio templates, shown in figures 7.6a and 7.6c were shown to retain the general features of the distributions. How well the features are retained depends on the smoothing threshold, which is an optimised parameter, discussed in the following section. The splines, shown in the same figures, were seen to fit the coarsely binned templates well, and produce smooth ratio distributions. The comparisons between the smooth and the original ratios are shown in figures 7.6b and 7.6d. The smooth ratios were seen to smoothly describe the features of the original ratios within the MC statistical uncertainties and mitigate unwanted fluctuations.

The Smoothing Threshold

It was important that the smooth ratios agreed well with the original ratios, such that no possible physical features were overlooked. The optimisation process iterated on small threshold differences of 0.5%, however, even under such slight variations,

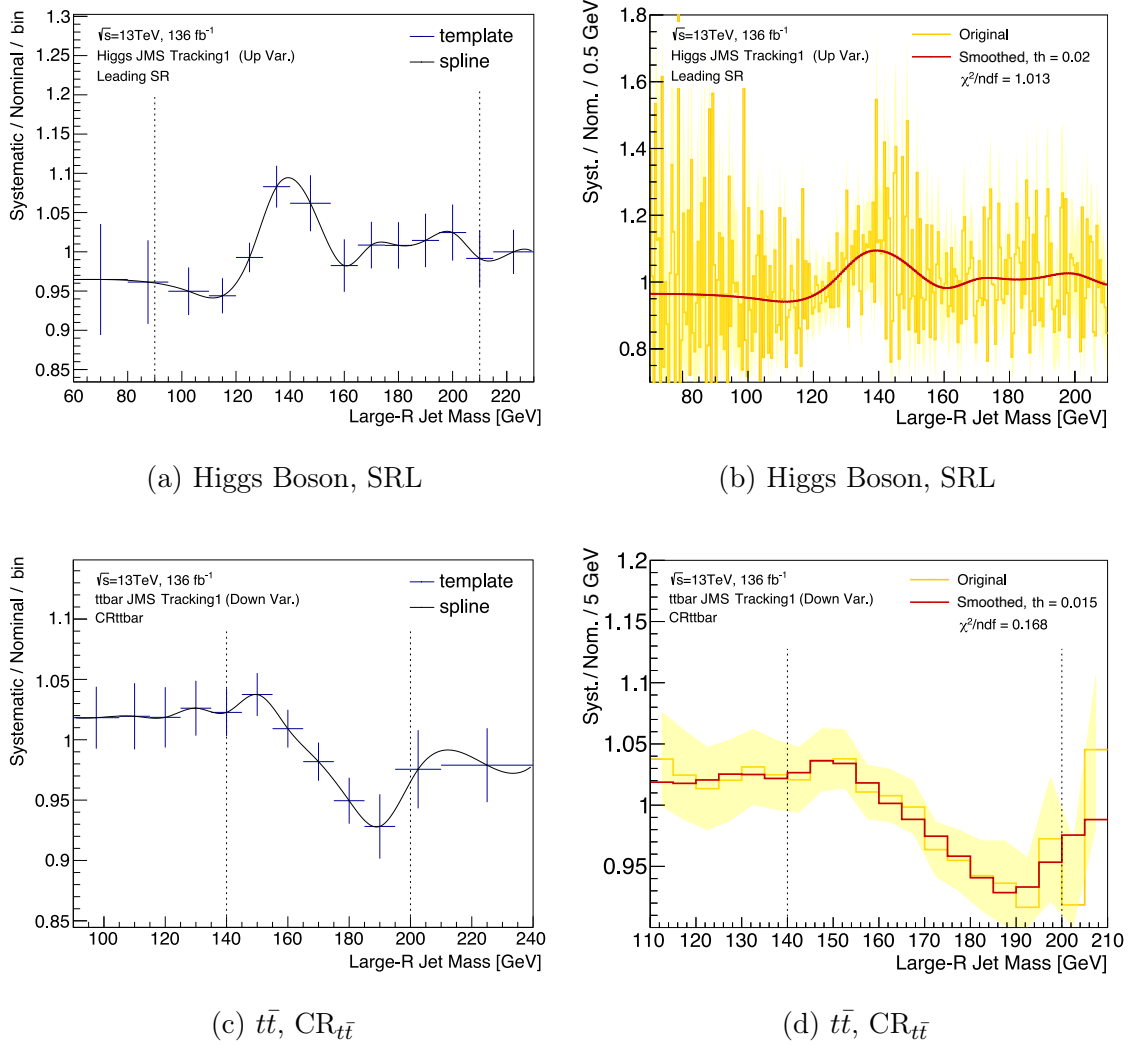


Figure 7.6: Plots illustrating the systematic uncertainty smoothing procedure using the JMS_Tracking_1 uncertainty of (top) the Higgs boson in SRL, and (bottom) $t\bar{t}$ in $CR_{t\bar{t}}$; (Left) variable-bin templates of the uncertainty-to-nominal m_{jet} template ratios and cubic splines fitted to them; (right) comparisons of the smoothed and original uncertainty-to-nominal ratios of the same distributions.

a flat, $t = \text{const.}$, threshold was found to be difficult to optimise, and the resulting shapes did not describe the ratios to a satisfactory standard. Figure 7.7a shows a comparison between the original uncertainty-to-nominal ratio and smoothed ratios produced using constant thresholds of 4.5%, 5% and 5.5% of the top-quark JMR uncertainty in the $CR_{t\bar{t}}1$ region ($p_T \in [450, 650]$ GeV), which illustrates the optimisation difficulties described next.

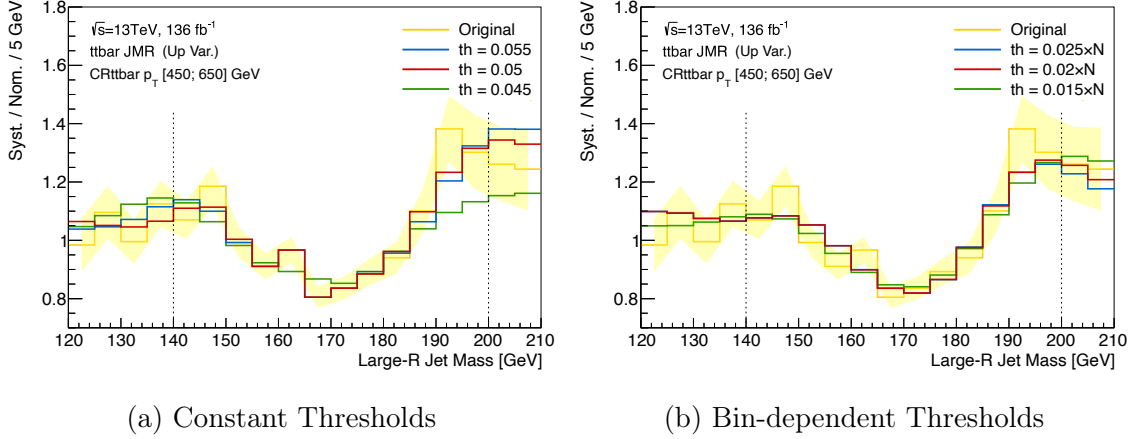


Figure 7.7: Comparisons of the smoothed and original uncertainty-to-nominal ratios of Top JMR uncertainty in the $CR_{t\bar{t}}$ region ($p_T \in [450, 650]$ GeV) with (a) constant, $t = \text{const.}$, and (b) bin-dependent, $t = cN_{\text{bins}}$, smoothing thresholds. The vertical lines indicate the $CR_{t\bar{t}}$ fit range.

It can be seen that even slight differences in the threshold lead to significantly different effects. The tighter (smaller) threshold tended to aggressively merge bins and lead to significant discrepancies between the smooth and original ratios, whereas slightly looser thresholds began retaining fluctuations in the regions around the peak of the resonance¹⁵ (where a smooth variation between the nominal process and mass resolution effects would be expected). Such behaviour was observed with many uncertainty ratios, and made a constant threshold difficult to optimise.

The issue was addressed by making the threshold proportional to the number of bins already merged: $t = cN_{\text{bins}}$, which loosened the condition for wider bins. As the initial binning was always set to 5 GeV, this corresponds to a threshold of c for a 5 GeV bin, $2c$ for a 10 GeV bin, etc. Making the threshold bin-dependent allowed for easier optimisation, as the thresholds could be tightened to achieve smooth descriptions, without losing features in regions with low statistics.

Overall, the use of a bin-dependent threshold produced more consistent results

¹⁵ The $t\bar{t}$ resonance peaks at $m_{\text{jet}} \approx 170$ GeV (due to energy losses) and drops relatively promptly beyond this point, see figure D.3 for an example.

as c was varied. Examples of comparisons between the original and smoothed ratios produced with bin-dependent thresholds are shown in figure 7.7b. The comparison shows more consistent descriptions between different threshold values, which were overall smooth and were in good agreement with the original. Such consistency was seen with other uncertainties as well. Because of these improvements a bin-dependent threshold was used in the final uncertainty smoothing procedure.

7.5.2 Threshold Optimisation

The smoothing procedure was applied to all of the systematic uncertainty templates of all processes in the SR and $\text{CR}_{t\bar{t}}$ regions. The optimal constant threshold factors (c in $t = cN_{\text{bins}}$) were determined for each process in each region separately. Henceforth c will be referred to as the *threshold* for simplicity.

The thresholds were optimised by comparing uncertainty ratio shapes of high-impact uncertainties (JMR, JMS and generator uncertainties) with $\pm 0.5\%$ increments in c . Once a preferred threshold was determined, all uncertainty templates were inspected to ensure good agreement with the original ratio. The tightest possible thresholds which did not result in significant discrepancies (with regards to the MC statistical uncertainty on the ratio) between the smooth and original ratios were regarded as the *optimal thresholds* as they would be expected to provide the smoothest acceptable description.

Examples of the smoothed template ratios inspected during the optimisation process are shown in figures 7.8a and 7.8b. The former compares $c = 1\%$, 1.5% and 2% for the $t\bar{t}$ process in the inclusive $\text{CR}_{t\bar{t}}$ region, and the latter compares $c = 1.5\%$, 2% and 2.5% for the Higgs boson process in the inclusive SR region. The middle values ($c = 1.5\%$ for $t\bar{t}$, and $c = 2\%$ for the Higgs boson) were the optimal thresholds.

In both examples good agreement can be seen between the ratios produced with the chosen (red) and the original ratios. Good agreement was also seen between

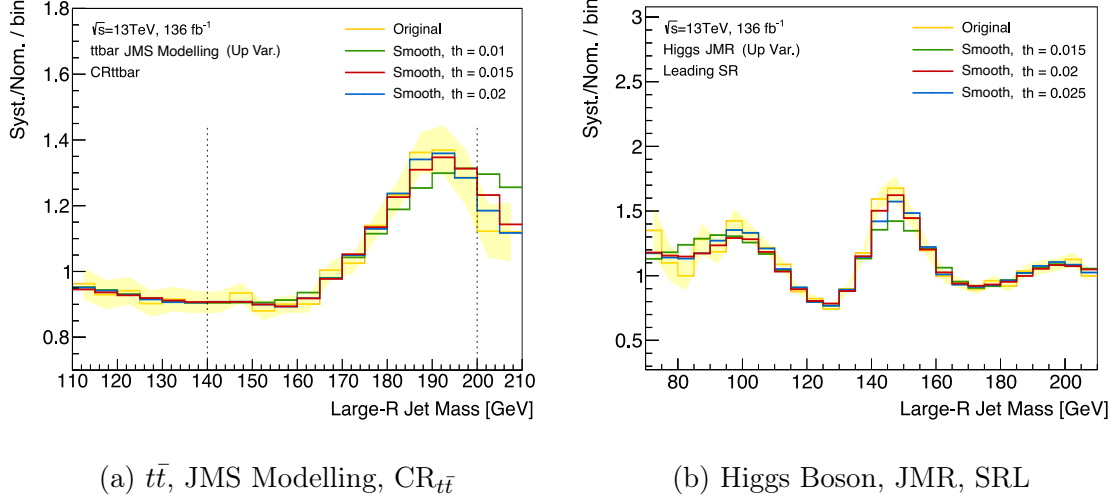


Figure 7.8: Comparisons of the smoothed and original uncertainty-to-nominal ratios of (a) $t\bar{t}$ JMS_Modelling + 1σ variation in $CR_{t\bar{t}}$, and (b) Higgs boson JMR + 1σ variation in SRL, with $c_{\text{chosen}} \pm 0.5\%$ smoothing threshold factors (c in $t = cN_{\text{bins}}$). The distribution produced with the chosen threshold factor is shown in red. The vertical lines in (a) indicate the $CR_{t\bar{t}}$ fit range.

the original ratio, and the ratios produced with the chosen (red) and the looser threshold (blue), showing consistency in the procedure, and supporting the validity of the threshold chosen to be optimal. Lastly, the ratios produced with a slightly tighter threshold (green) were seen to deviate from the original shape, as is expected by design of the optimisation procedure. Later this will be referred to as “over-smoothing”. Such threshold comparisons were observed for in high impact uncertainty distributions, until a preferred threshold was determined. The agreement was confirmed in all uncertainty ratios before finalising the threshold choice.

The author optimised the smoothing thresholds in all $CR_{t\bar{t}}$ regions, inclusive SRL, SRL regions, and p_T^{jet} binned SR regions for the Z boson differential measurement. The thresholds for the Higgs boson differential measurement were optimised by other members of the analysis team using the same methodology and technical implementation. The final threshold values are given in table G.2 in appendix G.5.

The impact of small and large threshold variations using a high statistics sample was studied to evaluate the stability and behaviour of the procedure. These studies

were made in inclusive $\text{CR}_{t\bar{t}}$ data, and are presented in appendix G.6. The procedure was seen to be stable. Differences between small changes in threshold were seen to be minor, whereas, a significant loosening of the threshold shows stronger similarities with a non-smoothed fit.

7.5.3 The Impact of Smoothing Systematic Uncertainties

The impact of systematic uncertainty smoothing was studied in the $\text{CR}_{t\bar{t}}$ regions which allowed the use of real data, where uncertainty constraint effects tend to be more prominent.

The smoothing procedure was applied on the systematic uncertainty templates before the uncertainty reduction procedure – *pruning* (described in section 7.6), such that the pruning conditions were applied on the smooth uncertainties. As a result, more uncertainties were pruned due to reduced differences between the nominal and uncertainty templates, simplifying the models. For example, an additional 12% – 29% of systematic uncertainty descriptions were pruned from the inclusive and differential $\text{CR}_{t\bar{t}}$ regions. The number of additionally pruned uncertainties was larger in the regions with lower MC statistics, which indicated that the smoothing procedure was fulfilling its purpose of reducing differences of statistical nature.

Biases in the model descriptions were probed by comparing the fit results found in Asimov fits (expectations) to those found in data. Using a well-behaved model was expected to yield similar results. As the Asimov fits always yield $\text{SF}_{t\bar{t}} = 1$, and the measurements in data fluctuated around $\text{SF}_{t\bar{t}} \approx 0.8$, the scaling differences were accounted for by rescaling σ_{data} as

$$\sigma_{\text{data}}^{\mu=1} = \frac{\sigma_{\text{data}}}{\text{SF}_{t\bar{t}}}. \quad (7.6)$$

The results were compared using a relative difference:

$$\frac{\sigma_{\text{data}}^{\mu=1} - \sigma_{\text{Asimov}}}{\sigma_{\text{Asimov}}}. \quad (7.7)$$

Table 7.3: Relative differences (equation 7.7) between $SF_{t\bar{t}}$ uncertainties in Asimov and real data fits in all $CR_{t\bar{t}}$ regions, with and without systematic uncertainty smoothing. Data uncertainties were rescaled to be equivalent to $SF_{t\bar{t}} = 1$, as described in equation 7.6. The differential measurement regions were defined in candidate jet p_T bins: $250 \text{ GeV} < B0 < 450 \text{ GeV} < B1 < 650 \text{ GeV} < B2 < 1 \text{ TeV}$.

	Inclusive	B0	B1	B2
Not Smoothed	11.9%	12.7%	16.0%	13.3%
Smoothed	3.0%	3.6%	0.7%	2.8%

The relative differences between total uncertainties from data and Asimov fits in $CR_{t\bar{t}}$ regions, with and without systematic uncertainty smoothing are shown in table 7.3. With the application of systematic uncertainty smoothing the agreement was better in all $CR_{t\bar{t}}$ regions, with differences ranging between $1\% - 4\%$ as opposed to $12\% - 16\%$. This was a clear indication that the smoothing improved the model description, resulting in better agreement between expected and observed results.

Uncertainty Behaviour

Examples of the candidate jet mass (m_{jet}) distributions of uncertainties discussed throughout this section can be found in figure G.5 in appendix G.3.

With the implementation of the systematic uncertainty smoothing, the alarming features in systematic uncertainty pulls and sizes, such as those seen in the standalone $CR_{t\bar{t}2}$ fit in figure 7.5, were mitigated. A comparison of the post-fit pulls and sizes of the systematic uncertainties with and without smoothing from the same fit (standalone $CR_{t\bar{t}2}$) are shown in figure 7.9. With the implementation of systematic uncertainty smoothing the expected (found in Asimov data) and measured (in real data) uncertainty sizes became more consistent, and no significant under-constraints were observed. Fewer significant pulls were seen, with none present amongst the low ranking uncertainties, which were all points of concern, discussed earlier in the section.

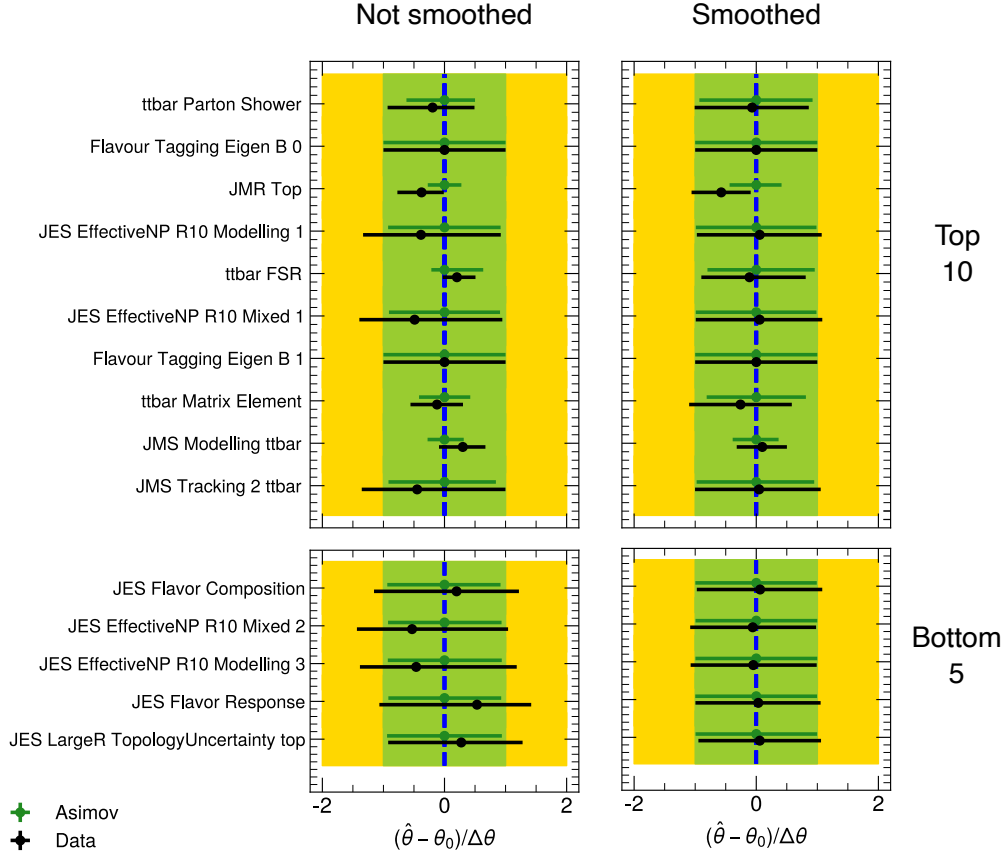


Figure 7.9: The post-fit pulls and width of the 10 highest ranking and 5 lowest ranking uncertainties from standalone $\text{CR}_{t\bar{t}}^2$ ($p_T^{\text{jet}} \in [650, 1000]$ GeV) fits to Asimov and real data, with and without systematic uncertainty smoothing. The uncertainties are shown in order of post-fit impact to $\text{SF}_{t\bar{t}, b2}$, highest-to-lowest shown top-to-bottom. The labels and descriptions of all uncertainties included in the fits are given in appendix G.1. After smoothing is introduced, the results in data are seen to agree better with expectations from the Asimov fit; and issues such as under-constraints, and pulls of low-impact uncertainties were mitigated.

The comparison in figure 7.9 also shows that some of the high-impact uncertainties which were strongly constrained beforehand, such as **FSR** (final state radiation modelling), and **Matrix_Element** and **Parton_Shower** modelling uncertainties¹⁶,

¹⁶ To a smaller extent this was also true for **JMR** and **JMS_Modelling** uncertainties. Note that the strong constraints of these uncertainties were not alarming, as they were some of the largest uncertainties under consideration, derived in general purpose calibrations. The statistical precision of the targeted $\text{CR}_{t\bar{t}}$ region was larger than these uncertainties, and sufficient to significantly constrain them.

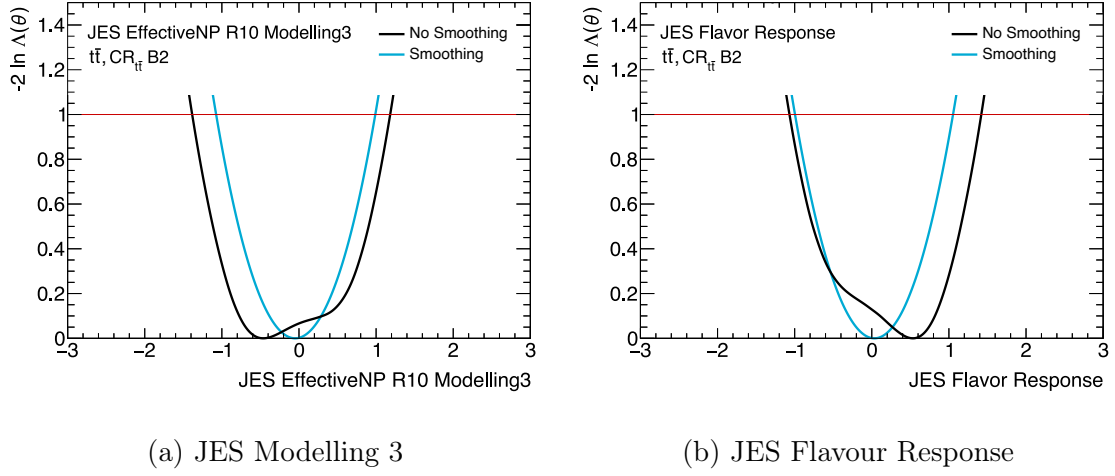


Figure 7.10: Profile likelihood scans of $t\bar{t}$ (a) `JES_Modelling_3` and (b) `JES_Flavour_Response` uncertainties in standalone fits to $CR_{t\bar{t}2}$ data. The minimum corresponds to best-fit value of the uncertainty ($\hat{\theta}$), and the θ values at $-2 \ln \Lambda(\theta) = 1$ correspond to the width of the uncertainty ($\pm 1\sigma$).

showed significantly reduced constraints after the smoothing. This, in context of other improvements, was seen as further evidence that the effects were caused by the fit interpreting statistical fluctuations as features and using them to falsely constrain the uncertainties, in particular as the agreement between the fit results in data and Asimov data was seen to be improved. Overall, all points of concern were mitigated with the implementation of the systematic uncertainty smoothing. The same behaviour was observed in the other investigated regions.

A closer look at the changes in the uncertainty treatment with the introduction of smoothing was provided by the *profile likelihood* of the uncertainties. The profile likelihood of a parameter θ is the distribution of the maximum likelihood values evaluated at different values of θ . Figure 7.10 shows the profile likelihoods¹⁷ for two low-impact uncertainties – `JES_Modelling_3` and `JES_Flavour_Response`, from standalone $CR_{t\bar{t}2}$ data fits with and without uncertainty smoothing, which

¹⁷ The *profile likelihood* of θ is described in terms of a negative log likelihood ratio between the likelihood evaluated at different values of θ ($\mathcal{L}(\theta)$), and the maximum likelihood estimate ($\mathcal{L}(\hat{\theta})$): $-2 \ln \mathcal{L}(\theta)/\mathcal{L}(\hat{\theta})$. Because a negative log expression is used, the best-fit value of θ is at the *minimum* of the distribution.

illustrate one of the key improvements introduced by the uncertainty smoothing.

In a simple $\text{CR}_{t\bar{t}}$ fit with only one process which was allowed to vary, the profile likelihoods for all parameters would *a priori* be expected to be parabolic. This was especially true for small uncertainties, as the data was not expected to have enough statistical power to constrain them. However, without the uncertainty smoothing, the shown uncertainties, and many others (mostly those which were seen to be under-constrained) displayed non-parabolic likelihood shapes.

Both profile likelihoods in figure 7.10 show strong pulls and non-parabolic “shoulders”. As these uncertainties were small, such profile likelihood features were unlikely to be due to real features of the uncertainties, and were more consistent with noise in the uncertainty shape, leading to artificial pulls of the nuisance parameter to compensate for differences between the model and data.

With the introduction of uncertainty smoothing all uncertainties were seen to have parabolic profile likelihoods. This indicated that the effects were introduced by the statistical differences in the nominal and systematic uncertainty templates. The parabolic profile likelihoods of nuisance parameters, observed after the introduction of uncertainty smoothing were seen as an improvement in the fit model.

7.5.4 Section Summary

Limited statistics of the MC simulations used in the measurement were seen to cause fluctuations in the ratios of the nominal processes and their systematic uncertainties, which were seen to bias the fits. Including MC statistical uncertainties into the fit model would have been unfeasible, so a procedure to smooth the ratios of m_{jet} distributions of uncertainties and their nominal processes was developed, called *systematic uncertainty smoothing*. This section discussed the implementation, impact and validation of the uncertainty smoothing. The smoothing was shown to mitigate the observed alarming fit result features seen without the smoothing.

A step-by-step description of the smoothing procedure, which relies on merging bins with low relative statistical uncertainties, was given. It was shown that the use of a constant smoothing threshold ($\sigma/y > t = \text{const.}$) resulted in smoothed distributions which were either incompatible with the original, or not smooth enough, so a more flexible bin-dependent threshold was used.

The implementation of the smoothing procedure was shown to greatly improve the consistency between the expected and observed results, and uncertainty pulls and sizes. The alarming features indicative of false constraints, such as under-constrained uncertainties and significant effects on low-impact uncertainties, were seen to be mitigated. Without the smoothing procedure, some uncertainties displayed non-parabolic profile likelihoods, indicating of tensions which were unlikely to be present in a simple fit. After the implementation of smoothing the profile likelihoods of all nuisance parameters were seen to be parabolic.

Strong constraints on several high-impact uncertainties were also reduced. In the context of all other findings, this was likely caused by the fit interpreting MC statistical fluctuations as physical features of uncertainties, which the fit would use to further constrain large uncertainties. Overall, the implementation of the systematic uncertainty smoothing procedure was vital for the analysis, as artificial constraints rising from statistical noise in the simulated samples could have significantly biased the final measurement.

7.6 Pruning of Systematic Uncertainties

This analysis considered a huge number of systematic uncertainties for all major resonant processes involved in the measurement. If all uncertainty descriptions¹⁸ (u.d.) were included, the standalone $\text{CR}_{t\bar{t}}$ fit would have had 49 u.d., the inclusive

¹⁸ For example, the top-quark JMR uncertainty had 1 description in a $\text{CR}_{t\bar{t}}$ standalone fit, 3 – in an inclusive measurement fit, and 8 – in a differential measurement fit (1 for each process ($t\bar{t}$), in each region it was included, not counting yield and shape components separately).

measurement¹⁹ fit would have had 419 u.d., and the differential measurement fit would have had 1116 u.d..

Many of the considered systematic uncertainties were small, and were not expected to have a large impact on the fit results. A procedure was developed to remove – *prune* – such uncertainties from the fit model, to reduce its complexity and computation time. The latter aspect was particularly important after the move from using a coarser 5 GeV binning in the signal regions²⁰, as the fit became much slower due to the software feature allowing the use of coarser bins.

A comparison performed by another member of the analysis team showed that without uncertainty pruning, the inclusive measurement fit took around 11 h to process, whereas with the pruning procedure, as optimised by the presented studies, the processing time was reduced to ~ 2 h. The improvement was even more important for the differential measurement fit, which, without pruning, took around 160 h (6.6 days) to process. When pruning was applied using the optimised thresholds, the computation time of the differential measurement fit was reduced to around 50 h (2.1 days), which was more feasible for studies.

The thresholds imposed by this procedure were optimised such that the removal of small uncertainties would not impact the fit results, or pulls and profiling of high-impact uncertainties.

The Pruning Procedure

In the model description, the uncertainty descriptions were decomposed into yield and shape components²¹. Therefore, two separate pruning procedures were implemented. *Yield pruning* imposed a minimum threshold (α_Y) on the relative difference

¹⁹ *Reminder:* the inclusive measurement fit consists of three regions fit simultaneously: SRL, SRS and $\text{CR}_{t\bar{t}}$; and the differential measurement fit consists of 8 regions binned in jet p_T : SRL 1/2, SRS 0/1/2, $\text{CR}_{t\bar{t}}$ 0/1/2. The measurements are defined in section 5.5.

²⁰ See section 5.7.1 for more details on the binning.

²¹ Described in section 7.3.

between the yield (Y) of the uncertainty (θ) and the nominal process:

$$\max \left[\frac{|Y_{+\theta} - Y_{\text{nom}}|}{Y_{\text{nom}}}, \frac{|Y_{-\theta} - Y_{\text{nom}}|}{Y_{\text{nom}}} \right] > \alpha_Y, \quad (7.8)$$

where $\pm\theta$ indicate the $\pm 1\sigma$ variations of the uncertainty.

The shape components of uncertainties were each described by two histograms ($\pm 1\sigma$) of the m_{jet} spectra, (called *mass templates*). The *shape pruning* imposed a minimum threshold α_S on the largest relative shape difference between the mass template of the uncertainty and the nominal process. First, the templates were normalised to an integral of 1 to isolate the shape components. Then the threshold was imposed as such:

$$\max_{i \in N} \left[\frac{|y_i^{+\theta} - y_i^{\text{nom}}|}{y_i^{\text{nom}}}, \frac{|y_i^{-\theta} - y_i^{\text{nom}}|}{y_i^{\text{nom}}} \right] > \alpha_S, \quad (7.9)$$

where N is the set of all bins in the m_{jet} template, and y_i is the normalised template yield in the i^{th} bin of the template. The pruning was applied separately, such that an uncertainty with a pruned yield component could enter the model as a shape-only uncertainty and vice versa.

The threshold values were optimised for each region. The following section describes the optimisation studies for the $\text{CR}_{t\bar{t}}$ region, performed by the author. The optimisation procedure developed by the author in $\text{CR}_{t\bar{t}}$, was later applied by other members of the analysis to optimise the pruning thresholds for the inclusive and differential signal regions.

For simplicity, the same threshold was applied for both yield and shape components ($\alpha_Y = \alpha_S = \alpha$) and for all processes in a region. The optimisation studies found that a 2% pruning threshold should be applied in all regions ($\text{CR}_{t\bar{t}}$ and SR). Using the finalised pruning threshold scheme, the number of uncertainty descriptions entering the standalone $\text{CR}_{t\bar{t}}$ fit, the inclusive measurement fit, and the differential SR measurement fit were reduced to 14, 152, and 456, respectively, which translates to a 71%, 64%, and 59% reduction to each group.

7.6.1 Pruning Optimisation for $\text{CR}_{t\bar{t}}$

The primary concern of the pruning optimisation studies was to find the largest pruning threshold which did not impact the fit results in any meaningful way. Various aspects of the $\text{CR}_{t\bar{t}}$ fit results produced with different pruning thresholds were compared. The section primarily presents the study of the inclusive $\text{CR}_{t\bar{t}}$ fit, but the same procedure was also used to optimise pruning thresholds for p_T^{jet} binned $\text{CR}_{t\bar{t}}$ regions used in the differential measurement fit. Pruning thresholds from 0.5% to 7% were investigated and results from 1% to 5% are shown for brevity.

The pruning thresholds were optimised by observing the changes in $\text{SF}_{t\bar{t}}$ measurements with varied thresholds. The comparisons were made in reference to a non-pruned model. The pruning effects on fit results were quantified in three aspects²²: the relative change in the measurement uncertainty $\Delta\sigma/\sigma$, the absolute shift in measured $\text{SF}_{t\bar{t}}$ value in terms of significance ($|\Delta\text{SF}_{t\bar{t}}|/\sigma$), and difference in measured $t\bar{t}$ scale factor significance ΔZ ($Z = \text{SF}_{t\bar{t}}/\sigma$). The minimum accepted differences induced by the pruning were defined as: $|\Delta\sigma/\sigma| < 5\%$, $|\Delta\text{SF}_{t\bar{t}}|/\sigma < 0.5\sigma$, and $|\Delta Z| < 0.5\sigma$.

The comparisons of the measurement changes induced by pruning with different thresholds in the inclusive $\text{CR}_{t\bar{t}}$ region are summarised in table 7.4. None of the shown pruning schemes induced significant shifts in the measured $\text{SF}_{t\bar{t}}$ value, showcasing the stability of the measurement. The 5% and 3% pruning thresholds were found to be too harsh, as they induced changes in significance $|\Delta Z| \geq 1.0\sigma$ and in uncertainty reduction $|\Delta\sigma/\sigma| > 8\%$, so a 2% threshold was chosen. A 2% threshold did not significantly affect the measured $\text{SF}_{t\bar{t}}$ value and total uncertainty, while still removing around 71% (35 out of 49) of uncertainty descriptions.

Equivalent comparisons for the p_T^{jet} -binned $\text{CR}_{t\bar{t}}$ regions are given in figure G.5 in appendix G.7. Following the same strategy the largest acceptable thresholds were

²² The differences were quoted between a pruned and a non-pruned model relative to the non-pruned model, e.g.: $\Delta\sigma/\sigma = (\sigma_{\text{prun}} - \sigma_{\text{no prun}})/\sigma_{\text{no prun}}$

Table 7.4: Comparison of $SF_{t\bar{t}}$ values and uncertainties measured in inclusive $CR_{t\bar{t}}$ data using models with different pruning thresholds. $\sigma = \sigma_{\text{total}}$, $Z = SF_{t\bar{t}}/\sigma_{\text{total}}$, NP_{rm} – number of pruned uncertainties (total - 49). All differences are shown in reference to the non-pruned model, such that the sign indicates reduction or increase in relation to it, e.g. $\Delta\sigma/\sigma = (\sigma_{\text{prun}} - \sigma_{\text{no prun}})/\sigma_{\text{no prun}}$. A 2% pruning threshold was chosen, as it did not significantly change the total uncertainty ($|\Delta\sigma/\sigma| < 5\%$), while removing a substantial number of nuisance parameters ($35/49 \approx 71\%$).

Pruning	$\Delta\sigma/\sigma$	$ \Delta SF_{t\bar{t}} /\sigma$	ΔZ	NP_{rm}
$< 1\%$	1.4%	$< 0.1\sigma$	-0.2σ	28
$< 2\%$	-2.1%	0.1σ	0.2σ	35
$< 3\%$	-8.2%	0.1σ	1.0σ	38
$< 5\%$	-21.0%	0.1σ	3.4σ	41

determined to be 3% for the lowest p_T^{jet} bin ($p_T^{\text{jet}} \in [250, 450]$ GeV) and 2% for the medium and high momentum bins. For simplicity, a 2% threshold was used in all regions, which removed 73%, 69% and 61% of uncertainty descriptions from the low, medium and high p_T^{jet} differential $CR_{t\bar{t}}$ regions, respectively. All fit results were also compared using Asimov data, which agreed with the findings in data.

Testing the Uncertainty Features

Changing the uncertainty model of a fit can impact other uncertainties, i.e. other nuisance parameters, as well as the primary parameter(s) of interest. As $t\bar{t}$ uncertainties were correlated between $CR_{t\bar{t}}$ and the signal regions in the measurement fits, it was important to observe any such effects before finalising the chosen threshold.

Figure 7.11 shows the pulls and widths of the 10 highest impact $t\bar{t}$ uncertainties in inclusive $CR_{t\bar{t}}$ data fits with different pruning thresholds. No significant differences were seen up to and including a 2% pruning threshold. Higher thresholds started showing some slight differences in the widths, as well as pruning a high ranking b -tagging uncertainty. These findings supported the choice of a 2% pruned

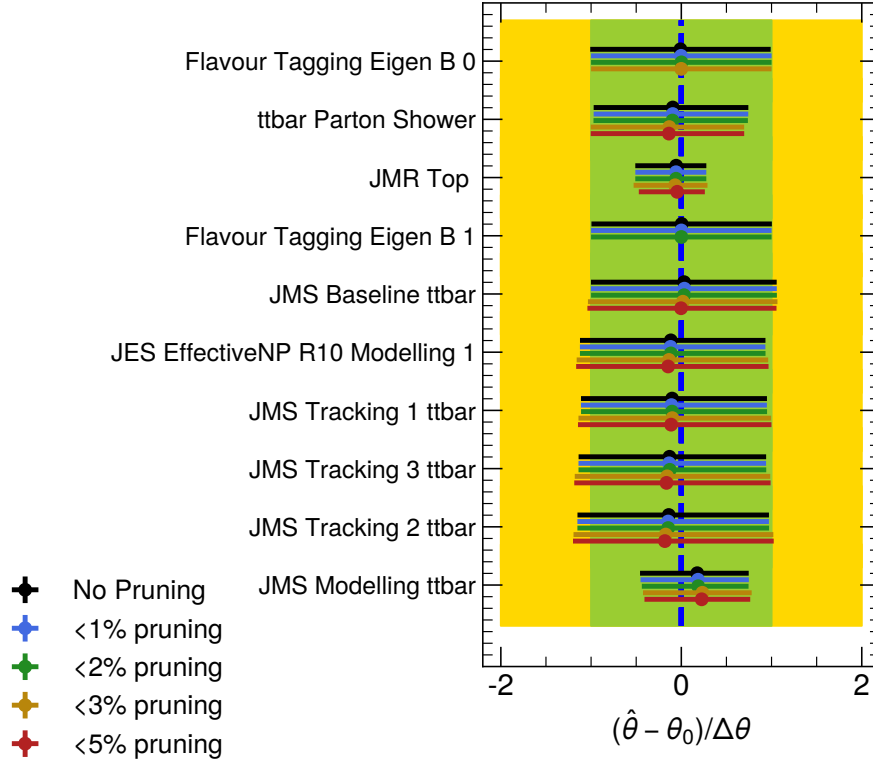


Figure 7.11: Comparison of systematic uncertainty pulls and widths in fits to inclusive $\text{CR}_{t\bar{t}}$ data with progressively tighter systematic uncertainty pruning thresholds. The 10 $t\bar{t}$ uncertainties with the highest impacts to the $\text{SF}_{t\bar{t}}$ measurement are shown in order of post-fit impact: highest-to-lowest shown top-to-bottom.

ing threshold. The same test was conducted in the p_T^{jet} -binned $\text{CR}_{t\bar{t}}$ regions, all of which displayed equivalent features and supported a 2% threshold. The corresponding plots are given in figure G.8 of appendix G.7.

Validation in the Inclusive Measurement Fit

Once a 2% threshold was established as the best choice in standalone fits to $\text{CR}_{t\bar{t}}$, it was tested in the inclusive measurement fit configuration (a simultaneous SRL, SRS and $\text{CR}_{t\bar{t}}$ fit). A 0.5 GeV m_{jet} template binning was used in the signal regions, as was done throughout most of the analysis development.

The differences in the expected μ_H , μ_Z and $\text{SF}_{t\bar{t}}$ uncertainties found using the

Table 7.5: Expected μ_H , μ_Z and $\text{SF}_{t\bar{t}}$ measurements as found from inclusive measurement fits (SRL, SRS and $\text{CR}_{t\bar{t}}$) to Asimov data without pruning, and with a 2% pruning threshold in $\text{CR}_{t\bar{t}}$. Differences are shown in reference to the non-pruned model, such that the sign indicates reduction or increase in relation to it, e.g. $\Delta\sigma/\sigma = (\sigma_{\text{prun}} - \sigma_{\text{no prun}})/\sigma_{\text{no prun}}$.

	Pruning	σ_{stat}	σ_{syst}	$\Delta\sigma$	$\Delta\sigma/\sigma$
$\text{SF}_{t\bar{t}}$	None	0.015	0.069	–	–
	< 2%	0.015	0.068	–0.001	–2.0%
μ_Z	None	0.13	0.10	–	–
	< 2%	0.13	0.10	$< \mathcal{O}(10^{-4})$	0%
μ_H	None	2.5	2.2	–	–
	< 2%	2.5	2.2	–0.01	–0.4%

Asimov data²³ are shown in table 7.5. In all cases, the effects of the pruning were minor. A 2% reduction in total $\text{SF}_{t\bar{t}}$ uncertainty was seen, which was consistent with the reduction seen in the standalone $\text{CR}_{t\bar{t}}$ fit. No effect was observed on the μ_Z measurement, and a minute reduction of 0.4% in total uncertainty was observed on the expected μ_H measurement, which was not seen as significant.

The impact on the $t\bar{t}$ scale factor measurement was also compared in blind fits to data²⁴, and are shown in table 7.6. No significant shift in the measured $\text{SF}_{t\bar{t}}$ value was observed, and only a small 2.7% reduction in total uncertainty was seen, which was consistent with findings in standalone $\text{CR}_{t\bar{t}}$ fits, as well as the inclusive SR measurement expectations in Asimov data.

Overall, the selection and validation tests showed that a 2% pruning threshold was a safe and optimal choice, removing 71% of uncertainty descriptions in the inclusive $\text{CR}_{t\bar{t}}$ region, and between 71% and 61% in the p_T^{jet} -binned $\text{CR}_{t\bar{t}}$ regions.

²³ Asimov data is an idealised dataset, built from the model itself, providing the expected results and sensitivity of the measurement. Described in section 5.7.2.

²⁴ The fit was performed with μ_H fixed to 1 (SM value), and only observing $t\bar{t}$ results.

Table 7.6: Comparison of $SF_{t\bar{t}}$ values and uncertainties found in blind²⁴ inclusive measurement fits (SRL, SRS and $CR_{t\bar{t}}$) to data without pruning, and with a 2% pruning threshold in $CR_{t\bar{t}}$. Differences are shown in reference to the non-pruned model, such that the sign indicates reduction or increase in relation to it, e.g. $\Delta\sigma/\sigma = (\sigma_{\text{prun}} - \sigma_{\text{no prun}})/\sigma_{\text{no prun}}$.

Pruning	$SF_{t\bar{t}}$	σ_{stat}	σ_{syst}	$\Delta\sigma$	$\Delta\sigma/\sigma$	$ \Delta SF_{t\bar{t}} /\sigma$
None	0.81	0.013	0.055	–	–	–
< 2%	0.81	0.013	0.053	–0.002	–2.7%	< 0.1 σ

7.6.2 Signal Region Pruning Scheme

The procedure developed in the $CR_{t\bar{t}}$ regions was later used to determine the optimal pruning for signal regions. As mentioned previously, pruning was particularly important to reduce the complexity of the measurement fits, due to their long computation time.

The optimisation studies were performed for both the inclusive and differential measurement fits. During the tests all signal regions in the fit were set to the same pruning threshold. The studies were performed using only Asimov data, as the signal region data had to be kept blind.

The studies found that 2% pruning thresholds were optimal for all regions, removing 64% of uncertainty descriptions from the inclusive measurement fit and 59% of uncertainty descriptions from the differential measurement fit. Plots summarising the uncertainties kept with a 2% pruning in the inclusive and differential measurement regions are shown in figures G.9 and G.10 in appendix G.7.

7.6.3 Section Summary

Considering all uncertainty components, the fit models had a huge number of uncertainty descriptions ranging from ~ 50 in a standalone $CR_{t\bar{t}}$ fit to ~ 1100 in

the differential measurement model, leading to complex, slow-to-compute fits. This section presented the uncertainty pruning procedure, and the pruning threshold optimisation for the $\text{CR}_{t\bar{t}}$ regions, performed by the author. The analytical machinery developed for the $\text{CR}_{t\bar{t}}$ pruning optimisation, was later used by other analysis members to optimise the pruning in the signal regions.

The pruning optimisation studies determined a 2% pruning threshold to be optimal as it had minimal impact on the $\text{SF}_{t\bar{t}}$ measured values and uncertainties, while removing 61% – 73% of the uncertainty descriptions. Comparisons of high ranking uncertainty post-fit pulls and widths showed no effect with the use of a 2% pruning threshold. Similar results and outcomes were seen with p_T^{jet} -binned $\text{CR}_{t\bar{t}}$ regions.

The same procedure was used to optimise the pruning thresholds in the signal regions. Overall, the systematic uncertainty pruning significantly simplified the fit models used in the analysis. The number of uncertainty descriptions was reduced by 71% in the standalone inclusive $\text{CR}_{t\bar{t}}$ fit model, 64% in the inclusive SR measurement fit model, and 59% in the differential SR measurement fit model. Furthermore, the introduction of the pruning procedure significantly reduced the computation times of the measurement fits: by around 9 hours for the inclusive measurement, and 110 hours for the differential measurement.

7.7 Constraining the JMR Uncertainty of W and Z bosons²⁵

The QCD background was described by a flexible parametric function. Because of this, it was highly sensitive to the shapes of the resonant backgrounds. The $t\bar{t}$ background was constrained well by the $\text{CR}_{t\bar{t}}$ region, as is described in detail in the following chapter. As a result, there were no strong correlations between the $t\bar{t}$ scale factor $\text{SF}_{t\bar{t}}$ and other processes. However, no such procedure was available for the Z +jets and W +jets processes.

²⁵ The studies presented in this section were the work of other analysis members [73] (internal).

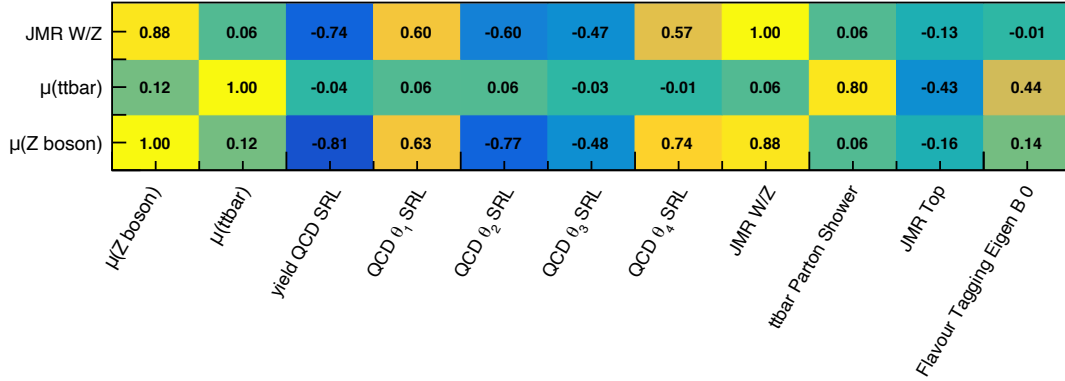


Figure 7.12: Isolated correlations of μ_Z , $\text{SF}_{t\bar{t}}$ and V boson JMR uncertainty from a data fit measuring μ_Z in a simultaneous SRL and $\text{CR}_{t\bar{t}}$ fit ($\mu_H = 1$), showing high correlations between μ_Z , V boson JMR uncertainty and the QCD parameters. Adapted from [73] (internal).

The inclusive Z +jets signal measurement²⁶ was used to validate the analysis. The initial tests, which did not include an external constraint of V boson jet mass resolution (JMR) uncertainty, showed large correlations between the Z +jets signal strength (μ_Z), V boson JMR uncertainty, and the QCD estimate function parameters. A reduced correlation plot of the simultaneous SRL and $\text{CR}_{t\bar{t}}$ fit to data shown in figure 7.12 illustrates this behaviour.

To quantify the impact of this interplay on the measurement, studies were conducted with 58 VRL_{hyb} data slices²⁷. Each slice was fit with the QCD estimate function, Z +jets signal strength (μ_Z), and the V +jets JMR uncertainty. A non negligible fraction of fits displayed large ($> 2\sigma$) pulls of the JMR uncertainty. This, in turn, broadened the Z peak, and returned larger values of μ_Z and downward-shifted QCD backgrounds. Given the large correlations between the JMR uncertainties, μ_Z and the QCD function parameters, this effect can be understood as a lack of constraint in the model. The flexible QCD function and the large JMR

²⁶ in these fits μ_H was fixed to SM expectation, $\mu_H = 1$

²⁷ The VR_{hyb} slices had an injected $\mu_Z = 1$ component. See section 6.4.1 for more information on VR_{hyb} .

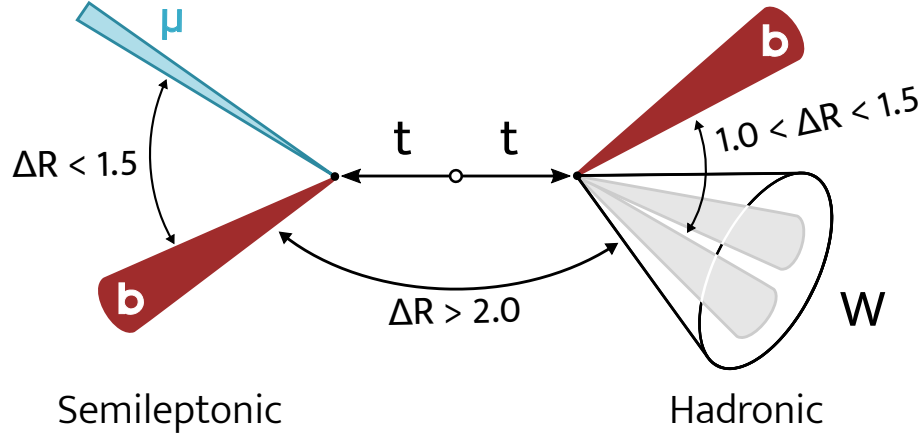


Figure 7.13: A diagram describing the topology of a CR_W event.

uncertainty allowed several acceptable descriptions of the data. The same studies were done with the jet mass scale (JMS) modelling uncertainty, which also showed strong correlations with μ_Z , however no such behaviour was observed.

The JMR uncertainty recommendation available at the time of the analysis was widely considered to be a rough, conservative estimate. Therefore an external CR_W control region²⁸ isolating W boson events was constructed to provide a more accurate estimate of the V +jets JMR uncertainty in the kinematic regime of this analysis.

7.7.1 W and Z boson JMR Control Region (CR_W)

The CR_W was designed to isolate a sample of $W \rightarrow qq$ decays from $t\bar{t}$ enriched events. Similarly to $\text{CR}_{t\bar{t}}$, the event selection was based on a back-to-back $t\bar{t}$ decay with one hadronic and one leptonic component. However, in this case, the focus was on isolating a $W \rightarrow qq$ candidate. A diagram of the topology of an event of interest is shown in figure 7.13.

As in $\text{CR}_{t\bar{t}}$, the events were identified using the semileptonic top decay. The

²⁸ The abbreviation of CR_W is used by author's choice in this thesis only, in the analysis documentation CR_W was called $\text{WCR}_{t\bar{t}}$

data was collected using a muon trigger and an isolated muon, matched with the trigger muon was required. The muon has to have $p_T^\mu > 27$ GeV to ensure full trigger efficiency over all years. A b -tagged VR track jet with $p_T > 25$ GeV was required within $\Delta R < 1.5$ of the muon to complete the semileptonic top decay topology.

At least one large- R calorimeter jet with $p_T > 200$ GeV was required in the event, and the large- R jet with the highest p_T was considered the $W \rightarrow qq'$ candidate. The candidate large- R jet had to have at least two associated VR track jets, and be $\Delta R > 2.0$ away from the b -tagged track jet in the semileptonic decay, to ensure a back-to-back topology. To make sure that the large- R jet contained only the W boson decay, a b -tagged VR track jet with $p_T > 10$ GeV was required within $1.0 < \Delta R < 1.5$ of the W boson candidate.

The inclusive m_{jet} and p_T^{jet} spectra of the candidate jets are shown in figures 7.14a and 7.14b. To isolate W +jets mass resonance, the $m_{\text{jet}} \in [60, 100]$ GeV range was used in the fits. This also made the CR_W region orthogonal to $\text{CR}_{t\bar{t}}$, which used a $m_{\text{jet}} \in [140, 200]$ GeV fitting range. It is notable that the Wt (single-top) background was negligible, which illustrates that the requirement for a near-by b -quark (to the W candidate) is powerful at reducing this background.

7.7.2 Method and Results

As the candidate p_T^{jet} distribution in figure 7.14b shows, few events were available in CR_W at high p_T ranges ($p_T > 750$ GeV). Therefore, the V boson JMR uncertainty measurement was also performed in VRL data, which provided a measurable V +jets resonant peak with excellent ($10\sigma - 13\sigma$, depending on the differential p_T^V bin) sensitivity, mostly made up of W +jets events²⁹. The regions were complementary as CR_W provided a clean W boson sample, and VRL provided high p_T^{jet} sensitivity.

The JMR uncertainty constraints were derived by performing fits in the CR_W

²⁹ The V +jets measurement in VRL data is discussed in section 9.5.1 and shown in figure I.4 in appendix I.

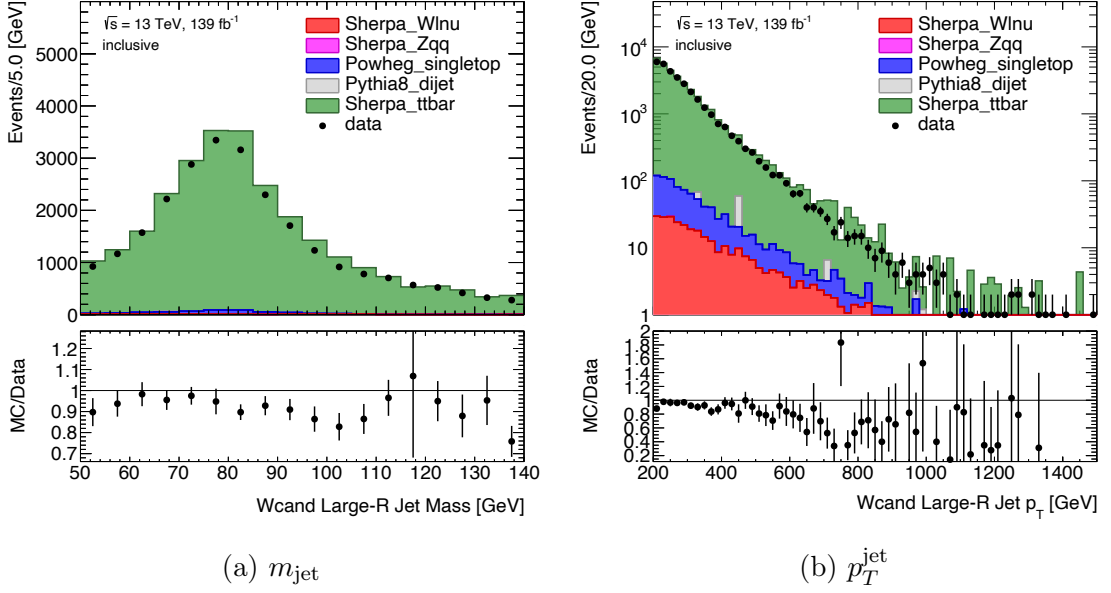


Figure 7.14: The (a) m_{jet} and (b) p_T^{jet} distributions of data and processes passing the CR_W event selection [73] (internal).

and VR regions, and extracting the post-fit values and widths of the V boson JMR uncertainty ($\hat{\theta}_{\text{JMR}} \pm \sigma$). The JMR constraints were propagated to the signal region fits as external Gaussian constraints on the V boson JMR uncertainties.

In the CR_W and VR fits only the JMR and JMS (which control the width and position of the V boson resonance peak) uncertainties were kept free, all other uncertainties were fixed to zero to prevent correlations with JMR. The floating parameters in the two types of fits were:

$$\begin{aligned} \text{CR}_W & - \text{SF}_{t\bar{t}} (W \text{ boson in } t\bar{t}), \theta_{\text{JMR}(V)}, \boldsymbol{\theta}_{\text{JMS}(V)}; \\ \text{VR} & - \boldsymbol{\theta}_{\text{QCD}}, \theta_{\text{JMR}(V)}, \boldsymbol{\theta}_{\text{JMS}(V)}; \end{aligned}$$

where θ denotes a nuisance parameter (NP), and $\boldsymbol{\theta}$ denotes a set of nuisance parameters. In the VR fits, μ_V was fixed to the SM expectation ($\mu_V = 1$) to prevent the correlation effects discussed previously. The compatibility of this assumption was tested and confirmed before the extraction of the JMR values.

The CR_W fits were performed in three p_T^{jet} bins: $[200, 275]$ GeV, $[275, 375]$ GeV, and $[375, 1500]$ GeV, and the VR fits were performed in two p_T^{jet} bins: $[450, 650]$ GeV,

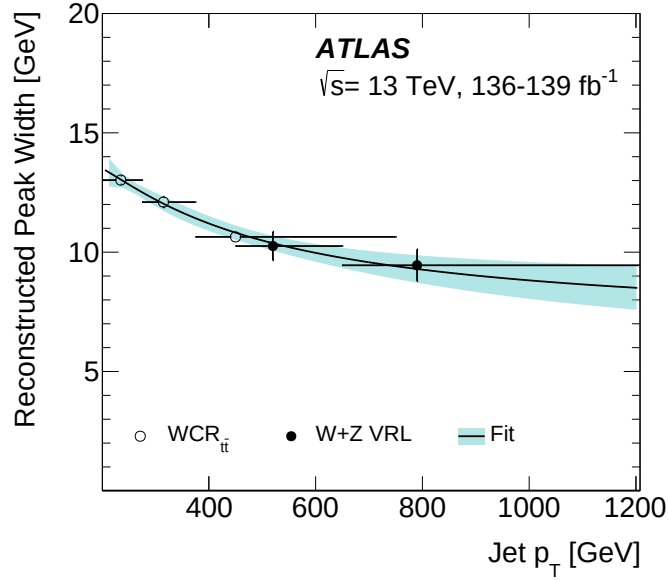


Figure 7.15: V boson mass resonance peak width as measured using the W boson resonance in CR_W ($WCR_{t\bar{t}}$ in figure) data and combined W and Z resonance in VR data [5]. The horizontal bars express the full range in which the measurement is made, and the points depict the average p_T^{jet} in the bin. The black curve and cyan bands depict a fit to the measurements and the uncertainties on the fit.

and $[650, 3000]$ GeV. The VR data sample was sliced into 5 datasets to maximise the fit precision, while retaining the QCD estimate statistical compatibility³⁰.

The results from the two regions were combined by fitting a $f(x) = a + bx + c/x$ functional form to the measured values expressed in terms of V boson resonance width. The results are shown in figure 7.15. The uncertainty behaviour was seen to be compatible with the results presented in the new JMR recommendations by ATLAS³¹ [78].

The constraints for each p_T^{jet} region were derived by sampling the constraint combination fit range 250×10^3 times and averaging the values within the p_T^{jet} ranges of each signal region, such that the larger uncertainties at higher p_T^{jet} values were

³⁰ The number of parameters needed to describe the QCD background tends to scale with available luminosity, see 6.4.1 for more details.

³¹ The procedure was also presented to, and approved by the dedicated group producing JMR uncertainties at ATLAS.

correctly obtained. Additional uncertainties accounting for the extrapolation from $W \rightarrow jj$ and $Z \rightarrow jj$ (j - jet) to $Z \rightarrow b\bar{b}$ were estimated to be $\sim 10\%$ of the original JMR uncertainty, which were added in quadrature to the uncertainty width obtained from the fit. Overall, the nominal values of the JMR uncertainties differed from the original values obtained from simulation by less than 2.5%, and was constrained to between 14% and 22% of its previous size [5], which was a great improvement from the previous estimate.

The implementation of this constraint successfully mitigated the unwanted correlation effects, for example, reducing the correlation between μ_Z and $\theta_{\text{JMR}(V)}$ in the inclusive SR measurement, from $\sim 90\%$ to $\sim 30\%$ [143].

JMR and the Higgs Boson

Despite the similar topologies of $Z \rightarrow q\bar{q}$ and $H \rightarrow b\bar{b}$ decays, the external constraint derived using $Z \rightarrow q\bar{q}$ decays could not be translated to the Higgs boson process without additional studies. Given that this procedure was introduced late in the analysis, this was not attempted.

In the differential fits, the correlations between $\mu_{H,i}$ and Higgs boson JMR ranged between 2% – 60%. To ensure against similar correlation-induced issues, the relative differences in measurement significance ($\mu_{H,i}/\sigma_{H,i}$) induced by fixing the JMR and JMS modelling uncertainties to $\theta = 0$ were observed in otherwise blind differential fits to SR data. No significant effects requiring additional measures were observed. In the future, additional studies could be done to attempt to extrapolate the JMR constraints derived in $Z \rightarrow q\bar{q}$ decays to the Higgs boson process, which would reduce the total uncertainties on the Higgs boson measurement.

7.8 Decorrelation of Systematic Uncertainties

In the differential measurement fits³², most uncertainties were fully correlated across p_T^{jet} bins by describing them with a single nuisance parameter (NP). As the uncer-

tainties are derived as functions of p_T^{jet} , there is no reason to expect large differences between bins. This treatment allows for simple fit models and is generally recommended in ATLAS. However, if the data has significant power to constrain certain uncertainties in some regions, this approach has to be tested so as not to introduce biases in the fit.

In the $H(\rightarrow b\bar{b}) + j$ measurement fit there are several high impact uncertainties constrained well in the fit. To check whether these uncertainties needed to be decorrelated across p_T^{jet} bins in the fit (i.e. be described by separate NPs in different p_T^{jet} bins), or if the fully correlated treatment was reasonable, studies looking into the impact of such decorrelation on fit results and uncertainty pulls were conducted.

This section focuses on the early decorrelation studies of Z boson and $t\bar{t}$ uncertainties, performed by the author. Brief discussions of the finalised Z and Higgs boson uncertainty decorrelation studies performed by other members of the analysis group [73] (internal) are also presented. The following uncertainties are discussed throughout this section:

<i>Label</i>	<i>Source</i>	<i>Size</i>
JMR	– jet mass resolution (top and V +jets)	large
JMS_	– jet mass scale:	
Baseline	– differences between data and simulation	moderate
_Modelling	– Nominal vs. alternative MC generators	large
Tracking_[1-3]	– various tracking-related uncertainties	moderate
TotalStat	– statistical uncertainty	small
V+jets_QCD_Scale	– V +jets generator uncertainties	moderate / large

The labels and descriptions of all uncertainties included in the fits are given in

³² *Reminder:* the differential measurement signal regions (and $\text{CR}_{t\bar{t}}$) were divided into corresponding candidate jet p_T bins: SRS0, SR*1, and SR*2 (* = L/S) – low, medium and high jet p_T . The process of interest (Z or Higgs boson) was measured in truth-level- p_T bins, e.g.: $\mu_{H,0}$, $\mu_{H,1}$, and $\mu_{H,2}$, corresponding to the low, medium and high truth- p_T bins defining the fiducial regions. Other resonant processes in the differential measurement were measured in jet p_T bins, e.g. $\text{SF}_{t\bar{t},b1}$ describes the $t\bar{t}$ scale factor in SRL1, SRS1, and $\text{CR}_{t\bar{t}}1$.

appendix G.1. Examples of the JMR, JMS and V +jets modelling uncertainties in the inclusive signal regions are given in figures G.1, G.2 and G.3 in appendix G.3.

7.8.1 Z boson Uncertainties

Early Studies

The early uncertainty decorrelation studies were performed before the V +jets JMR uncertainty was constrained using a data-driven method. These studies were an important precursor to the final decorrelation studies, which are presented in the following section. The studies were performed with a 0.5 GeV binning in the signal regions, as was used throughout most of the analysis development.

The highest-impact uncertainties on the V +jets processes were investigated: Z boson JMR, all JMS uncertainties (as a group), and V +jets generator uncertainties. The study was conducted by running differential Z +jets ($\mu_{Z,i}$) measurement fits with each of the listed uncertainties decorrelated between candidate p_T^{jet} bins (i.e. described by separate nuisance parameters, rather than a single one), and comparing the results to the baseline (fully correlated) model. The Higgs boson process was included in the fit model with μ_H fixed to its SM value ($\mu_H = 1$). The effects on the measurement uncertainties were observed using Asimov data. The effect on the measured $\mu_{Z,i}$ values was observed in blinded data fits by looking at the shift in $\mu_{Z,i}$ relative to the size of the uncertainty of the non-decorrelated model ($|\Delta\mu|/\sigma$).

The results are shown in table 7.7. Expected measurement significance comparisons ($\Delta Z = \mu/\sigma$) are also given to provide context of the size of the uncertainties. Further understanding was gained by comparing the uncertainty pulls and widths found in data, shown in figure 7.16. The tables and plots also include Top JMR uncertainties, which will be discussed later in section 7.8.2.

Large effects on the $\mu_{Z,i}$ measurements were observed when decorrelating V +jets JMR uncertainties, as shown in table 7.7. The total expected uncertainties on

Table 7.7: μ_Z measurement shifts in data, and differences in expected uncertainties (σ) and signal significances ($Z = \mu/\sigma$) found in Asimov data, induced by decorrelating a given uncertainty (or unc. group, i.e. JMS) across p_T^{jet} bins. Differences are given in reference to non-decorrelated model, such that the sign indicates reduction or increase in relation to it, e.g. $\Delta\sigma/\sigma = (\sigma_{\text{dc}} - \sigma_{\text{no dc}})/\sigma_{\text{no dc}}$. Minute differences are shown in grey. Without decorrelation, the expected uncertainties measured in an Asimov fit were: $\sigma_{\mu,0}^{\text{no dc}} = 0.72$, $\sigma_{\mu,1}^{\text{no dc}} = 0.24$, $\sigma_{\mu,2}^{\text{no dc}} = 0.40$.

Decorr. Unc.	μ	Asimov (Expectation)		Data
		$\Delta\sigma/\sigma$	ΔZ	$ \Delta\mu /\sigma$
V+jets JMR	$\mu_{Z,0}$	5%	−0.07	0.55
	$\mu_{Z,1}$	13%	−0.47	0.34
	$\mu_{Z,2}$	35%	−0.65	1.58
JMS (All)	$\mu_{Z,0}$	7%	−0.09	0.22
	$\mu_{Z,1}$	< 1%	−0.02	0.12
	$\mu_{Z,2}$	< 1%	−0.01	0.01
V+jets Generator	$\mu_{Z,0}$	< 1%	−0.01	0.01
	$\mu_{Z,1}$	< 1%	0.00	0.07
	$\mu_{Z,2}$	< 1%	−0.01	0.02
Top JMR	$\mu_{Z,0}$	< 1%	0.00	0.07
	$\mu_{Z,1}$	< 1%	0.00	0.05
	$\mu_{Z,2}$	< 1%	−0.01	0.00

the measured $\mu_{Z,i}$ values increased by up to 35% after decorrelation. The JMR decorrelation also induced $\Delta\mu_{Z,i}$ shifts of 0.55σ , 0.34σ and 1.58σ in low, medium and high p_T^{truth} bins, respectively. To understand whether the larger constraint in the correlated model was valid, the JMR uncertainty pulls were observed, given in figure 7.16a. The pulls show that the medium momentum bin (bin 1) with the largest statistics was able to strongly constrain the JMR uncertainty, whereas the low and high momentum bins could not. Therefore, when correlated, the medium momentum bin dominated the JMR measurement. This constrained and shifted the best-fit values of the JMR uncertainties in the other bins. As the JMR uncertainties

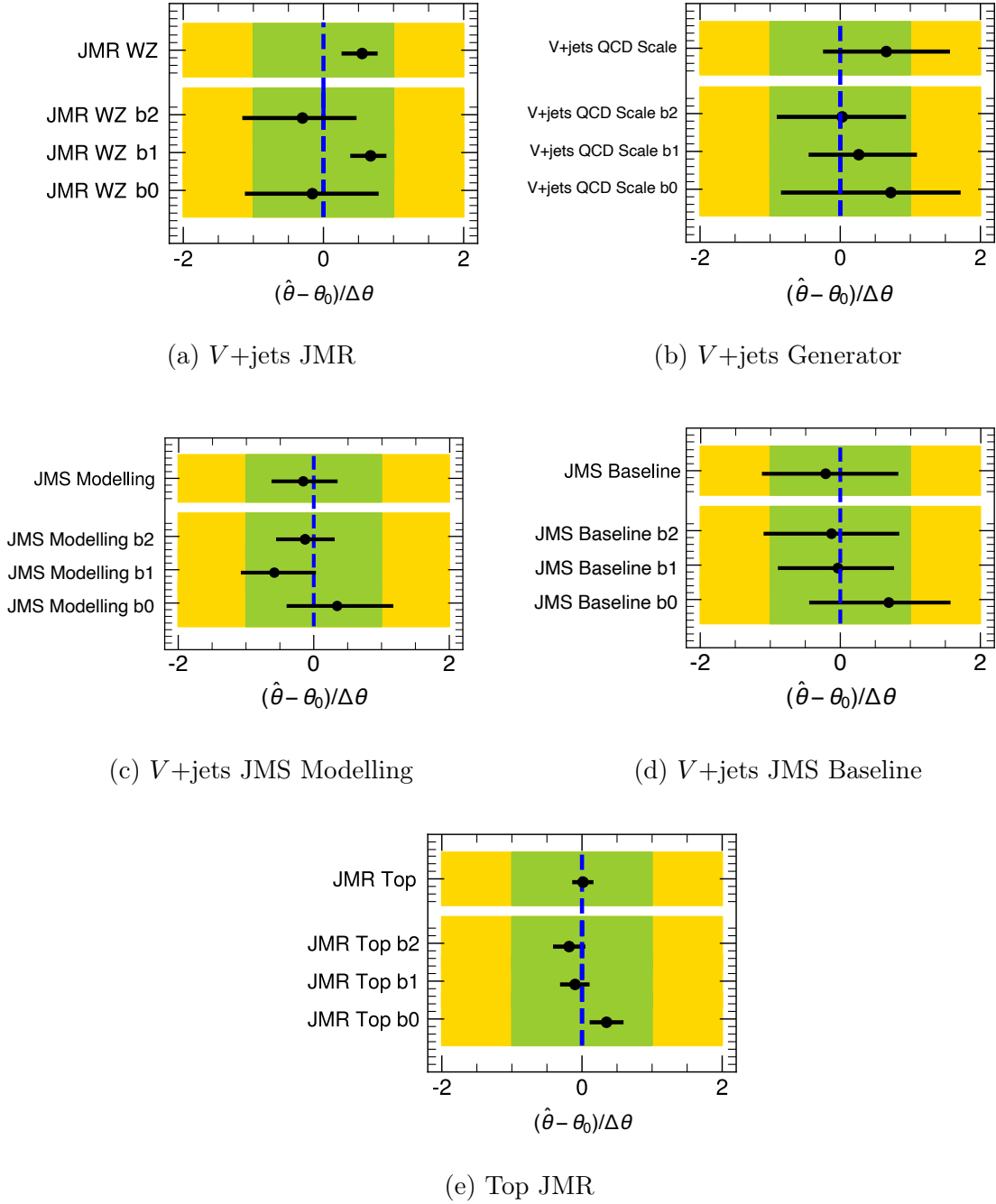


Figure 7.16: Post-fit pulls and widths of high impact uncertainties from differential measurement fits in data with and without decorrelation of each uncertainty across p_T^{jet} bins. The JMS uncertainties were decorrelated as a group, and the uncertainties with the most significant changes are shown. The (a) V boson JMR and (e) $t\bar{t}$ JMR uncertainties show significant differences in pulls between p_T^{jet} bins; the (c, d) V boson JMS Modelling and JMS Baseline uncertainties show slight pull differences; and the (b) V +jets MC generator (QCD Scale) uncertainties show no significant differences.

were the largest systematic uncertainties on the Z +jets process, the additional constraint lead to a decrease in uncertainty and shifts in the measured μ_Z values.

The significant differences in the pull directions between the JMR uncertainty in the dominant medium p_T^{jet} bin, and the other two bins, indicated that the constraint from the medium bin might not be applicable to the other bins. Therefore, in light of these differences and the large impact on the fit, the JMR uncertainties were decorrelated across p_T^{jet} bins in the fit model. Once the external JMR constraints were introduced (described in section 7.7), these findings motivated the use of separate JMR constraints for different p_T^{jet} bins. As the Higgs boson and V +jets processes have similar topologies, this was also done for Higgs boson JMR uncertainties.

The decorrelation of JMS or V +jets generator uncertainties across p_T^{jet} bins, did not have a large effect on the $\mu_{Z,i}$ measurements. Slight differences between the pulls in different p_T^{jet} bins were seen for `JMS_Modelling` and `JMS_Baseline` uncertainties (figures 7.16c and 7.16d). As the studies were produced at a period of flux in the analysis³³, further studies were postponed, and later conducted by other members of the analysis team. These studies are presented in the following passage.

In summary, the studies showed a need to decorrelate JMR uncertainties across p_T^{jet} bins for the V +jets (and Higgs boson) processes due to differences seen in the JMR nuisance parameter pulls, and large effects on the measurement. The `JMS_Modelling` and `JMS_Baseline` uncertainties showed possible indications for the need of decorrelation, which required further investigation. No other investigated V +jets uncertainties displayed significantly different behaviours between correlated and decorrelated models requiring further study or decorrelation.

Further Studies

Further studies regarding V +jets uncertainty decorrelation over p_T^{jet} bins were conducted by other analysis members, following the addition of external JMR con-

³³ Other studies produced in the group at the same time indicated the need of external JMR constraints, which lead to the development of the CR_W region.

Table 7.8: Relative shifts of differential μ_Z measurements in data, induced by the decorrelation of listed uncertainties between p_T^{jet} bins. $\Delta(i) = |\Delta\mu_{Z,i}|/\sigma_{Z,i}$. The decorrelation is applied to all processes in the entry. Adapted from [73] (internal). The only significant differences were induced by decorrelating the **JMS_Modelling** uncertainty.

Decorrelated NP	$\Delta(1)$	$\Delta(2)$	$\Delta(3)$
JMS Modelling	0.22	0.28	0.42
JMS Modelling & Baseline	0.18	0.26	0.42
JMS Modelling, Baseline & JES Topology	0.14	0.26	0.40
JMS Modelling & V +jets Generator	0.25	0.30	0.40
JMS All	0.22	0.23	0.40
JMS All, $t\bar{t}$ ME/PS, & V +jets Generator	0.24	0.22	0.40

straints discussed in section 7.7. The **JMS_Modelling** and **JMS_Baseline** uncertainties were studied, as they displayed slight differences between uncertainty pulls in p_T bins during the initial studies, as shown in figures 7.16c and 7.16d. Other high-impact V +jets uncertainties were also investigated. The studies were performed in blind differential measurement fits to SR data.

The relative $\mu_{Z,i}$ measurement shifts ($\Delta(i) = |\Delta\mu_{Z,i}|/\sigma_{Z,i}$) induced by decorrelating uncertainties, are given in table 7.8. The decorrelation of **JMS_Modelling** uncertainties induced moderately large shifts ($0.22\sigma - 0.42\sigma$) in all $\mu_{Z,i}$ measurements. Further decorrelation of other uncertainties did not have significant impact. The effects induced by decorrelated JMS uncertainties were stronger than seen previously, likely due to the reduced freedom in the fit, as the largest V +jets uncertainty – V boson JMR – was now constrained externally.

The correlations between **JMS_Modelling** nuisance parameters and $\mu_{Z,i}$ measurements were also observed, and are shown in table 7.9. Decorrelating JMS Modelling uncertainties across p_T^{jet} bins reduced the correlations between this uncertainty and

Table 7.9: Correlations between $\mu_{Z,i}$ and **JMS_Modelling** nuisance parameter(s), from differential measurement fits to SR data with the **JMS_Modelling** uncertainty on V +jets processes correlated and decorrelated across p_T^{jet} bins. Clear differences in correlation values and signs were observed after decorrelation. Adapted from [73] (internal).

Decorrelated NP	Corr(μ_Z , JMS Modelling)		
	$\mu_{Z,0}$	$\mu_{Z,1}$	$\mu_{Z,2}$
None	0.20	0.33	0.53
JMS Modelling	-0.12	-0.23	0.39

all of the $\mu_{Z,i}$ parameters, and for correlations with $\mu_{Z,0}$ and $\mu_{Z,1}$ induced a change in sign. The reduction and change in correlation, showed that the independent behaviour of the **JMS_Modelling** uncertainties across p_T^{jet} bins was not well described with a correlated model, and therefore this uncertainty had to be decorrelated across p_T^{jet} bins. To simplify implementation the **JMS_Modelling** uncertainties were decorrelated across p_T^{jet} bins for all processes.

7.8.2 $t\bar{t}$ Uncertainties

As discussed previously, the correlation of most uncertainties across p_T jet bins can be a safe assumption for most uncertainties. However, it needs to be explicitly tested for uncertainties which are highly constrained in the fit, so as not to introduce biases. The $\text{CR}_{t\bar{t}}$ region used in the measurements had the power to significantly constrain the top-quark JMR uncertainty – one of the largest and highest impact uncertainties for the $t\bar{t}$ process.

The impact of decorrelating the top-quark JMR uncertainty across p_T^{jet} bins was investigated by observing the impact on the $\mu_{Z,i}$ and $\text{SF}_{t\bar{t},\text{bi}}$ values. They were observed in differential Z boson measurement fits³⁴, and are shown in tables 7.7

(impact on $\mu_{Z,i}$) and 7.10 (impact on $\text{SF}_{t\bar{t},bi}$). The decorrelation of the top-quark JMR uncertainty across p_T^{jet} bins did not affect either resonance measurements significantly. No shifts in the measured values $> 0.5\sigma$ were induced, and differences in uncertainty were $< 5\%$ in all cases.

Despite the minimal impact on the measurements, the top-quark JMR uncertainty pulls with and without decorrelation were compared, and shown earlier in figure 7.16e. Significant differences in uncertainty pulls were observed. For example, the best-fit value of the JMR nuisance parameter in the lowest p_T^{jet} bin (bin 0), $\hat{\theta}_{b0}$, was found to be $1.4\sigma_{b0}$ widths away from the best-fit value in the correlated model. Describing this uncertainty by a single nuisance parameter, despite such discrepancies in different p_T^{jet} regions, could have affected other parameters and biased the fit. As each region was seen to have excellent constraint on the Top JMR uncertainty individually (therefore not affecting the uncertainties on the $\text{SF}_{t\bar{t}}$ measurement significantly), the safest approach was to decorrelate the top-quark JMR uncertainties across p_T^{jet} bins.

Table 7.10: Differences in $\text{SF}_{t\bar{t}}$ values and uncertainties found in differential Z boson measurement fits to SR data, induced by decorrelating **Top_JMR** uncertainties across p_T^{jet} bins. Differences are given in reference to non-decorrelated model: such that the sign indicates reduction or increase in relation to it, e.g. $\Delta\sigma/\sigma = (\sigma_{\text{dc}} - \sigma_{\text{no dc}})/\sigma_{\text{no dc}}$. Without decorrelation, the expected uncertainties measured in an Asimov fit were: $\sigma_{b0}^{\text{no dc}} = 0.06$, $\sigma_{b1}^{\text{no dc}} = 0.07$, $\sigma_{b2}^{\text{no dc}} = 0.07$.

μ	$\Delta\sigma/\sigma$	$(\Delta\sigma/\sigma)_{\text{syst}}$	$ \Delta\text{SF}_{t\bar{t}} /\sigma$
$\mu_{t\bar{t},b0}$	0.8%	0.8%	0.05
$\mu_{t\bar{t},b1}$	3.4%	3.9%	0.32
$\mu_{t\bar{t},b2}$	0.2%	0.3%	0.04

³⁴ The study was conducted at the same time (and using the same model) as the early Z boson uncertainty decorrelation studies described previously.

7.8.3 Higgs boson Uncertainties

In the default model, the JMS uncertainties were fully correlated between Higgs boson and V +jets processes, as could be allowed by their similar jet topologies. However, given that in this analysis the Higgs boson signal is very small compared to the immense and *flexible* QCD background estimate, the measurement fit model has to be particularly precise, as the Higgs boson measurement could be easily biased. Given the flexibility of the fit, if the JMS uncertainties were to be correlated between Higgs boson and V +jets processes, the larger Z boson resonance would likely constrain the uncertainties. However, the Higgs boson and V +jets samples were generated using different MC generators, which could mean that the values of uncertainties could be different for the two estimates, in which case such correlation could bias the Higgs boson measurement.

After the inclusive Z boson measurement was made, a relatively strong pull in the `JMS_Modelling` uncertainty on the V +jets processes was observed. It was decided that decorrelating this uncertainty between V +jets and Higgs processes was a safer choice, as it was unclear whether the resonances derived from different generators would be pulled in the same way.

The need for decorrelation of other JMS uncertainties between Higgs and V +jets processes, and p_T bins was also investigated in blinded differential fits to SR data (by other members of the analysis team). The default (fully correlated) model was compared to a model wherein all JMS uncertainties were decorrelated between the Higgs boson and V +jets processes and the Higgs boson uncertainties were further decorrelated across p_T^{jet} bins.

The relative differences in μ_H measurement significance ($|\Delta\mu|/\sigma$) induced by the uncertainty decorrelation were seen to be 7%, 10% and 0.6% for the low, medium and high p_T^H bins, respectively. Compared to the 0.05σ , 0.30σ and 0.16σ expected significances for each measurement, such induced changes were seen as insignificant, and did not require further complication of the fit model.

7.8.4 Section Summary

The description of the same uncertainty by a single nuisance parameter across p_T^{jet} bins or similar processes, is a reasonable treatment for most uncertainties and can significantly simplify fit models. However, when doing so for high-impact uncertainties, studies need to be made to make sure the correlated model agrees with the individual behaviour of the uncertainties in the regions in question. Otherwise, biases in the fits can be introduced. Therefore the impact of decorrelating high impact uncertainties across p_T^{jet} bins for the Z +jets, $t\bar{t}$, and Higgs boson processes was investigated.

Early studies in Z +jets differential measurement fits showed the need to decorrelate JMR uncertainties across p_T^{jet} bins for all processes, and motivated the use of separate external V +jets JMR constraints in different p_T^{jet} bins. Later studies of JMS and other high-impact uncertainties in the differential Z +jets measurement indicated the need to decorrelate JMS modelling uncertainties across p_T^{jet} bins, and for simplicity of implementation, this was applied to all processes. No further decorrelation was seen to be required.

Given the significant ability for the $\text{CR}_{t\bar{t}}$ fits to constrain top-quark JMR uncertainties, it was important to observe whether correlating this uncertainty across p_T^{jet} bins in the differential measurement was not introducing biases in the fit. No significant effects on the μ_Z or $\text{SF}_{t\bar{t}}$ measurements were seen, but the pulls between some of the uncertainty components in the p_T^{jet} -bins significantly disagreed with the correlated value. If overlooked, this discrepancy could have affected other fit parameters and biased the fit. Therefore, the top-quark JMR uncertainties were decorrelated in the measurement.

Lastly, the decorrelation of JMS uncertainties between the Higgs boson and V +jets processes was investigated, as well as the decorrelation of JMS uncertainties on the Higgs boson process across p_T^{jet} bins. The **JMS_Modelling** uncertainty was decorrelated between the Higgs boson and V +jets processes, but no other JMS

uncertainties were seen to require such treatment.

7.9 Chapter Overview

This chapter discussed the sources and treatment of the systematic uncertainties in the $H(\rightarrow b\bar{b}) + j$ measurement fit. In section 7.2, four main sources of uncertainties were discussed: jet uncertainties, b -tagging uncertainties, spurious signal uncertainties and theoretical uncertainties.

The details of the treatment were discussed in section 7.3. The uncertainties were included in the likelihood description as nuisance parameters (NP). Section 7.4 described the concepts of NP *pulls* and *impact*, which were used to study uncertainties throughout the analysis.

Section 7.5 presented issues caused by statistical limitations of the simulated mass templates used to model the processes and uncertainties, and the smoothing procedure used to mitigate them. MC statistical fluctuations in the templates lead to uneven variation between the nominal process and uncertainty descriptions, which were reinterpreted as features by the fit, and caused false constraints of fit parameters. A procedure was used to smooth the ratios between the uncertainty and nominal templates. It was seen to mitigate the observed alarming features in the fit results, such as under-constrained uncertainties and non-parabolic uncertainty profile likelihoods, and lead to more consistency between the expected and measured uncertainties. The procedure was successfully validated in $\text{CR}_{t\bar{t}}$ data.

Section 7.6 presented the uncertainty *pruning* procedure and optimisation studies, which enabled a significant simplification of the model, and reduced computation times. The optimisation procedure was developed and used by the author to optimise the pruning thresholds in the $\text{CR}_{t\bar{t}}$ regions. The same procedure was employed by other members of the analysis to optimise pruning in the signal regions. The optimised uncertainty pruning successfully removed large fractions of uncertainty

descriptions across all fits: 61% – 73% of uncertainty descriptions were removed from standalone $\text{CR}_{t\bar{t}}$ fits, 64% – from the inclusive measurement fit, and 59% – from the differential measurement fit. This reduced the inclusive measurement processing time by around 9 hours, and the differential measurement processing time by around 110 hours.

The large size of the V boson JMR uncertainty, and the strong correlation between this uncertainty and the Z boson signal strength (μ_Z) was seen to introduce ambiguities in the fit results, making them unreliable. To mitigate this issue, external constraints for the V boson JMR uncertainty were derived using data from a dedicated CR_W control region and the validation regions. The issue, and constraint derivation was described in section 7.7.

In the differential measurement many uncertainties are fully correlated across p_T^{jet} bins, which can be a good approximation for many uncertainties, allowing to simplify complex fits. However, for uncertainties which have a large impact on the fit measurement, such approximations can be too broad and neglect behaviour which could scale with jet p_T . Studies presented in section 7.8 investigated the impact of decorrelating high-impact uncertainties across p_T^{jet} bins. Early studies performed by the author indicated the need to decorrelate JMR uncertainties across p_T^{jet} bins for all processes. Further studies, performed after the introduction of external V boson JMR constraints, showed the need to decorrelate the JMS modelling uncertainties across p_T^{jet} bins as well.

Overall, this chapter provided an in-depth discussion of systematic uncertainties and their treatment in the $H(\rightarrow b\bar{b}) + j$ measurement. A robust uncertainty treatment is essential to the reliability of the results of the analysis, and the contribution the author made to the analysis through these studies has been crucial for the progression of the analysis.

Chapter 8

Studies of the $t\bar{t}$ Background

The largest resonant background in this analysis was contributed by $t\bar{t}$ decays. By utilising the muon-tagging capabilities of the ATLAS experiment, this analysis was able to construct a kinematically similar region to the signal region - $\text{CR}_{t\bar{t}}$, which was enriched in $t\bar{t}$ decays and was used to substantially constrain this background. The $\text{CR}_{t\bar{t}}$ region provided excellent constraints of high-impact $t\bar{t}$ systematic uncertainties, and the $t\bar{t}$ process could be estimated with $9\sigma - 14\sigma$ sensitivity¹. Because of the significant constraining power of the $\text{CR}_{t\bar{t}}$ region, its usage and fit results had to be thoroughly vetted and understood.

The $t\bar{t}$ background and $\text{CR}_{t\bar{t}}$ fits were introduced in section 6.6, which presented the expected and measured $t\bar{t}$ scale factor ($\text{SF}_{t\bar{t}}$) values in standalone $\text{CR}_{t\bar{t}}$ fits. This chapter focuses on more in depth studies of $\text{CR}_{t\bar{t}}$ fits, both as a standalone fit, and as part of the combined measurement fit. Section 8.1 presents detailed studies of the standalone $\text{CR}_{t\bar{t}}$ fit results, made to validate the $\text{CR}_{t\bar{t}}$ fit for use in various studies and the measurements. The studies include comparisons of the observed and expected results, and an in depth look at the uncertainty behaviour.

Section 8.2 explores different methods of incorporating the constraints from the $\text{CR}_{t\bar{t}}$ region into the Higgs boson measurement. Two different ways of combining

¹ Depending on the p_T^{jet} -binned region. $\text{CR}_{t\bar{t}}$ regions are: inclusive $\text{CR}_{t\bar{t}}$: $p_T^{\text{jet}} > 250$ GeV, and differential p_T^{jet} bins: $250 \text{ GeV} < \text{CR}_{t\bar{t}}0 < 450 \text{ GeV} < \text{CR}_{t\bar{t}}1 < 650 \text{ GeV} < \text{CR}_{t\bar{t}}2 < 1 \text{ TeV}$.

$\text{CR}_{t\bar{t}}$ and SR fits were investigated: performing the $\text{CR}_{t\bar{t}}$ fit separately and using the measured $t\bar{t}$ scale factor value to construct a Gaussian constraint on the $t\bar{t}$ yield in SR; or fitting the $\text{CR}_{t\bar{t}}$ simultaneously with the SR. The studies presented in this section showcase the excellent constraining capabilities achieved through the implementation of a simultaneous SR and $\text{CR}_{t\bar{t}}$ fit, which resulted in substantially reduced expected uncertainties of $t\bar{t}$ and QCD backgrounds.

As well as the studies presented in this chapter, the author provided continuous support for the $\text{CR}_{t\bar{t}}$ region fits throughout the development of the analysis, by conducting validation studies of the $\text{CR}_{t\bar{t}}$ region fits when relevant changes were implemented in the analysis. She also performed various studies which involved the region, such as uncertainty pruning and smoothing in the $\text{CR}_{t\bar{t}}$ region, presented in sections 7.5 and 7.6.

All studies and figures in this chapter were the original work of the author. The studies show results made with a late-stage fit set-up, presenting the status of the $\text{CR}_{t\bar{t}}$ fit and the impact of different $\text{CR}_{t\bar{t}}$ treatment in context of the final measurement setup. Any differences from the final fit set-up are stated explicitly in the study discussion, or in section 9.1.1 which outlines the changes in the analysis implemented during the writing of this thesis. Regardless of these changes, the presented studies finalised the usage of the $\text{CR}_{t\bar{t}}$ region, and the outcomes and conclusions presented in this chapter remained valid.

The first studies comparing the $\text{CR}_{t\bar{t}}$ fit combination with the signal regions were made in the initial stages of the analysis. The author used the dataset and fit model from the Higgs boson interpretation of the BSM $X(\rightarrow b\bar{b}) + j$ search [4] to validate and study the impact of moving from a $t\bar{t}$ Gaussian constraint method, used in the $X(\rightarrow b\bar{b}) + j$ search, to a simultaneous SR and $\text{CR}_{t\bar{t}}$ fit configuration. This built upon and improved the simple treatment in the previous Higgs boson probe, and contributed to building the foundation for the current measurement model. These studies were a precursor to the studies presented in this chapter.

The $t\bar{t}$ scale factor ($SF_{t\bar{t}}$) can be thought of as the $t\bar{t}$ signal strength ($\mu_{t\bar{t}}$) in this high p_T regime. For better readability, it will be referred to as such throughout this chapter. This chapter also contains several discussions of $t\bar{t}$ uncertainty behaviour. The most commonly discussed uncertainties in the chapter are:

<i>Label</i>	<i>Source</i>	<i>Size</i>
JMR	– jet mass resolution	large
JMS_	– jet mass scale:	
_Modelling	– nominal vs. alternative MC generators	large
Eigen_B_[0-4]	- b -jet b -tagging scale factor uncertainties	large
ttbar_PartonShower	– alternative parton shower generator	large
ttbar_MatrixElement	– alternative matrix element calculation	moderate / large

The labels and descriptions of all uncertainties included in the fits are given in appendix G.1.

8.1 CR_{t $\bar{t}$} Standalone Fit Validation

Due to its purity ($t\bar{t}$ made up $> 96\%$ of events in all CR_{t $\bar{t}$} regions), the CR_{t $\bar{t}$} region had excellent constraining power of the $t\bar{t}$ process, and as will be seen in the following section, primarily determines the $\mu_{t\bar{t}}$ measurement. As well as this, the CR_{t $\bar{t}$} fit was much simpler than the signal region fits, and provided a great testing ground for the fitting software and various fit features, particularly as the free use of data in this region was allowed. Therefore, it was crucial to observe and understand various aspects of the standalone CR_{t $\bar{t}$} fit results, and compare them to expectations. Such studies were conducted multiple times throughout the development of this analysis, following any relevant changes to the fit model or the samples used.

As well as serving as validation of the $t\bar{t}$ measurement in CR_{t $\bar{t}$} , the studies discussed in this section provided a baseline for studies on the combination of CR_{t $\bar{t}$}

and SR fits. The standalone $\text{CR}_{t\bar{t}}$ fit results helped to distinguish between SR and $\text{CR}_{t\bar{t}}$ effects in simultaneous SR and $\text{CR}_{t\bar{t}}$ fits. The results presented in this section discuss the inclusive $\text{CR}_{t\bar{t}}$ fits, however, the studies were also performed on p_T -binned $\text{CR}_{t\bar{t}}$ regions used in the differential measurement fit, which displayed similar behaviour.

An important feature of the fit results was the shape of the $\mu_{t\bar{t}}$ profile likelihood (introduced in section 7.5.3). For a simple fit model, such as this one, where only the $t\bar{t}$ component was allowed to float to fit the data² – a smooth, parabolic shape was expected. Significant deviations from the parabolic shape such as multiple minima would have been symptomatic of issues in the fit³, and would have needed to be understood. Figures 8.1a and 8.1b show the $\mu_{t\bar{t}}$ profile likelihoods in fits to Asimov⁴ and real $\text{CR}_{t\bar{t}}$ data, respectively. In both cases the profile likelihoods were seen to be parabolic and agreed with the expected (Asimov) and observed (data) fit results, given in tables 6.4 and 6.5, in section 6.6.1, showing no reasons for concerns.

Comparing the expected and observed fit results, shown previously in tables 6.4 and 6.5, the total uncertainties (σ) on the $\mu_{t\bar{t}}$ values measured in data were seen to be smaller than the expectations obtained from the fits to Asimov data. This is also visible comparing the widths of the profile likelihoods in figure 8.1. This effect can be explained by taking into account the scaling of $\mu_{t\bar{t}}$. In data, the measured $\mu_{t\bar{t}} \approx 0.8$. This meant that the normalisation components of all systematic uncertainties on $\mu_{t\bar{t}}$ were expected to be scaled down by the same amount⁵. In fact, if the uncertainties measured in data (σ_{data}) were scaled up to correspond to $\mu_{t\bar{t}} = 1$, by

$$\sigma_{\text{data}}^{\mu=1} = \frac{\sigma_{\text{data}}}{\mu_{t\bar{t}}}, \quad (8.1)$$

² The single-top and $W(\ell\nu)$ components were fixed to SM expectations, which together made up between 1.6% – 4.5% of the total yield in the region.

³ An example of this was discussed in section 7.5.

⁴ Asimov data is an idealised dataset, built from the model itself, providing the expected results and sensitivity of the measurement. Described in section 5.7.2.

⁵ The $t\bar{t}$ measurement was dominated by systematic uncertainties. The normalisation of each systematic uncertainty scaled with $t\bar{t}$ yield ($N_{t\bar{t}}$) as $\propto N_{t\bar{t}}$. The statistical uncertainties in data made up almost entirely by $t\bar{t}$ events would scale with $t\bar{t}$ yield as $\sigma_{\text{stat}} \approx \sqrt{N_{t\bar{t}}}$.

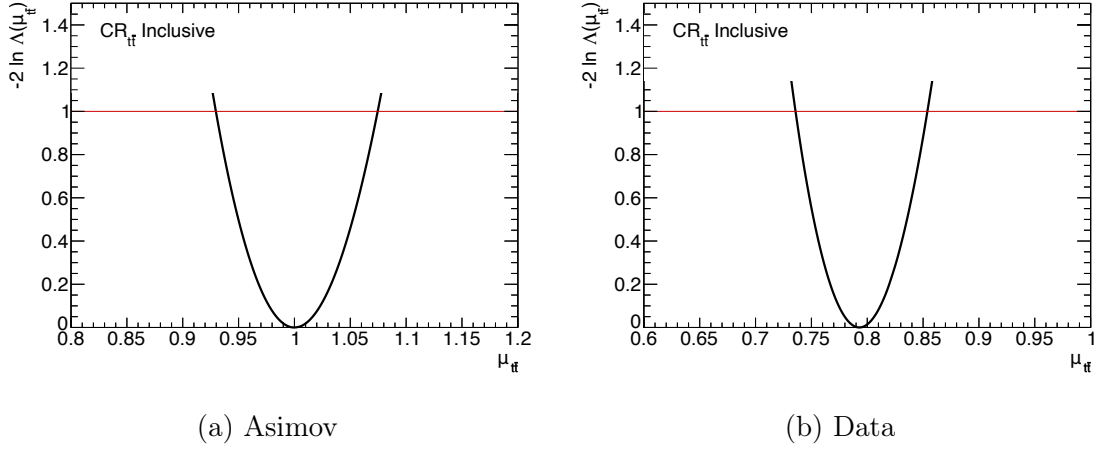


Figure 8.1: Profile likelihood scans of $t\bar{t}$ scale factor ($\mu_{t\bar{t}}$) from standalone $\text{CR}_{t\bar{t}}$ fits to (a) Asimov data, and (b) real data. The minimum corresponds to best-fit value of $\mu_{t\bar{t}}$ ($\hat{\mu}_{t\bar{t}}$), and the $\mu_{t\bar{t}}$ values at $-2 \ln \Lambda(\mu_{t\bar{t}}) = 1$ correspond to $\hat{\mu}_{t\bar{t}} \pm 1\sigma$.

the difference between the $\sigma_{\text{data}}^{\mu=1}$ and σ_{Asimov} was only $\mathcal{O}(10^{-3})$.

The hypothesis that the differences between expected and measured uncertainties were due to scaling, was further confirmed by looking at the relative impacts the individual systematic uncertainties had on the $\mu_{t\bar{t}}$ measurement⁶. The uncertainty impacts seen in Asimov data and real data are shown in the nuisance parameter (NP) ranking plots, in figures 8.2 and 8.3, respectively. The impacts are described by the top x -axis, and are shown in block blue and green colours, depending on whether the nuisance parameter is positively or negatively correlated with $\mu_{t\bar{t}}$. Comparing the two plots, the impacts of the individual nuisance parameters relative to the best-fit values of $\mu_{t\bar{t}}$, were seen to be highly similar in both data and Asimov fits, when taking into account the natural differences expected from fitting different datasets.

The ranking plots also show the systematic uncertainty pulls and widths⁷. No pulls were observed in the Asimov fit. This was expected, as the “data” and the nominal model were the same, and no preference for systematic uncertainties should

⁶ Nuisance parameter impact was described in section 7.4. The impact of parameter θ on μ is found by comparing the measured μ values when θ is a free parameter ($\hat{\mu}_{t\bar{t}}$), and is fixed to $\pm 1\sigma$. The *relative impact* is the ratio of the impact and $\mu_{t\bar{t}}$ as found when θ is free: $(\mu_{t\bar{t}}(\theta_{\text{fixed}}) - \hat{\mu}_{t\bar{t}}) / \hat{\mu}_{t\bar{t}}$.

⁷ The concepts of nuisance parameter pulls and widths were presented in section 7.4.

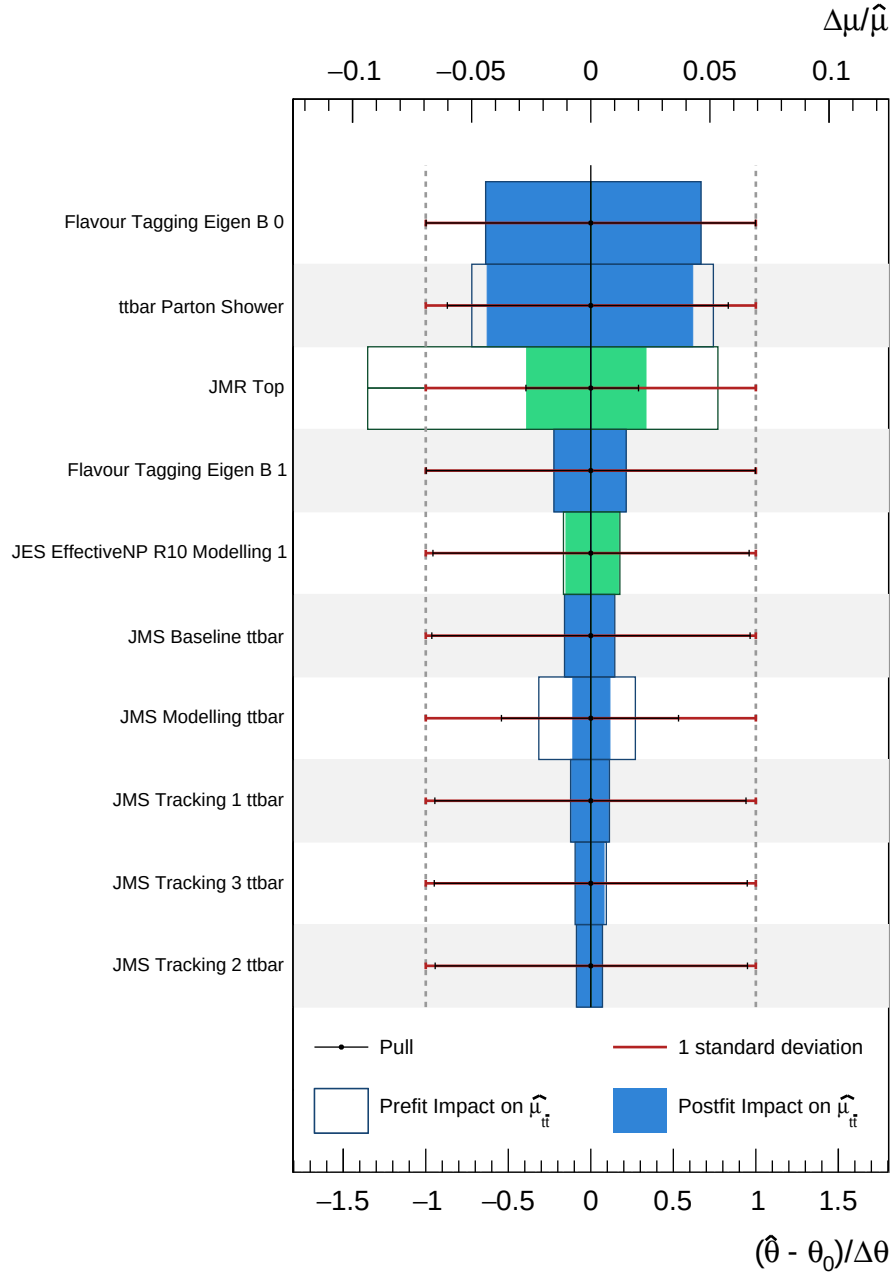


Figure 8.2: Ranking and pull plot of the 10 highest-impact systematic uncertainties on the $t\bar{t}$ signal strength ($\mu_{t\bar{t}}$) as measured in $\text{CR}_{t\bar{t}}$ Asimov data (built from MC samples). Impact relative to best-fit $\mu_{t\bar{t}}$ value is shown.

How to read the plot: the pre-fit and post-fit impact on μ is described by the top axis. It is found by fixing each uncertainty (θ) to $\pm 1\sigma$, extracting the resulting μ value and comparing it to the best-fit value, $\hat{\mu}$, such that $\Delta\mu = \mu - \hat{\mu}$. Blue (green) colour indicates (anti-)correlation between θ and μ . Also shown are pulls and widths of the systematic uncertainties, described by the bottom axis. $\hat{\theta}$ - best-fit value of the NP, θ_0 - pre-fit value of the NP, and $\Delta\theta$ - pre-fit width of the NP.

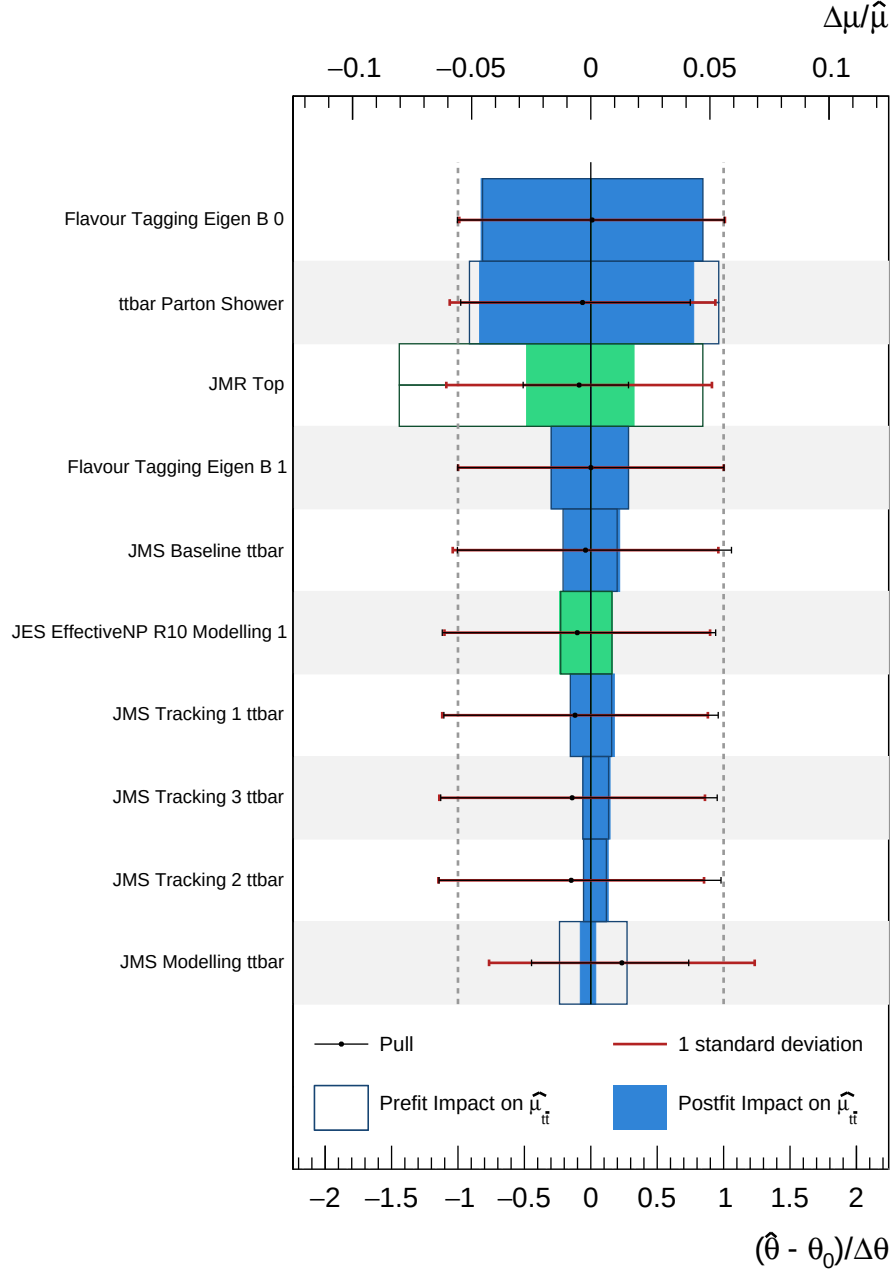


Figure 8.3: Ranking and pull plot of the 10 highest-impact systematic uncertainties on the $t\bar{t}$ signal strength ($\mu_{t\bar{t}}$) as measured in $\text{CR}_{t\bar{t}}$ data. Impact relative to best-fit $\mu_{t\bar{t}}$ value is shown.

How to read the plot: the pre-fit and post-fit impact on μ is described by the top axis. It is found by fixing each uncertainty (θ) to $\pm 1\sigma$, extracting the resulting μ value and comparing it to the best-fit value, $\hat{\mu}$, such that $\Delta\mu = \mu - \hat{\mu}$. Blue (green) colour indicates (anti-)correlation between θ and μ . Also shown are pulls and widths of the systematic uncertainties, described by the bottom axis. $\hat{\theta}$ - best-fit value of the NP, θ_0 - pre-fit value of the NP, and $\Delta\theta$ - pre-fit width of the NP.

be observed. A presence of pulls in the Asimov fit results would indicate issues with the model or fitting software. In the data fit some pulls were expected, induced by differences between the data and the initial model. No large pulls ($> 0.5\sigma$) requiring further investigation were observed.

The post-fit widths of the uncertainties showed strong constraints of the JMR⁷ (60%)⁸ and JMS modelling (41%) uncertainties, and a notable constraint of the Parton Shower (PS) generator uncertainty (14%). The constraints were seen both in data and Asimov fits, indicating that the constraining power was from the data statistics, rather than induced by differences between the data and model.

The large post-fit constraints on these uncertainties were not worrying as the uncertainties in question are initially large, as indicated by the pre-fit impact on $\mu_{t\bar{t}}$. The high purity and statistics available in the $\text{CR}_{t\bar{t}}$ region constrained the large uncertainties derived in general calibrations, as the data precision was higher than that of the uncertainties. This attests to the benefit of using targeted external regions in the phase-space of the analysis to aid the constraint of backgrounds.

Figure 8.4 shows the fit parameter correlations from the $\text{CR}_{t\bar{t}}$ standalone data fit. $\mu_{t\bar{t}}$ was seen to have the largest (anti-)correlations with the b -tagging (63%), PS (59%), and JMR (-34%) uncertainties. Such behaviour was entirely reasonable, as these were the three highest-impact uncertainties, and the correlation size followed the ordering of impact strength.

Large interactions were also seen between strongly constrained uncertainties: JMR, PS and JMS. The JMR uncertainty (the largest pre-fit uncertainty) had anti-correlations of -64% and -66% with the PS and JMS modelling uncertainties, respectively, whereas the PS and JMS uncertainties were positively correlated by 35%. Figure 8.5a shows a comparison between the JMR and PS uncertainties, and figure 8.5b shows a comparison between the JMR and JMS modelling uncertainties. Both the PS and JMR uncertainties, shown in figure 8.5a, had similar shapes and

⁸ The quoted values are from fits to data.

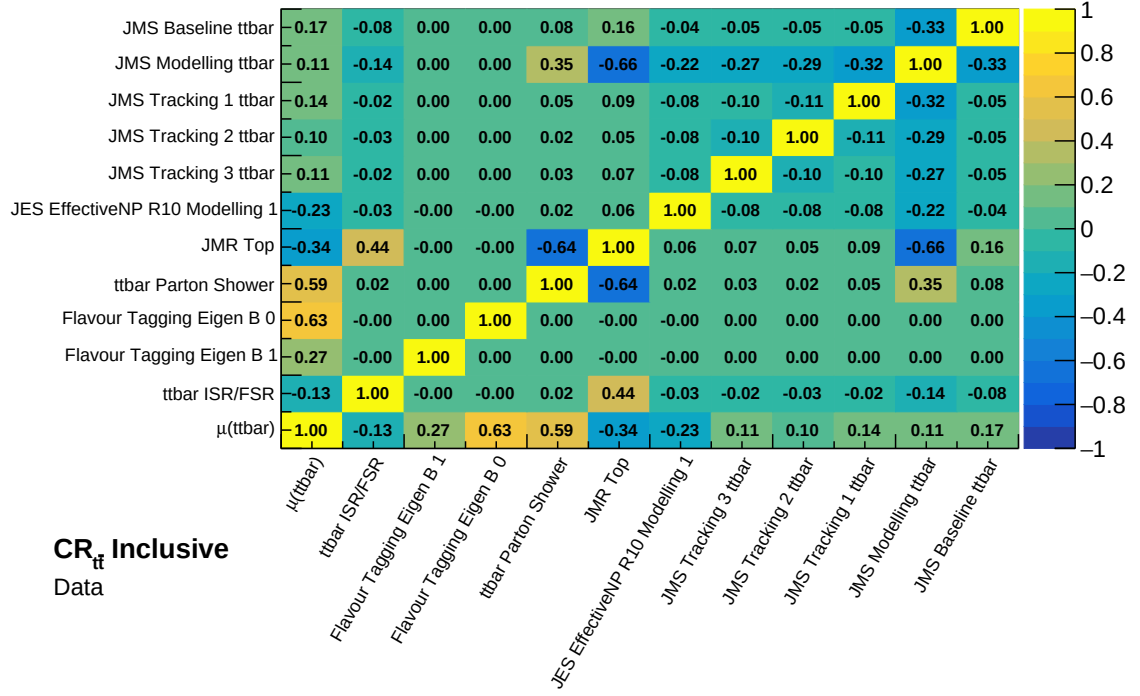


Figure 8.4: Fit parameter correlations from the standalone $\text{CR}_{t\bar{t}}$ data fit. Nuisance parameters with all correlation coefficients $|r| < 0.2$ are not shown.

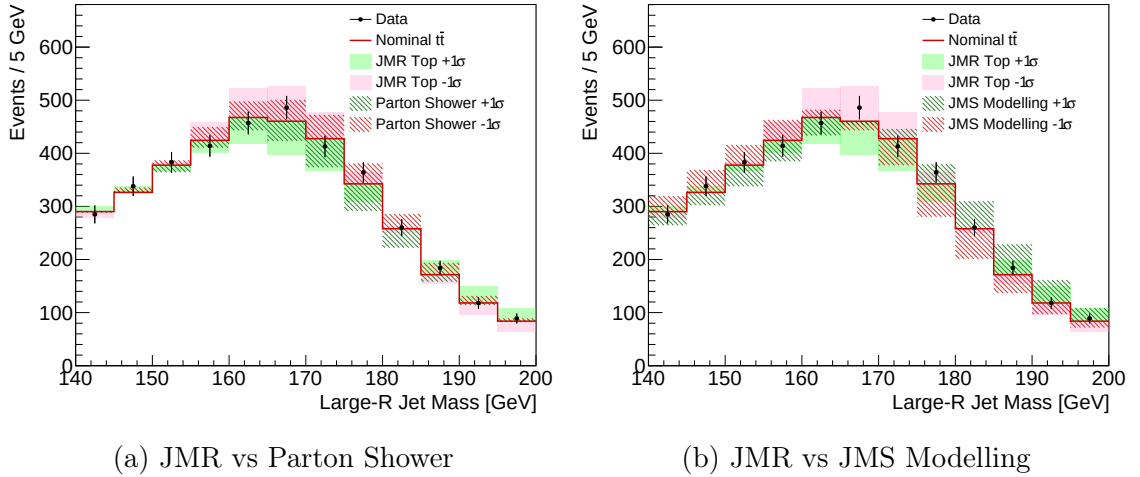


Figure 8.5: Candidate jet mass distributions of $\text{CR}_{t\bar{t}}$ data, the nominal $t\bar{t}$ MC template, and (a) the JMR and parton shower generator uncertainties, and (b) the JMR and JMS modelling uncertainties. All $t\bar{t}$ MC templates are scaled by $\mu_{t\bar{t}} = 0.79$ and have single-top and $W(\ell\nu)$ components added at the SM rate, to be comparable with data.

regions of largest effect, with the same directionality (i.e. effect of $\pm\sigma$) in many bins, which explains the strong anti-correlations. The JMR and PS uncertainties had similar effects around the peak of the $t\bar{t}$ distribution, but not in the high mass tail, whereas the JMR and JMS modelling overlap was seen between $m_{\text{jet}} = 150$ GeV and 165 GeV (just below the mass peak), and in the high mass tail. Such complementary overlap of these two uncertainties with the JMR uncertainty reflected in the positive correlation between the two uncertainties.

To summarise, the standalone $\text{CR}_{t\bar{t}}$ fit was thoroughly investigated, as was required for the use of this region in the Higgs boson measurement, and other studies. No indications of biases were seen, and good agreement between data and expectation was displayed. The $\text{CR}_{t\bar{t}}$ region showed excellent statistical power to significantly constrain the $t\bar{t}$ yield and some of the largest $t\bar{t}$ uncertainties, which, as will be seen in the following section, was highly beneficial for the signal region fit.

8.2 Simultaneous Fitting of SR and $\text{CR}_{t\bar{t}}$

The primary purpose of the $\text{CR}_{t\bar{t}}$ region was to control the $t\bar{t}$ background during the measurement of Higgs and Z boson signal strengths (μ_H and μ_Z). Therefore, the measurement was performed by fitting the signal regions (SRL and SRS) and the $\text{CR}_{t\bar{t}}$ region simultaneously, and fully correlating (100%) the $t\bar{t}$ scale factor ($\mu_{t\bar{t}}$ or $\text{SF}_{t\bar{t}}$) between all regions by describing it as a single parameter.

The technique of using an external control region to get a more precise estimate of the $t\bar{t}$ yield, was also used in the BSM $X(\rightarrow b\bar{b}) + j$ search, from which this analysis was derived. However, the BSM analysis took a simpler approach, by performing the $\text{CR}_{t\bar{t}}$ fit separately, and using the measured $\mu_{t\bar{t}}$ and $\sigma_{t\bar{t}}$ to construct a Gaussian prior for the $t\bar{t}$ yield in the signal region (SR). The prior entered the fit as another nuisance parameter, acting on the $t\bar{t}$ yield. Despite being simpler, this approach had limitations which will be explored in this section, and were overcome by using a simultaneous SR and $\text{CR}_{t\bar{t}}$ fit set-up.

The ability to construct and use an external data region, with high statistics of a significant background can be a powerful aid to a measurement. This section discusses the impact of using information from the external $\text{CR}_{t\bar{t}}$ region to benefit the Higgs boson measurement, and compares the use of a Gaussian prior in the SR, as was done in the parent BSM analysis, to simultaneous fitting of SR and $\text{CR}_{t\bar{t}}$. The simultaneous fit configuration was also validated through the observation of various fit features and comparison with the results from standalone $\text{CR}_{t\bar{t}}$ fits.

The studies presented in this section discuss results from inclusive SR fits with 0.5 GeV binning, as was used throughout a large part of the analysis development process⁹. Most results discussed in this section were extracted from Asimov data in order to keep the signal region data blind. Where results from data were quoted, the Higgs boson component in the fit had been fixed to the SM value ($\mu_H = 1$), and only results concerning the $t\bar{t}$ process were observed. In the following, the different fit configurations are referred to as:

- SR+CR_{t $\bar{t}$} fit* – simultaneous SR and $\text{CR}_{t\bar{t}}$ fit (inclusive measurement set-up);
- SR+Gauss fit* – SR fit with a Gaussian prior on the $t\bar{t}$ yield derived from $\text{CR}_{t\bar{t}}$;
- SR-only fit* – SR fit with no information from $\text{CR}_{t\bar{t}}$;
- CR_{t $\bar{t}$} -only fit* – standalone $\text{CR}_{t\bar{t}}$ fit.

In all listed cases, SR denotes a simultaneous SRL and SRS fit. The most important difference to be understood between the SR+Gauss configuration and SR+ $\text{CR}_{t\bar{t}}$ configuration, was that the former effectively decorrelates all $t\bar{t}$ uncertainties between $\text{CR}_{t\bar{t}}$ and the signal regions, and the latter correlates them fully.

⁹ See section 5.7.1 for more details on the binning.

8.2.1 Impact on the $t\bar{t}$ Background

The power to constrain the $t\bar{t}$ background of different fit configurations can be most easily compared by observing the resulting $\mu_{t\bar{t}}$ uncertainties from each fit. A comparison of expected uncertainties found by fitting Asimov data is shown in table 8.1, where the two rightmost columns show the difference in total uncertainties achieved by using SR+ $\text{CR}_{t\bar{t}}$ fit instead of the listed one.

Utilising the $\text{CR}_{t\bar{t}}$ region together with the signal regions, as opposed to using only SR, resulted in a striking 80.9% reduction of $t\bar{t}$ uncertainties (more than 5 times smaller). The result was not surprising given the purity of $\text{CR}_{t\bar{t}}$ compared to the signal regions, however, the extent of improvement signified the importance of utilising the $\text{CR}_{t\bar{t}}$ region.

A small, 4.4% reduction in uncertainties was also seen when comparing the combined model to a $\text{CR}_{t\bar{t}}$ -only fit. In equivalent data fits, shown in table 8.2, the relative uncertainty reduction increased to 7.8%. Such results indicated that the combination of regions was beneficial to improving the uncertainty on the $t\bar{t}$ component. The reasons for the $\mu_{t\bar{t}}$ measurement improvement are discussed later in this section.

Table 8.1: The uncertainty breakdown of $\mu_{t\bar{t}}$ measurements in Asimov data fits with different SR and $\text{CR}_{t\bar{t}}$ configurations. $\Delta\sigma/\sigma = (\sigma' - \sigma)/\sigma$, where σ' is the uncertainty from SR+ $\text{CR}_{t\bar{t}}$ fit, describes the change in uncertainty from using SR+ $\text{CR}_{t\bar{t}}$ as opposed to the alternative configuration.

Fit	σ_{stat}	σ_{syst}	$\Delta\sigma_{\text{total}}$	$\Delta\sigma_{\text{total}}/\sigma_{\text{total}}$
SR + $\text{CR}_{t\bar{t}}$	0.02	$^{+0.07}_{-0.07}$	—	—
SR Only	0.12	$^{+0.39}_{-0.29}$	−0.29	−80.9%
$\text{CR}_{t\bar{t}}$ Only	0.02	$^{+0.07}_{-0.07}$	−0.003	−4.4%

In the SR+Gauss fit, a constraint was used for the $t\bar{t}$ yield, and no $\mu_{t\bar{t}}$ measurement was made. As the Gaussian prior was included in the fit as a nuisance parameter, the fit could enlarge or reduce its width. The SR+Gauss fit reduced the initial $t\bar{t}$ uncertainty (taken from $\text{CR}_{t\bar{t}}$) by 2% in Asimov data, and 1% in data – notably smaller than the change seen when comparing the $\text{CR}_{t\bar{t}}$ -only and SR+ $\text{CR}_{t\bar{t}}$ configurations. This suggested that the interplay of uncertainties in a simultaneous SR and $\text{CR}_{t\bar{t}}$ fit, which was lost by decoupling these regions with the SR+Gauss model, was beneficial to reducing $t\bar{t}$ uncertainties.

Measurement Stability

Table 8.2 shows the $\mu_{t\bar{t}}$ measurements made in a simultaneous SR+ $\text{CR}_{t\bar{t}}$ fit, and a standalone $\text{CR}_{t\bar{t}}$ fit in data. It also highlights the relative shifts induced in the $\mu_{t\bar{t}}$ values by performing a simultaneous fit, as opposed to a $\text{CR}_{t\bar{t}}$ -only fit ($|\Delta\mu_{t\bar{t}}|/\sigma_{\text{CR}}$). It was notable, that the measured $\mu_{t\bar{t}}$ values in SR+ $\text{CR}_{t\bar{t}}$ and $\text{CR}_{t\bar{t}}$ -only data fits closely agreed, differing only by $|\Delta\mu| = 0.02$, which equates to a 0.3σ shift in reference to the uncertainty on the $\mu_{t\bar{t}}$ from the $\text{CR}_{t\bar{t}}$ -only fit. This indicated that the $t\bar{t}$ yield measurement was stable and largely determined by the $\text{CR}_{t\bar{t}}$ region. Once again, no comparison for $\mu_{t\bar{t}}$ values can be made with SR+Gauss method, as it imposed a constraint on the yield of the $t\bar{t}$ process equivalent to the standalone $\text{CR}_{t\bar{t}}$ measurement.

Table 8.2: Comparison of $\mu_{t\bar{t}}$ measurements from SR+ $\text{CR}_{t\bar{t}}$ and $\text{CR}_{t\bar{t}}$ -only fits to data. $|\Delta\mu_{t\bar{t}}|/\sigma = |\mu'_{t\bar{t}} - \mu_{t\bar{t}}|/\sigma$, where $\mu_{t\bar{t}}$ and σ are the $t\bar{t}$ scale factor measurement and uncertainty from the $\text{CR}_{t\bar{t}}$ -only fit, and $\mu'_{t\bar{t}}$ is from a SR+ $\text{CR}_{t\bar{t}}$ fit.

Fit	$\mu_{t\bar{t}}$	σ_{stat}	σ_{syst}	$ \Delta\mu_{t\bar{t}} $	$ \Delta\mu_{t\bar{t}} /\sigma_{\text{total}}$
SR + $\text{CR}_{t\bar{t}}$	0.81	0.01	$^{+0.06}_{-0.05}$	–	–
$\text{CR}_{t\bar{t}}$ Only	0.79	0.01	$^{+0.06}_{-0.06}$	0.02	0.30σ

$t\bar{t}$ Uncertainties

A more in-depth perspective was offered by comparison of the post-fit widths of the individual $t\bar{t}$ systematic uncertainties under different fit configurations in Asimov data, shown in figure 8.6. The SR-only configuration was seen to provide the least constraint. The SR+Gauss configuration showed stronger constraints than the SR-only fit, likely due to the tightly bound $t\bar{t}$ yield.

As seen in figure 8.6, fitting the SR and $\text{CR}_{t\bar{t}}$ simultaneously (SR+ $\text{CR}_{t\bar{t}}$) offered the most constraint out of all fit configurations, particularly for generator – parton shower (PS) and matrix element (ME) uncertainties, JMR uncertainties, and to a smaller extent, JMS modelling uncertainties. The JMR and PS uncertainties were the largest $t\bar{t}$ uncertainties entering the fit, therefore stronger constraints on these uncertainties translated into an uncertainty reduction for $\mu_{t\bar{t}}$.

As will be discussed later in this section, the combination of SR and $\text{CR}_{t\bar{t}}$ regions imposed strong nuisance parameter (NP) correlations dominated by $\text{CR}_{t\bar{t}}$. This was likely the reason behind the stronger constraints in the SR+ $\text{CR}_{t\bar{t}}$ fit, because any additional constraints from the SR had to be compatible with the constraints imposed by $\text{CR}_{t\bar{t}}$. Otherwise, if the additional constraints were solely driven by the knowledge of $\mu_{t\bar{t}}$, and the SR features, the same uncertainty widths would be seen in SR+ $\text{CR}_{t\bar{t}}$ and SR+Gauss configurations. This hypothesis was investigated further in the following.

The reason behind the increased constraints in the simultaneous fit were understood by comparing the constrained uncertainties between the SR and $\text{CR}_{t\bar{t}}$ regions, shown in figure 8.7. Due to the purity and high statistics of the $\text{CR}_{t\bar{t}}$ region most constraints were expected to be provided by the $\text{CR}_{t\bar{t}}$ region. However, looking at uncertainty comparisons in figure 8.7, it was evident that the SR could offer additional constraining power.

Firstly, the generator uncertainties – parton shower (PS) and matrix element (ME) were much larger in the signal regions compared to the $\text{CR}_{t\bar{t}}$ region. In the

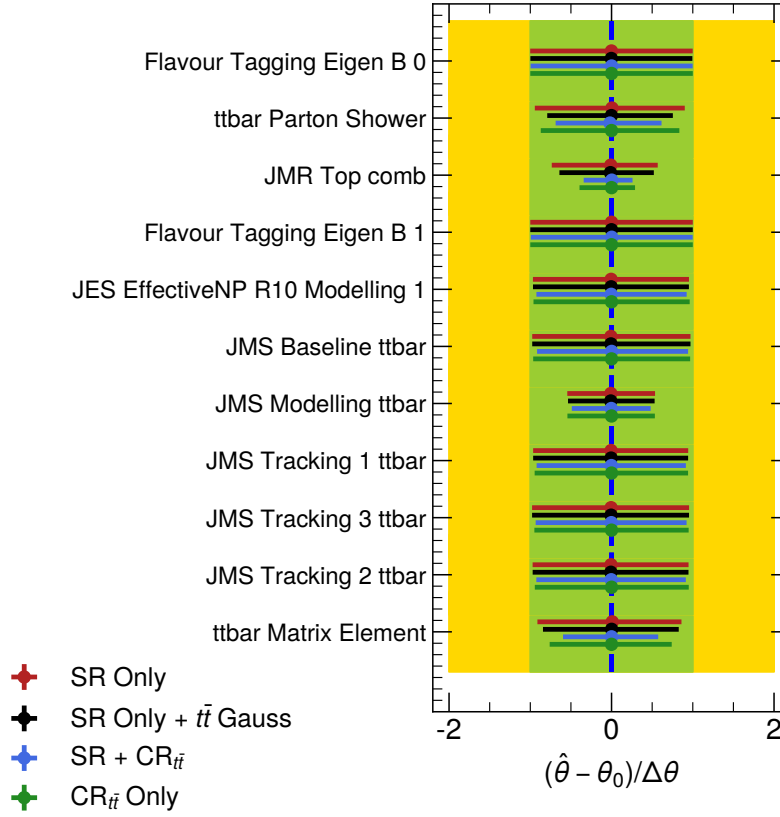


Figure 8.6: Systematic uncertainty pull and width comparison of Asimov fits with different SR and $\text{CR}_{t\bar{t}}$ configurations, for the top 10 highest impact $t\bar{t}$ uncertainties in $\text{CR}_{t\bar{t}}$ in order of post-fit impact (see figure 8.2): highest-to-lowest shown top-to-bottom. Matrix Element uncertainty (ranking 14th) is also included to show both generator uncertainties. The SR+ $\text{CR}_{t\bar{t}}$ fit configuration (blue) was seen to have the strongest constraints, which were understood to arise from the excellent constraining power of $\text{CR}_{t\bar{t}}$, and the $t\bar{t}$ nuisance parameter correlation across SR and $\text{CR}_{t\bar{t}}$ regions. The stronger constraints were seen as a benefit of using the SR+ $\text{CR}_{t\bar{t}}$ configuration.

signal regions the PS and ME uncertainties had normalisation effects ranging between 13% – 19%, and included shape components, whereas in the $\text{CR}_{t\bar{t}}$ the ME normalisation effects were < 2% (and therefore pruned), and PS had a 7% effect. The large extent of these uncertainties would make them easier to constrain, given the precise estimate of the $t\bar{t}$ yield and other high-ranking uncertainties provided

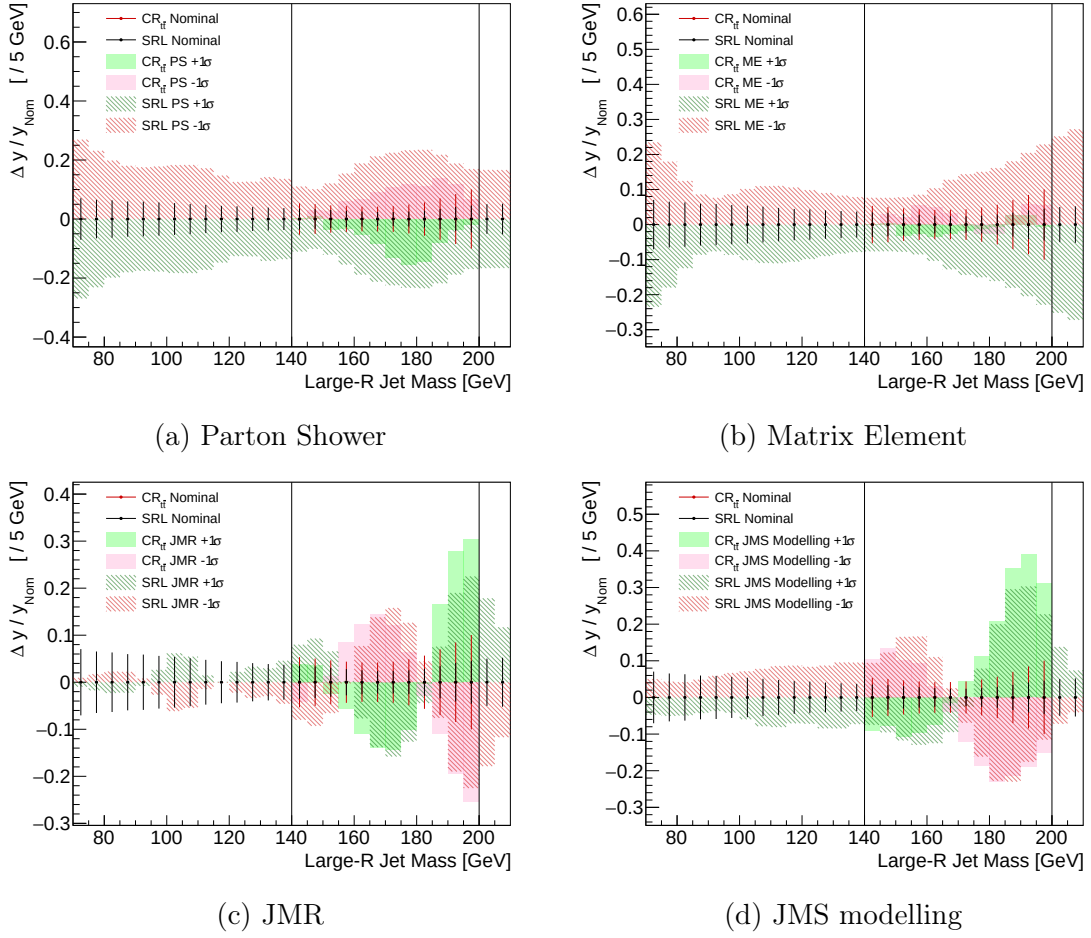


Figure 8.7: Comparisons of the bin-by-bin differences between the nominal $t\bar{t}$ templates and (a) parton shower, (b) matrix element (c) JMR, and (d) JMS modelling uncertainty $\pm 1\sigma$ variations, illustrating the extent of these uncertainties, in the SRL and $\text{CR}_{t\bar{t}}$ regions. The vertical lines indicate the fit range of $\text{CR}_{t\bar{t}}$. The uncertainties shown at the points at zero are the MC statistical uncertainties on the nominal templates. The m_{jet} templates of these uncertainties can be found in figures G.4 (a, b) and G.6 (c, d) in appendix G.3.

by $\text{CR}_{t\bar{t}}$. To a smaller extent this could also be true for JMR and JMS uncertainties which also had regions of the m_{jet} spectra where their uncertainties were larger in the SR as compared to $\text{CR}_{t\bar{t}}$. Furthermore, the SR fit range was also wider than the $\text{CR}_{t\bar{t}}$ range, which could have provided additional shape constraints in the tails of the $t\bar{t}$ distribution.

Despite the lower sensitivity of the signal regions, the additional constraints

from the signal regions could be obtained due to the excellent control of the $t\bar{t}$ scale factor and strong constraints on high-impact NPs provided by the $\text{CR}_{t\bar{t}}$, which restricted the freedom of the large nuisance parameters. The correlation of NPs between the SR and $\text{CR}_{t\bar{t}}$ required that any constraints between these regions were compatible, which allowed the large nuisance parameters to be constrained further using information from the signal regions.

This is further supported by the NP pull plot in figure 8.6. None of the constraints would have been possible by solely using the SR information, given the large backgrounds in the SR. The sole addition of the $\mu_{t\bar{t}}$ constraint in the SR+Gauss configuration also did not provide as good NP constraints as seen in the $\text{CR}_{t\bar{t}}$. Hence, it was understood that allowing the nuisance parameters to interact across the SR and $\text{CR}_{t\bar{t}}$ regions was the driving force behind the stronger NP constraints, and was seen as a benefit of using the simultaneous fit configuration.

8.2.2 Impact on Other Processes in the Signal Region

The impact of different SR and $\text{CR}_{t\bar{t}}$ configurations on the expected μ_H and μ_Z measurement accuracy was also investigated using Asimov data, and shown in table 8.3. No substantial effect was seen on the Z boson uncertainties with any configuration, due to the large separation of the Z boson and $t\bar{t}$ resonances, and resulting small interplay between these processes. A small, $\sim 4\%$ relative reduction of Higgs boson uncertainties was seen in a simultaneous SR+ $\text{CR}_{t\bar{t}}$ fit, as compared to SR-only or SR+Gauss configurations, implying that the active interplay between the SR and $\text{CR}_{t\bar{t}}$ regions was beneficial to the Higgs boson measurement as well.

Another important relationship to explore was the one between the $t\bar{t}$ constraints and the QCD function parameters¹⁰. Table 8.4 shows the relative uncertainties (σ_{rel}) on the QCD yield and $N = 1, 2, 3$ QCD function parameters as measured using the

¹⁰ The QCD background was estimated using a parametric function, described in section 6.4. The description is a polynomial exponential function, which in the inclusive SR has $N = 5$ parameters.

Table 8.3: The uncertainty breakdown of μ_H and μ_Z measurements in Asimov data fits with different SR and CR_{t $\bar{t}$} configurations. $\Delta\sigma/\sigma = (\sigma' - \sigma)/\sigma$, where σ' is the uncertainty from SR+CR_{t $\bar{t}$} fit, describes the relative change in σ from using SR+CR_{t $\bar{t}$} as opposed to the alternative configuration.

	Fit	σ_{stat}	σ_{syst}	$\Delta\sigma_{\text{total}}$	$\Delta\sigma_{\text{total}}/\sigma'_{\text{total}}$
μ_H	SR + CR _{t$\bar{t}$}	2.5	$^{+2.4}_{-2.0}$	—	—
	SR + Gauss	2.5	$^{+2.6}_{-2.2}$	−0.14	−3.9%
	SR Only	2.5	$^{+2.5}_{-2.2}$	−0.14	−4.0%
μ_Z	SR + CR _{t$\bar{t}$}	0.13	$^{+0.11}_{-0.08}$	—	—
	SR + Gauss	0.13	$^{+0.11}_{-0.08}$	$-\mathcal{O}(10^{-4})$	−0.06%
	SR Only	0.14	$^{+0.11}_{-0.08}$	$-\mathcal{O}(10^{-4})$	−0.2%

Table 8.4: Uncertainty breakdown of the yield and 3 lowest order QCD estimate function parameters as measured in Asimov data fits. The QCD estimate function form is given in equation 6.1 of section 6.4. Numbers for SR+CR_{t $\bar{t}$} show the total relative uncertainty on each parameter ($\sigma_{\text{rel}} = \sigma/\theta$), whereas the values given for the two alternative configurations describe the relative change in σ_{rel} achieved by using SR+CR_{t $\bar{t}$} (σ'_{rel}), instead of the alternative (σ_{rel}). $\Delta\sigma_{\text{rel}} = \sigma'_{\text{rel}} - \sigma_{\text{rel}}$.

Fit		SRL				SRS			
		Yield	θ_1	θ_2	θ_3	Yield	θ_1	θ_2	θ_3
SR + CR _{t$\bar{t}$}	σ'_{rel}	0.6%	3.9%	49.2%	49.3%	0.6%	2.5%	13.1%	103.1%
SR + Gauss	$\frac{\Delta\sigma_{\text{rel}}}{\sigma_{\text{rel}}}$	−21%	−8%	−20%	−7%	−25%	−7%	−6%	−5%
SR Only	σ_{rel}	−44%	−32%	−20%	−16%	−47%	−24%	−14%	−11%

SR+ $\text{CR}_{t\bar{t}}$ fit configuration, and the percentage change in the relative uncertainties on these parameters achieved by using SR+ $\text{CR}_{t\bar{t}}$ instead of the two alternative configurations (SR+Gauss, and SR-only) in Asimov data.

An impressive reduction of σ_{rel} was seen in both comparisons, with an average of 12% reduction when moving from SR+Gauss to SR+ $\text{CR}_{t\bar{t}}$, and an average of 26% reduction between SR-only, and SR+ $\text{CR}_{t\bar{t}}$. Such changes show that the constraint of the $t\bar{t}$ background and its uncertainties plays a important role in controlling the QCD estimate.

Improvements in the control of the QCD background were especially important as the QCD estimate directly impacts the determination of the Higgs boson signal strength. The QCD background was an immense presence in the signal region, ~ 550 times larger than the Higgs boson signal in the Higgs resonance region ($m_{\text{jet}} \in [105, 140]$ GeV). In a fit to real data, where the model does not perfectly agree with the data, like it does in an Asimov fit, any improvement to the control of this immense background was crucial to improve stability and convergence in the fit, as well as the sensitivity for the μ_H measurement.

The causes of the large impact on QCD uncertainties through constraint of $t\bar{t}$ were investigated to deem the fit model safe for the Higgs boson measurement. This was done by comparing the fit parameter correlations between different fit configurations as found in Asimov data. Figure 8.8 shows the correlations of the three resonance signal strengths - $\mu_{H/Z/t\bar{t}}$, with important fit parameters parameters. A clear trend was seen in the correlations between $\mu_{t\bar{t}}$ and the shown QCD parameters. In the SR-only fit $\mu_{t\bar{t}}$, was highly (anti-)correlated with the QCD parameters, by up to 71%. With the introduction of a $t\bar{t}$ yield constraint in SR+Gauss fit, the interaction between $\mu_{t\bar{t}}$ and QCD parameters reduced to $\leq 18\%$. When the correlation of $t\bar{t}$ uncertainties between SR and $\text{CR}_{t\bar{t}}$ regions was introduced in the SR+ $\text{CR}_{t\bar{t}}$ fit, the extent of the interaction was further reduced to $\leq 12\%$. This showed that as the $t\bar{t}$ constraints were improved, the QCD parameters had less freedom to fluctuate

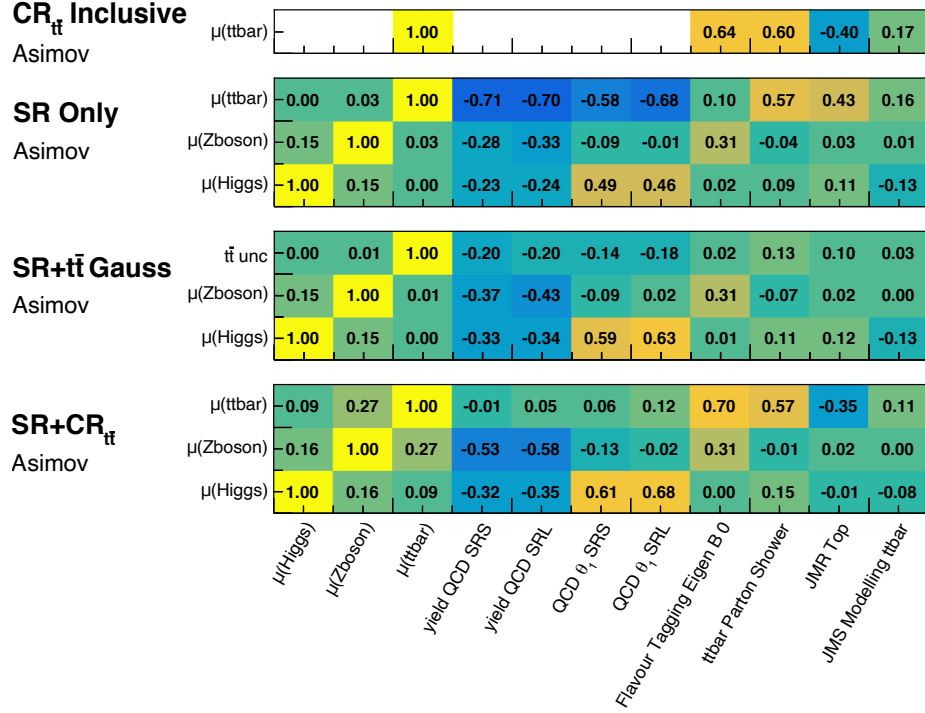


Figure 8.8: Fit parameter correlations in Asimov fits with different SR and $\text{CR}_{t\bar{t}}$ configurations, focusing on the correlations of the H , Z and $t\bar{t}$ signal strengths ($\mu_{H/Z/t\bar{t}}$) between themselves, with low order QCD parameters, and with three highest-impact $t\bar{t}$ uncertainties and the JMS modelling, which was known to have strong correlations in the $\text{CR}_{t\bar{t}}$ -only fit. Note that in the SR+Gauss fit, instead of $\mu_{t\bar{t}}$ parameter there is a Gaussian uncertainty on the $t\bar{t}$ yield called $t\bar{t}$ unc.

by altering the $t\bar{t}$ yield, which resulted in reduced QCD uncertainties, and a much more accurate estimate of the two largest backgrounds in the signal regions – QCD and $t\bar{t}$.

Figure 8.9 shows the correlations of the three highest ranking $t\bar{t}$ uncertainties, and the JMS Modelling uncertainty (7th in the ranking), which was highly correlated with high ranking NPs in the $\text{CR}_{t\bar{t}}$ -only and constrained by the simultaneous fit set-up. It was notable that in the simultaneous fit configuration, the inter-correlations between the shape uncertainties – JMR, PS and JMS modelling have increased, as compared to the SR-only, or SR+Gauss fit configurations, and were very similar to those seen in the standalone $\text{CR}_{t\bar{t}}$ fit. As was discussed previously, the strong NP

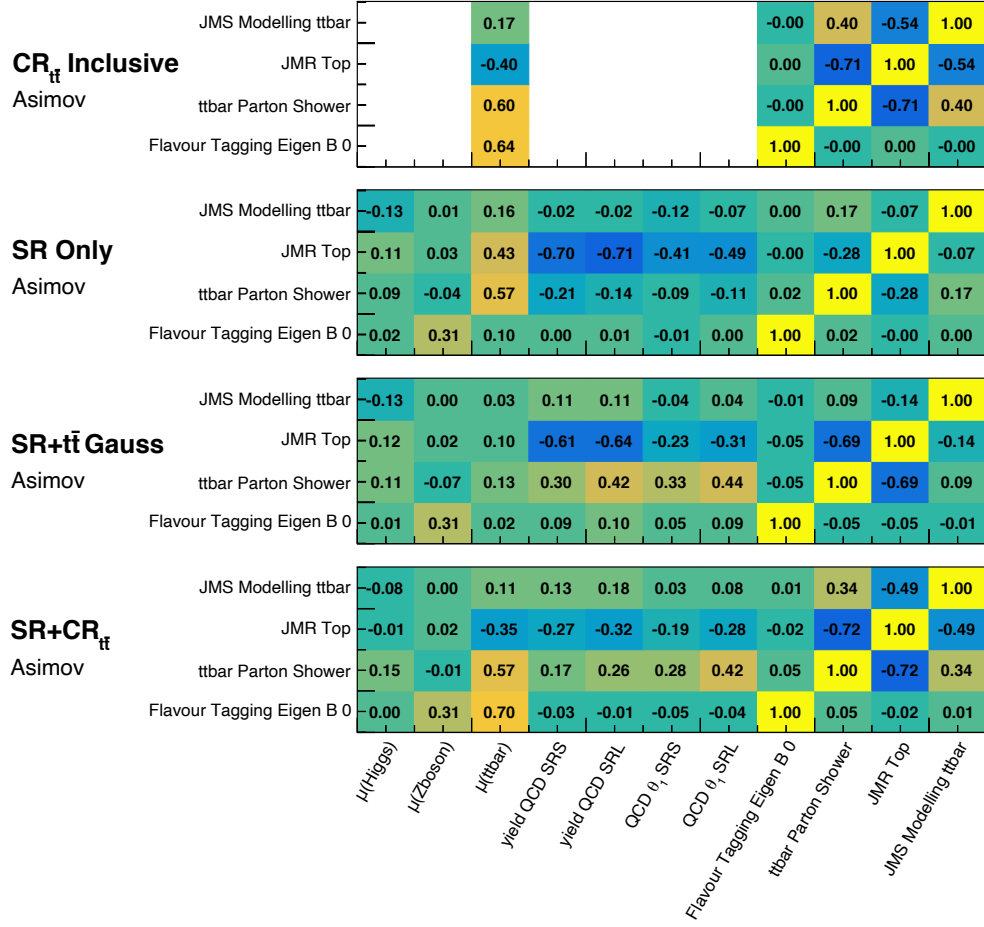


Figure 8.9: Fit parameter correlations in Asimov fits with different SR and $\text{CR}_{t\bar{t}}$ configurations, focusing on the correlations of the three highest-impact $t\bar{t}$ uncertainties and the JMS modelling uncertainty, which was known to have strong correlations in the $\text{CR}_{t\bar{t}}$ -only fit, with H , Z and $t\bar{t}$ signal strengths ($\mu_{H/Z/t\bar{t}}$), and low order QCD parameters. In the SR+Gauss fit, instead of $\mu_{t\bar{t}}$ parameter there is a Gaussian uncertainty on the $t\bar{t}$ yield called $t\bar{t} \text{ unc}$.

correlations imposed by the $\text{CR}_{t\bar{t}}$ region, which were transferred to the SR in the simultaneous fit, allowed the SR to further constrain some large nuisance parameters.

For all fit parameters, the SR+ $\text{CR}_{t\bar{t}}$ correlations were largely seen to follow the correlations of $\text{CR}_{t\bar{t}}$, which was expected due to the high purity and statistics of the $\text{CR}_{t\bar{t}}$ region. This behaviour was also consistent with the $\mu_{t\bar{t}}$ measurements in data shown previously, which indicated that the $t\bar{t}$ measurement was dominated by the

$\text{CR}_{t\bar{t}}$ region. Overall, the results between the $\text{CR}_{t\bar{t}}$ -only and the simultaneous SR and $\text{CR}_{t\bar{t}}$ fit were seen to be compatible with no observed tensions between the $t\bar{t}$ descriptions derived in either fit.

The studies presented in this section showcased the benefits of using a simultaneous SR and $\text{CR}_{t\bar{t}}$ fit for the Higgs boson measurement, as opposed to using only SR information, or including the $\mu_{t\bar{t}}$ measurement from $\text{CR}_{t\bar{t}}$ as a Gaussian prior on the $t\bar{t}$ yield. The $\text{CR}_{t\bar{t}}$ was shown to provide excellent constraint on $\mu_{t\bar{t}}$ and some of the highest-impact $t\bar{t}$ nuisance parameters, and the simultaneous fit set-up improved these constraints by allowing the interplay of NPs between SR and $\text{CR}_{t\bar{t}}$ regions. The simultaneous fit set-up also provided the strongest constraints on QCD nuisance parameters, by decoupling the QCD and $t\bar{t}$ backgrounds, which in turn lead to better fit stability, convergence, and sensitivity to the Higgs boson signal.

The author implemented the simultaneous SR and $\text{CR}_{t\bar{t}}$ fit setup into the analysis framework, and produced early studies of this fit configuration, similar to those presented in this section. These early studies presented the possibility to use the simultaneous SR and $\text{CR}_{t\bar{t}}$ fit setup for the measurement, showcased similar benefits, and validated it, such that the simultaneous fit setup could be used for the Higgs boson measurements.

8.3 Chapter Overview

This chapter discussed the features of the $\text{CR}_{t\bar{t}}$ standalone fit, showcased the excellent constraining power of the inclusion of the $\text{CR}_{t\bar{t}}$ region in the Higgs boson measurement fit, and validated the $\text{CR}_{t\bar{t}}$ standalone and simultaneous SR and $\text{CR}_{t\bar{t}}$ fits for use in the Higgs boson measurement and analysis development studies.

Section 8.1 presented validation studies of standalone $\text{CR}_{t\bar{t}}$ fits, comparing various features of the $\text{CR}_{t\bar{t}}$ data fit with expectations from fits to Asimov data. No features indicative of issues in the fitting software or the fit model were observed.

The $\mu_{t\bar{t}}$ profile likelihoods were seen to be parabolic. Small differences in $\mu_{t\bar{t}}$ uncertainties between measurement and expectation were seen to arise from $\mu_{t\bar{t}}$ scaling. No large systematic uncertainty pulls ($> 0.5\sigma$) were observed, which would require further understanding. The $\text{CR}_{t\bar{t}}$ region was seen to have great statistical power to constrain some of the largest $t\bar{t}$ uncertainties.

Section 8.2 explored the impact of including information from $\text{CR}_{t\bar{t}}$ to the signal region fit. The studies also compared two different ways to include $\text{CR}_{t\bar{t}}$ information in the signal region fit: by performing the $\text{CR}_{t\bar{t}}$ fit separately and constraining the $t\bar{t}$ yield in the signal region with a Gaussian prior derived from the $\text{CR}_{t\bar{t}}$ fit result; and by performing a simultaneous fit, with $\mu_{t\bar{t}}$ fully correlated between all regions.

Overall, any inclusion of $\text{CR}_{t\bar{t}}$ information to the signal region fit was seen to be beneficial: the expected uncertainties on the $t\bar{t}$ yield were reduced by more than a factor of 5. The expected relative uncertainties on the QCD parameters were also seen to be largely reduced, which was determined to be due to the reduced freedom in the fit. Fitting the SR and $\text{CR}_{t\bar{t}}$ regions simultaneously was seen to be the most beneficial approach, providing the largest reduction of expected $t\bar{t}$ and QCD uncertainties, and a small reduction of expected Higgs boson uncertainties.

Furthermore, the simultaneous SR and $\text{CR}_{t\bar{t}}$ fit configuration enabled the interaction of $t\bar{t}$ uncertainties between the regions, which provided more information to the fit and lead to improved $t\bar{t}$ constraints. The studies also showed consistency between the $t\bar{t}$ descriptions in the standalone $\text{CR}_{t\bar{t}}$ fit and the simultaneous SR and $\text{CR}_{t\bar{t}}$ fit. The $t\bar{t}$ scale factor and uncertainty behaviour was primarily governed by the $\text{CR}_{t\bar{t}}$ region, which was expected given its high statistics and purity.

Overall, combining the $\text{CR}_{t\bar{t}}$ region with the signal region fit was shown to lead to excellent improvements in the constraints on the two largest backgrounds in the signal region - $t\bar{t}$ and QCD, which was vital for fit stability, and also had positive effects on the expected Higgs boson results. The following chapters will return to the previous notation for the $t\bar{t}$ scale factor, $\text{SF}_{t\bar{t}}$, instead of $\mu_{t\bar{t}}$.

Chapter 9

The Results

The analysis aimed to make three types of Higgs boson measurements: a Higgs boson signal strength (μ_H) measurement over the entire accessible candidate jet transverse momentum (p_T^{jet}) spectra, called the **inclusive measurement**; a Higgs boson cross-section measurement within a fiducial phase space defined by the fully accessible Higgs boson phase-space, called the **fiducial measurement** and a measurement of the p_T^H -binned Higgs boson cross-sections, called the **differential measurement**. The results from these measurements are presented in sections 9.3, 9.4 and 9.5, respectively. A differential measurement of the Z boson signal strengths was also performed following the same procedure.

The measurements were described in detail in section 5.5, and a brief reminder is given in section 9.1. As the thesis was written while the analysis was being finalised, some changes in the measurement configurations have been made. These changes did not impact the outcomes of the studies presented in this thesis, and are summarised in section 9.1.

Validation studies for particularly relevant changes, which could have had an impact on the studies are given in appendix H. The studies did not show any significant differences, and confirmed that the analysis developments presented in this thesis did not need to be revisited.

The results were produced by other members of the analysis team using the

framework and methodology that has been developed in large part by the author. As well as being the main contributor to the analysis framework, the author produced many fit development and validation studies, which were paramount to the making of these measurements, and the methodology of which was used by other members of the analysis team.

Most results shown throughout the chapter have been taken from the published analysis paper [5] or corresponding internal documentation [73]. Where not cited, the results or figures were produced by the author using output files from the measurement fits produced by the group for the paper. The measurement comparison between using 5 GeV and 0.5 GeV binning in the SR discussed in appendix H.1 was produced by the author.

9.1 Fit Set-up and Evolution

All measurements were made by performing binned likelihood fits of SM processes expected in the Higgs boson candidate jet mass spectra, and extracting the Higgs boson signal strength(s)¹ μ_H ($\mu_H = 1$ in SM). In the **fiducial** and **differential** Higgs boson cross-section measurements the measured signal strengths were interpreted as cross-sections, as described in section 9.2.

The measurements were made by fitting leading-jet and subleading-jet signal regions (SRL and SRS), and the $t\bar{t}$ control region, $\text{CR}_{t\bar{t}}$, simultaneously. The SM processes considered in the regions were:

SR : H , Z , W , $t\bar{t}$, single top-quark, QCD;

$\text{CR}_{t\bar{t}}$: $t\bar{t}$, single top-quark, $W(\ell\nu)$.

A detailed description of the binned likelihood fits used to make the measurements is given in section 5.7.

¹ The differential measurement extracted Higgs boson signal strengths in several p_T^H bins simultaneously.

Table 9.1 shows the signal region definitions (left) and fiducial volumes in which measurements were made (right). In the differential measurement, the Higgs boson signal strength in each p_T^H volume was described by a different free parameter in the fit (i.e. was measured separately), with each $\mu_H^{p_T}$ fully correlated across all signal regions. The resonant background components were treated independently in regions with different p_T^{jet} ranges, and the QCD backgrounds were treated independently in each region.

The differential measurement setup was also used to determine Z boson signal strengths in bins of truth-level Z boson p_T (p_T^Z), and compare them to SM predictions. In this case the Z +jets process was treated as the signal and measured in p_T^Z bins, whereas the Higgs boson process was described as a background (defined inclusively within candidate p_T^{jet} bins) and fixed to the SM prediction in each p_T^{jet} bin. The Higgs boson signal was expected to be around 50 – 130 times smaller under the Z boson resonance ($m_{\text{jet}} \in [70, 110]$ GeV), so the effects of fixing it to the SM contribution were negligible.

Table 9.1: (Left) the signal region definitions in terms of p_T used in the Higgs or Z boson measurements, and (right) the fiducial volumes in which the H or Z measurements are made ($X = H, Z$). Each SR had corresponding $\text{CR}_{t\bar{t}}$ and VR regions. The maximum jet p_T in all regions was 3 TeV. “bin 0/1/2” – differential p_T^{jet} -binned signal region labels. Adapted from [5].

Region		SRL	SRS	Measurement	
		Cand. jet p_T [GeV]		p_T^X [GeV]	$ y_X $
Inclusive		> 450	> 250	–	–
Fiducial		> 450	> 450	> 450	< 2
Diff.	bin 0	–	250 – 450,	300 – 450,	< 2
	bin 1	450 – 650,	450 – 650,	450 – 650,	
	bin 2	650 – 1000	650 – 1000	650 – 1000,	
	bin 3	> 1000	–	> 1000	

All results quoted as “Expected” in this chapter were found from identical fits to Asimov data, constructed using MC samples representing SM expectations of considered processes, i.e. $\mu_H = 1$, $\mu_Z = 1$, and $SF_{t\bar{t}} = 1$.

9.1.1 Overview of Changes

Observing the region definitions in table 9.1, some small differences between the previously described fit model, and the current model can be seen. Firstly, the fiducial volume definition was changed from using truth-level particle pseudorapidity ($|\eta_{H/Z}| < 2$) to rapidity ($|y_{H/Z}| < 2$).

It was recognised that several Higgs boson candidates with $p_T^{\text{jet}} > 1$ TeV passed the event selection of the analysis, so an additional differential measurement region, SRL ($p_T^{\text{jet}} > 1$ TeV) was added, along with a corresponding measurement volume – $\mu_{H/Z}$ ($p_T^{\text{truth}} > 1$ TeV). The addition of this ultra-high p_T fiducial volume, is novel for Higgs boson analyses, and probes yet unexplored regions of reconstructed Higgs and Z bosons.

It was also found that the contribution from single top-quark (later, single-top) production was non-negligible in the signal region, with a relevant contribution in the m_{jet} spectrum in the Higgs boson resonance range – $0.65\times$ the Higgs boson yield in SRL, and $1.34\times$ the Higgs boson yield in SRS. Therefore the single-top contribution was included in the SR models, set to the expected SM yield with a 50% acceptance and efficiency uncertainty, and was fully correlated with the single-top production in the $\text{CR}_{t\bar{t}}$ regions. A 30% acceptance and efficiency uncertainty, was also included for the $W(\ell\nu)$ process, which was only present in the $\text{CR}_{t\bar{t}}$.

Previously only the Wt contribution to the single-top production was considered, as it was by far the dominant one in $\text{CR}_{t\bar{t}}$. However, with its inclusion in the SR, other single-top production modes were considered. The t -channel production was found to be non-negligible and included in all regions, whereas the s -channel production was found to be negligible.

As well as the changes discussed so far, the transition from a 0.5 GeV binning to a 5 GeV binning in the signal regions proceeded after most of the studies presented in this thesis were conducted, the impact of this change is discussed in appendix H.1. No relevant differences, which would require a review of the analysis developments made with 0.5 GeV binning, were observed.

A summary of the changes in the analysis between the presented studies and the results are:

- a $p_T^{\text{jet}} > 1$ TeV leading-candidate jet signal region (SRL3), and a corresponding $p_T^{\text{truth}} > 1$ TeV fiducial measurement region for μ_H or μ_Z was added to the differential measurement;
- truth-level *rapidity* ($|y_H| < 2$) was used to define the fiducial and differential regions instead of *pseudorapidity* ($|\eta_H| < 2$);
- single top-quark production process added to the SR;
- t -channel production included to the single top-quark process modelling;
- acceptance and efficiency uncertainties included for single-top (50%) and W ($\ell\nu$) (30%) processes.

The impact from all relevant changes to the $\text{CR}_{t\bar{t}}$ fits, which were discussed in detail in this thesis, was also studied and presented in appendix H.2. No significant differences in results were found.

9.2 Cross-sections and Limit Setting

The main goals of the fiducial and differential measurements were to measure the Higgs boson *production cross-sections* in certain fiducial volumes. This was done by measuring the Higgs boson signal strengths μ_H in those volumes, and deriving the cross-sections as:

$$\sigma_H = \frac{\mu_H N_{\text{SM}}}{L \cdot A\epsilon}$$

where N_{SM} is the Higgs boson yield as predicted by the Standard Model, and hence, $\mu_H N_{\text{SM}}$ is the observed Higgs boson yield in data, L is the integrated luminosity, A is the fiducial acceptance and ε is the selection efficiency. The $A\varepsilon$ values for all considered Higgs boson production modes used in the fiducial and differential measurements are given in tables I.1 and I.2 of appendix I.

As the sensitivity of this analysis is not large enough to make Higgs boson cross-section measurements with high significance, upper limits at a 95% confidence level (CL) were set using the CL_s method [138, 144].

9.3 The Inclusive Measurement

The **inclusive measurement** probed the Higgs boson signal strength (μ_H) over the entire accessible p_T^{jet} spectra, i.e., the signal regions were fully inclusive in p_T^{jet} . The inclusive Higgs boson signal strength was found to be

$$\mu_H = 0.8 \pm 2.5 \text{ (stat)} \pm 2.0 \text{ (syst)}.$$

The summary of the expected and observed measurements of the Higgs boson signal and Z boson and $t\bar{t}$ backgrounds is given in table 9.2.

The Higgs and Z signal strengths were seen to agree with the expected values. The Higgs boson measurement had an expected sensitivity of 0.32σ and an observed sensitivity of 0.25σ . The Z +jets process had an expected sensitivity of 5.8σ and an observed sensitivity of 5.7σ , showing great agreement for both processes.

The measured $t\bar{t}$ scale factor was seen to agree with the value observed in standalone $\text{CR}_{t\bar{t}}$ fits ($\text{SF}_{t\bar{t}} = 0.78 \pm 0.06$). This is in line with the observations discussed in chapter 8, indicating that $\text{CR}_{t\bar{t}}$ should dominate the measurement. The $\text{SF}_{t\bar{t}}$ measurement also agrees well with a dedicated ATLAS $t\bar{t}$ cross-section measurement in a similar kinematic region [133] (figure 54). The post-fit yields of the processes in all regions (SRL, SRS and $\text{CR}_{t\bar{t}}$), are given in table I.3 of appendix I.

Table 9.2: (Left) the expected and observed values of the Higgs boson signal strength (μ_H), Z boson signal strength (μ_Z), and the $t\bar{t}$ scale factor ($\text{SF}_{t\bar{t}}$), as found by an inclusive measurement in SRL, SRS and $\text{CR}_{t\bar{t}}$ regions [5]. (Right) the corresponding measurement sensitivities in terms of measurement uncertainty ($Z = \mu/\sigma$). The expected results were found in identical fits to Asimov data constructed from SM expectations with μ_H , μ_Z , $\text{SF}_{t\bar{t}} = 1$. The measured $\text{SF}_{t\bar{t}}$ value is in line with the findings of [133].

Result	μ_H	μ_Z	$\text{SF}_{t\bar{t}}$	Z_H	Z_Z	$Z_{t\bar{t}}$
Expected	1.0 ± 3.2	1.0 ± 0.17	1.0 ± 0.07	0.31σ	5.8σ	14.2σ
Observed	0.8 ± 3.2	1.29 ± 0.22	0.80 ± 0.06	0.25σ	5.7σ	14.3σ

Estimates of the μ_H uncertainty contributions from each uncertainty group are given in table 9.3. The μ_H measurement is statistically limited, however the systematic uncertainty contribution is comparable. The largest systematic uncertainty contribution is from jet uncertainties.

Table 9.3: Estimated uncertainty contributions to the inclusive Higgs boson signal strength measurement, $\mu_H = 0.8 \pm 2.5$ (stat) ± 2.0 (syst), from considered uncertainty groups [5].

Uncertainty Contribution	$\sigma(\mu_H)$
Total	3.2
Statistical	2.5
Systematic	2.0
Jet Systematics	1.9
Modelling and Theory Sysys.	0.5
Flavor Tagging Sysys.	0.4

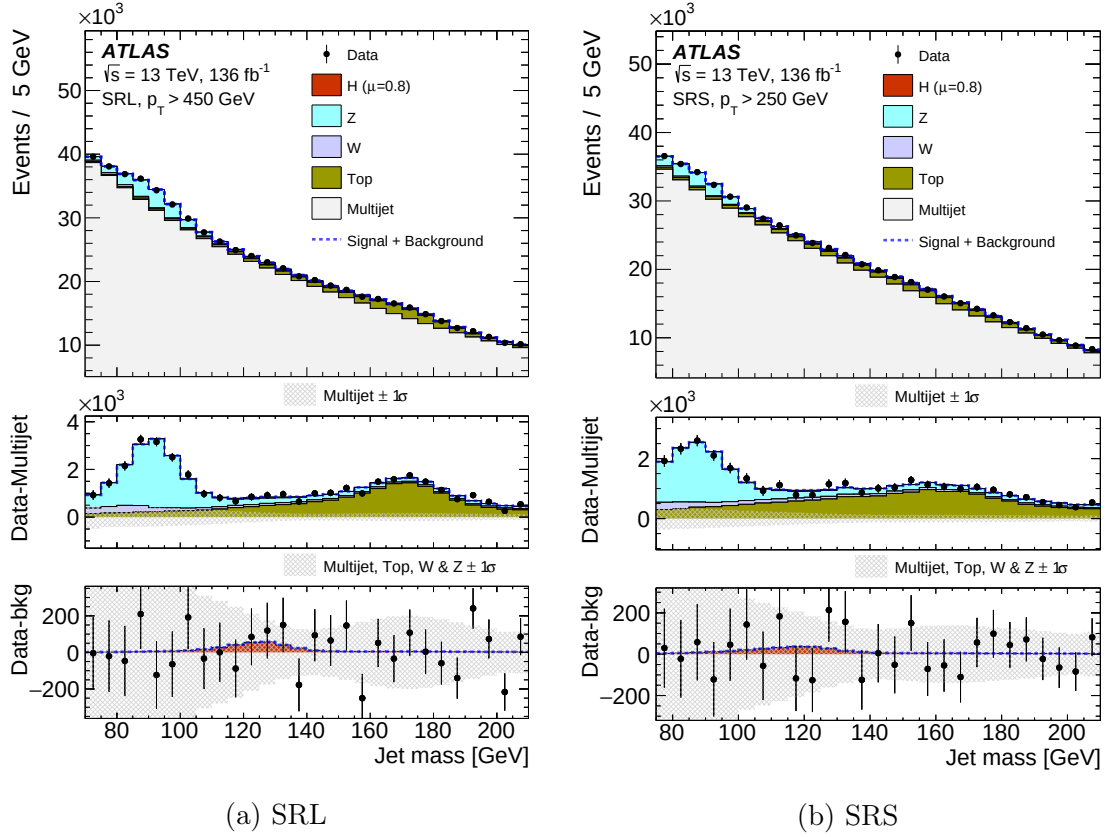


Figure 9.1: The post-fit distributions of data and model processes in inclusive (a) SRL and (b) SRS regions as found by the inclusive Higgs boson measurement [5]. The top panel shows all data and backgrounds, the middle panel shows the distributions with the QCD background subtracted such that the resonant processes are visible, and the bottom panel shows data with all resonant backgrounds subtracted such that the Higgs boson component is visible. The single top-quark production and $t\bar{t}$ process are combined as *Top*.

The post-fit distributions of the SRL and SRS regions are shown in figure 9.1. The top panels show all signals and backgrounds compared to data; the middle panel shows the data and backgrounds with the QCD component subtracted, such that the resonant processes are visible; and the bottom panel shows the data with all backgrounds subtracted, such that the Higgs boson component is visible. Good overall agreement was seen with reduced χ^2 goodness-of-fit values of 0.19 and 0.67 in SRL and SRS, respectively [5].

9.4 The Fiducial Measurement

A Higgs boson cross-section measurement over the entire fully accessible Higgs boson phase-space ($p_T^{\text{jet}} > 450$ GeV) was made, called the **fiducial measurement**. The SRL, SRS and $\text{CR}_{t\bar{t}}$ data with $p_T^{\text{jet}} > 450$ GeV were fit simultaneously. The Higgs boson signal strength and cross-section was measured for Higgs bosons within the fiducial volume, with $p_T^H > 450$ GeV and $|y_H| < 2$.

The Higgs boson mass templates in each SR were separated into two components: events with $p_T^H < 450$ GeV, and events with $p_T^H > 450$ GeV. The former were fixed to the SM expectation, whereas the latter, accounting for $> 80\%$ of the expected Higgs boson events [5], were used to fit the Higgs boson signal strength μ_H in the fiducial region, which was used to calculate the Higgs boson cross-section.

The measured Higgs boson signal strength in the fiducial region was

$$\mu_H = -0.1 \pm 2.6 \text{ (stat)} \pm 2.3 \text{ (syst)}, \quad (9.1)$$

corresponding to an upper limit of the Higgs boson cross-section at a 95% CL_s of [5]

$$\sigma_H (p_T^H > 450 \text{ GeV}) < 115 \text{ fb.}$$

The measured Higgs boson and Z boson signal strengths, and the $t\bar{t}$ scale factors are given in table 9.4. The measured μ_Z agrees with the inclusive measurement, and $\text{SF}_{t\bar{t}}$ is consistent with the standalone $\text{CR}_{t\bar{t}}$ measurements in the $p_T^{\text{jet}} > 450$ GeV bins (table H.2). The post-fit yields of all considered processes in the SRL, SRS and $\text{CR}_{t\bar{t}}$ are given in table I.4 of appendix I.

The contribution of the main groups of systematic uncertainties to the total uncertainty on μ_H are given in table 9.5. The values show the same order of impact as those found by the inclusive measurement. The μ_H measurement was dominated by statistical uncertainties, with comparable systematic uncertainties dominated by jet uncertainty contributions.

Table 9.4: The expected and observed values of the signal strength of Higgs bosons with $|y_H| < 2.0$ and Higgs boson $p_T > 450$ GeV (μ_H); total Z boson signal strength (μ_Z); and the $t\bar{t}$ scale factor ($\text{SF}_{t\bar{t}}$), as found by the Higgs boson fiducial measurement in SRL, SRS and $\text{CR}_{t\bar{t}}$ regions with candidate jet $p_T > 450$ GeV [5]. The expected results were found in identical fits to Asimov data constructed from SM expectations with μ_H , μ_Z , $\text{SF}_{t\bar{t}} = 1$. The measured $\text{SF}_{t\bar{t}}$ value is in line with the findings of [133].

Result	μ_H	μ_Z	$\text{SF}_{t\bar{t}}$
Expected	1.0 ± 3.4	1.0 ± 0.18	1.0 ± 0.08
Observed	-0.1 ± 3.5	1.30 ± 0.22	0.75 ± 0.06

Table 9.5: Estimated uncertainty contributions from all considered uncertainty groups to the fiducial Higgs boson signal strength measurement, $\mu_H = -0.1 \pm 2.6$ (stat) ± 2.3 (syst), in the phase space defined by Higgs boson $p_T > 450$ GeV and $|y_H| < 2$.

Uncertainty Contribution	$\sigma(\mu_H)$
Total	3.5
Statistical	2.6
Systematic	2.3
Jet Systematics	2.2
Modelling and Theory Sysys.	0.8
Flavor Tagging Sysys.	0.2

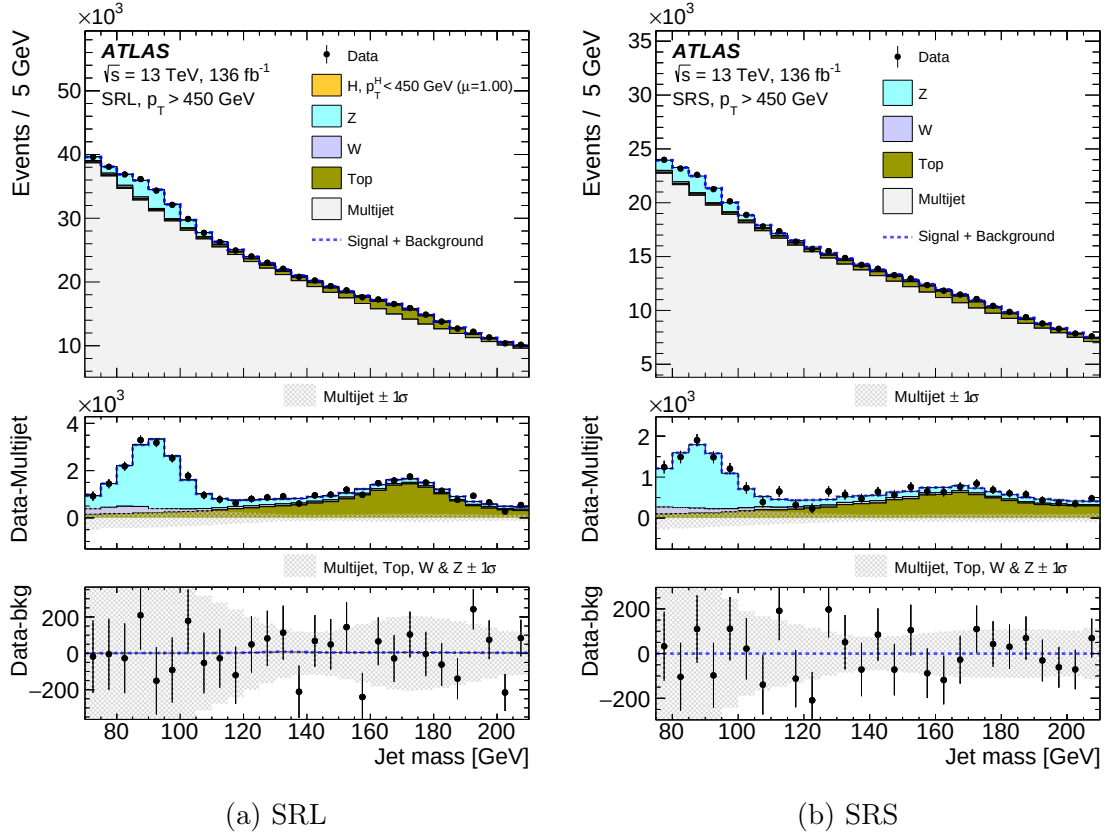


Figure 9.2: The post-fit distributions of data and model processes in fiducial (a) SRL and (b) SRS regions (jet $p_T > 450$ GeV), as found by the fiducial Higgs boson measurement in the phase space defined by Higgs boson $p_T > 450$ GeV and $|y_H| < 2$ [5]. The top panel shows all data and backgrounds, the middle panel shows the distributions with the QCD background subtracted such that the resonant processes are visible, and the bottom panel shows data with all resonant backgrounds subtracted such that the Higgs boson component is visible. The single top-quark production and $t\bar{t}$ process are combined as Top .

The post-fit distributions of the data and expected process contributions in the fiducial SRL and SRS are given in figure 9.2. As previously, panels with the QCD background removed and all backgrounds removed are shown in the middle and bottom panels, respectively. No Higgs boson signal is visible in the bottom panels as the $p_T^H < 450$ GeV contribution (fixed to SM) is very small, and the $p_T^H > 450$ GeV contribution was estimated to have a signal strength of $\mu_H = -0.1$.

9.5 The Differential Cross-section Measurement

As discussed in chapter 1, a BSM enhancement to the Higgs boson production would increase with Higgs boson p_T . Hence, it is beneficial to make a **differential measurement** of the Higgs boson production cross-section in bins of p_T^H .

The Higgs boson m_{jet} templates were divided into bins of Higgs boson p_T , and the signal regions and $\text{CR}_{t\bar{t}}$ were divided into corresponding p_T^{jet} bins (ten regions in total, see table 9.1). The signal strengths of each of the p_T^H -binned Higgs boson templates were free parameters in all p_T^{jet} -binned signal regions, and the μ_H for each p_T^H bin were fully correlated across them. The components with $p_T^H < 300$ GeV in all regions were fixed to their SM expectations. More details on the measurement configuration are given in section 5.5.

The signal regions with $p_{T,i}^{\text{jet}}$ were expected to have the strongest constraining power to μ_H measurements with corresponding $p_T^{H,i}$, as the event leakage to neighbouring bins due to resolution effects was seen to be relatively small. The measurements were expected to be the most sensitive to the $p_T^H \in [450, 650]$ GeV component, as the corresponding p_T^{jet} bin had the highest expected signal yields. The expected (pre-fit) Higgs boson event yield distribution across p_T^H and p_T^{jet} bins, and the fractional contributions of p_T^H templates within p_T^{jet} bins are given in tables I.1 and I.1b in appendix I.

9.5.1 The Z boson Measurement

The differential measurement framework was also used to determine Z boson signal strengths in bins of p_T^Z , and compare them to SM predictions. In this case, the Higgs boson components were treated as backgrounds fixed to their SM expectations. As well as using the signal regions, the signal strengths of the combined V +jets processes (Z +jets and W +jets), μ_V , were also determined using the leading-jet validation regions (VRL)². The VRL dataset was randomly split into 5 “slices” such

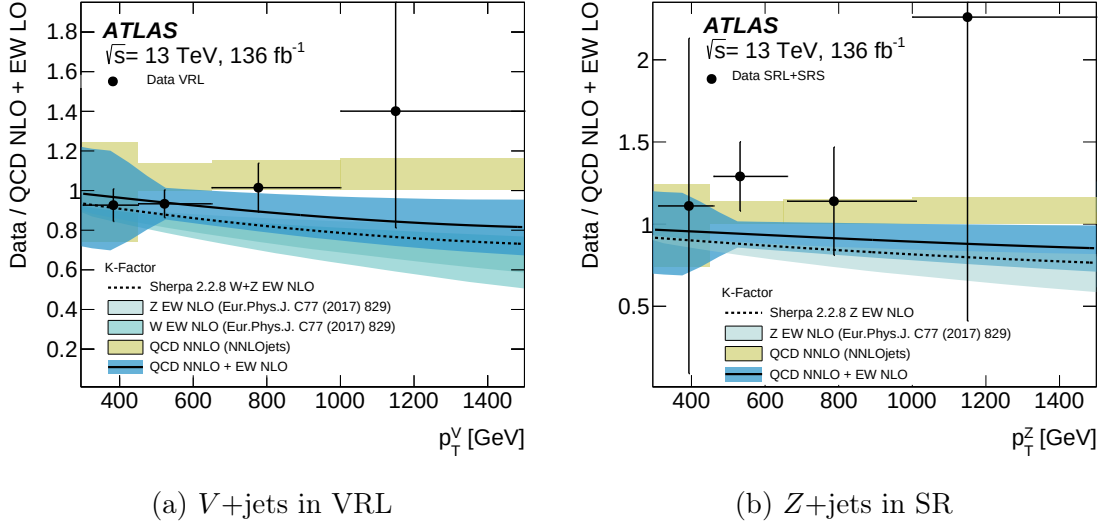


Figure 9.3: Signal strength measurements of the (a) V +jets process in VRL data, and the (b) Z +jets process in SRL and SRS data, with respect to the SM prediction obtained using NLO QCD and LO EW predictions [5]. The results are compared to SM predictions with NLO EW corrections generated by SHERPA [126, 127], NNLO QCD corrections provided by the NNLOJET group [129–131], their product, and state-of-the-art NLO EW calculations from [142].

that the QCD background in each slice could be described by the same functional form as used in the signal regions³.

The results, shown in figure 9.3 (left – VRL, right – SR), are compared to SM expectations with higher-order QCD and EW corrections⁴. The measured μ_V and μ_Z values (data points) represent the data agreement with SM predictions with QCD corrections at NLO, and EW corrections at LO precision⁵. The results were compared to higher-order-precision SM predictions obtained using NLO EW cor-

² In this case, the $t\bar{t}$ backgrounds were constrained using the Gaussian prior method described in section 8.2.

³ The number of parameters needed to describe the QCD background tends to scale with available luminosity, see section 6.4.1 for more details.

⁴ EW – electro-weak; (N)LO – (next-to-)leading order.

⁵ In the μ_H measurements, NNLO QCD and NLO EW corrections are used, as discussed in section 5.3.2. Here, for the purposes of comparison, the results have been scaled to represent the lowest common precision order of the compared SM estimates.

rections and NNLO QCD corrections. The results were seen to agree with the SM predictions.

9.5.2 The Higgs boson Measurement

The Higgs boson differential measurement fit results are given in table 9.6. These include, Higgs boson signal strengths in truth- p_T^H bins; and the scale factors of background processes: μ_Z and $SF_{t\bar{t}}$ measured in candidate p_T^{jet} bins. The Higgs and Z boson measurements were seen to be compatible with SM predictions, however the overall sensitivity of the Higgs boson measurements was low. The $t\bar{t}$ SF measurements were in-line with the standalone $CR_{t\bar{t}}$ measurements (table H.2 in appendix H), and a dedicated $t\bar{t}$ cross-section study in a similar kinematic regime [133].

The post-fit distributions of the data and process estimates in the SRL and SRS are given in figures I.2 and I.3 in appendix I, respectively. A good overall agreement with data was seen, however, the sensitivity to the Higgs boson signal was clearly small. The results were used to set upper limits on Higgs boson production cross-section values at 95% CL_s in probed fiducial regions, which were found to be [5]

$$\begin{aligned}\sigma_H (300 < p_T^H < 450 \text{ GeV}) &< 2.9 \text{ pb;} \\ \sigma_H (450 < p_T^H < 650 \text{ GeV}) &< 89 \text{ fb;} \\ \sigma_H (650 < p_T^H < 1000 \text{ GeV}) &< 39 \text{ fb;} \\ \sigma_H (p_T^H > 1000 \text{ GeV}) &< 9.6 \text{ fb.}\end{aligned}$$

The limits are shown along with the measured production cross-sections and uncertainties on them in figure 9.4. The lowest p_T^H bin had comparably poor sensitivity, as the most sensitive region to this component was only SRS0 (subleading-jet SR, $p_T^{\text{jet}} \in [250, 450] \text{ GeV}$). The most sensitive measurement was for Higgs bosons with $p_T^H \in [450, 650] \text{ GeV}$. It was primarily determined in SRL1 and SRS2 regions, which had the largest event yields of all regions determined in both SRL and SRS. The sensitivity is then seen to deteriorate with increasing p_T^H , as event yields drop and

Table 9.6: The expected and observed values of the Higgs boson signal strengths (μ_H) measured in Higgs boson p_T bins; and Z boson signal strengths (μ_Z) and the $t\bar{t}$ scale factors ($\text{SF}_{t\bar{t}}$) measured in candidate p_T^{jet} bins, as found by the Higgs boson differential measurement in p_T^{jet} -binned SRL, SRS and $\text{CR}_{t\bar{t}}$ regions [5]. The expected results were found in identical fits to Asimov data constructed from SM expectations with μ_H , μ_Z , $\text{SF}_{t\bar{t}} = 1$. The measured $\text{SF}_{t\bar{t}}$ values are in line with the findings of [133].

p_T^H [GeV]	μ_H	
	Exp.	Obs.
300 – 450	1 ± 18	−6 ± 18
450 – 650	1.0 ± 3.3	−3 ± 5
650 – 1000	1 ± 6	5 ± 7
> 1000	1 ± 30	18 ± 32

Jet p_T [GeV]	μ_Z		$\text{SF}_{t\bar{t}}$	
	Exp.	Obs.	Exp.	Obs.
250 – 450	1.0 ± 1.1	1.8 ± 1.1	1.00 ± 0.07	0.85 ± 0.06
450 – 650	1.00 ± 0.17	1.28 ± 0.22	1.00 ± 0.07	0.76 ± 0.06
650 – 1000	1.00 ± 0.33	1.4 ± 0.4	1.00 ± 0.09	0.74 ± 0.08
> 1000	1.0 ± 1.6	2.4 ± 1.7	1.00 ± 0.22	0.57 ± 0.18

statistical uncertainties increase. The summary of the post-fit yields of all considered processes is given in table I.5 in appendix I.

The contributions from all uncertainty groups to the measurement are given in table 9.7. The measurement in the $p_T^H \in [450; 650]$ GeV bin was seen to be dominated by systematic uncertainties. This was reasonable as the inclusive measurement showed statistical and systematic uncertainties of similar extent, and the measurement in this p_T^H bin was known to be primarily constrained by the signal regions with the largest statistics. The measurements in all other p_T^H bins were seen

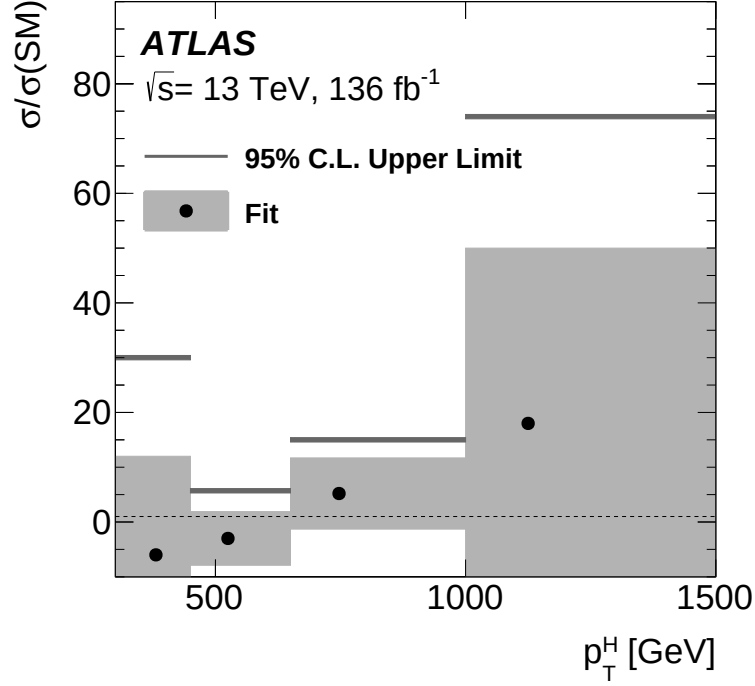


Figure 9.4: Measured Higgs boson signal strengths and upper limits corresponding to a 95% CL_s , extracted by the Higgs boson differential measurement in fiducial volumes defined in bins of Higgs boson p_T [5]. The dotted line marks the SM expectation at $\mu_H = 1.0$.

Table 9.7: Estimated uncertainty contributions from all considered uncertainty groups to the differential μ_H measurements (SM $\mu_H = 1$) in the phase space defined by Higgs boson p_T : $p_T^{H,0/1/2/3} \equiv p_T = 300 - 450, 450 - 650, 650 - 1000, > 1000$ GeV.

	$p_T^{H,0}$	$p_T^{H,1}$	$p_T^{H,2}$	$p_T^{H,3}$
Measured μ_H	-6	-3	5	18
Total Uncertainty	18	5.0	6.5	32
Statistical	16	3.0	5.5	30
Systematic	7	3.9	3.4	10
Jet Systematics	6	3.8	3.4	9.5
Modelling and Theory Sys.	4	0.7	0.7	2
Flavor Tagging Sys.	0.2	0.4	0.4	2

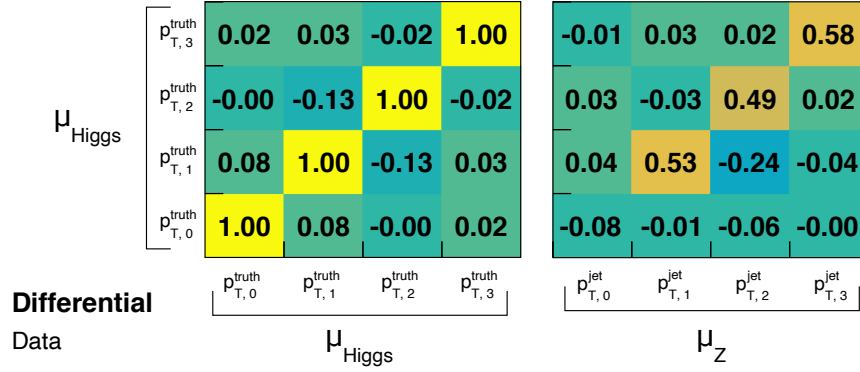


Figure 9.5: Correlations between Higgs boson signal strengths μ_H measured in Higgs boson p_T bins, and Z +jets signal strengths measured in candidate jet p_T bins, in the differential Higgs boson measurement fit. $p_{T,0/1/2/3}^{\text{truth}} \equiv p_T = 300 - 450, 450 - 650, 650 - 1000, > 1000$ GeV, $p_{T,0/1/2/3}^{\text{jet}} \equiv p_T = 250 - 450, 450 - 650, 650 - 1000, > 1000$ GeV.

to be dominated by statistical uncertainties. In all cases jet uncertainties were the dominant systematic uncertainties, driven by the jet mass scale (JMS) uncertainties.

The inter-correlations between the differential μ_H measurements in p_T^H bins, and correlations between the μ_H measurements and μ_Z measurements in p_T^{jet} bins are shown in figure 9.5. Interactions between μ_H measurements in different p_T^H domains, shown in figure I.1b, were seen to be minor, attesting to the expectantly low migration of events from one truth- p_T bin to a non-corresponding p_T^{jet} bin due to resolution effects.

The interactions between μ_H and μ_Z measurements were primarily limited to the processes in corresponding p_T^H and p_T^{jet} bins, which was also expected given the low event migration to non-corresponding p_T^{jet} bins. The μ_H and μ_Z measurements in corresponding p_T bins were positively correlated due to interaction through the QCD background. For the fit to increase one of these signal strengths, the QCD background yield needs to be reduced. This, in turn, forms a deficit underneath the other resonance, requiring the other signal strength to be increased as well.

9.6 Future Outlook

Currently, the extracted Higgs boson signals in all regimes were limited by statistical uncertainties, meaning that with increasing sample sizes from *Run 3* of the LHC (throughout 2022–2024) these uncertainties should decrease. However, as the LHC enters the High-Luminosity-LHC stage [145, 146], where luminosity is expected to be increased to $5 - 7 \times$ the luminosity of 2015, improvements to object reconstruction and background reduction techniques will be vital.

Technical Improvements

The current $H(\rightarrow b\bar{b}) + j$ analysis was started in early 2019, and the object reconstruction and identification techniques used by the analysis followed the early 2019 ATLAS recommendations. Throughout the development of the analysis many improvements were made to ATLAS tools and calibrations, which will be implemented in the future.

One important advancement was the development of the dedicated double- b tagging algorithm (D_{Xbb}) [81], briefly introduced in section 4.2.9. The algorithm is based on a deep neural network (machine learning (ML) technique), using the outputs of a new ML-based single b -tagging algorithm DL1r [87] for up to 3 leading p_T track jets within the large- R jet, and the p_T and η of the large- R jet itself.

Figure 9.6 shows the QCD multi-jet and top-jet background rejection⁶ of the D_{Xbb} tagger (blue) compared to two individual b -tags with the MV2 algorithm (grey), used in this analysis, and the newer DL1r algorithm (green). The D_{Xbb} algorithm significantly outperformed both of the single b -tagging algorithms in top rejection, and performed generally better in multi-jet rejection for $p_T^{\text{jet}} > 500$ GeV.

In August 2021, the first preliminary calibrations of the D_{Xbb} tagger have been made public [3], which used $Z(\rightarrow b\bar{b}) + \gamma$ and $Z(\rightarrow b\bar{b}) + j$ events. The calibration

⁶ Rejection is the inverse of the mis-tagging “efficiency” at which a top or QCD jet is tagged as a double- b -jet, introduced in section 3.3.

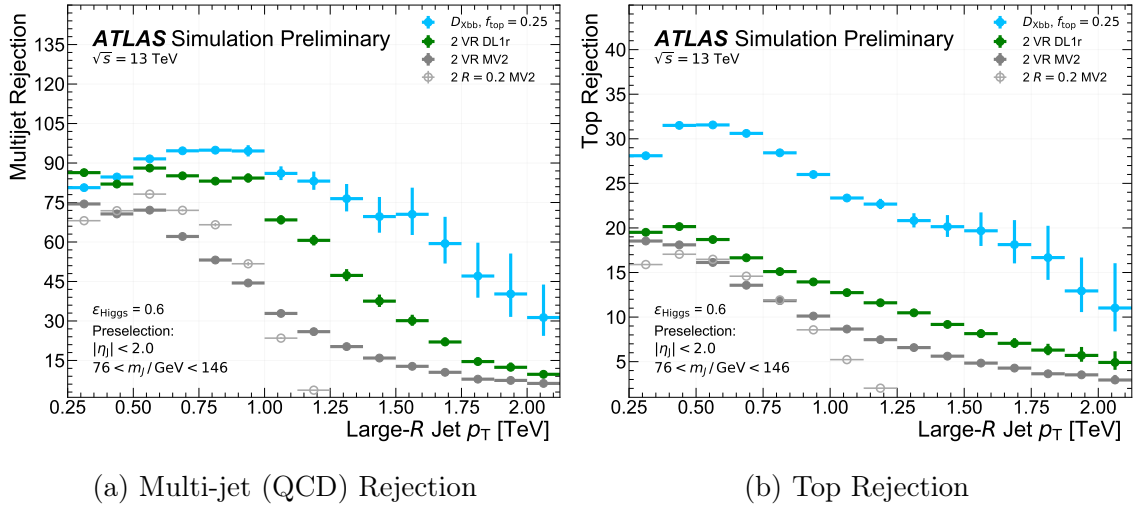


Figure 9.6: (a) Multi-jet (QCD) and (b) top-jet background rejection by various double- b -tagging strategies at a 60% Higgs boson tagging efficiency [81]. Strategies: ML-based $X \rightarrow b\bar{b}$ tagging algorithm (D_{Xbb}); and 2 single b -tags using the DL1r, and the MV2 algorithms. D_{Xbb} and DL1r use variable-radius track jets, and the MV2 algorithm is shown using variable and fixed radius track jets. Error bars show statistical uncertainties.

in $g \rightarrow b\bar{b}$ events, presented in chapter 4, is also well underway. It is also notable, that the calibrations in $Z(\rightarrow b\bar{b}) + \gamma/j$ events repurposed the $H(\rightarrow b\bar{b}) + j$ fitting framework developed by the author of the thesis.

In the future this analysis will certainly make use of greatly improved b -tagging capabilities provided by the D_{Xbb} tagger. Other technical advancements include new jet mass and energy resolution uncertainties [78], and precision large-radius jet collections currently under research [147].

Analysis Strategy

As the analysis has been published very recently, no studies for future analysis improvements have yet been made, however some points of significant interest can be identified. Firstly, the complementary study published by the CMS experiment in 2020 [104] has shown better sensitivity through stronger background reduction. This was likely heavily influenced by using a dedicated double- b -tagger and more

aggressive event selection. Therefore, an important focus for the analysis going forward is background reduction. Studies of including variables characterising jet substructure, such as discriminants quantifying the distribution of energy within the jet [148–150], or number of associated tracks [151,150] could help further reduce backgrounds.

Many of the challenges in the measurement fit arose from the parametric treatment of the QCD background in combination with the binned-template treatment of the resonances. The fix in the *RooFit* software⁷ which enabled the use of 5 GeV binning in the signal regions had also massively increased the computation time from $\mathcal{O}(\text{min})$ to $\mathcal{O}(\text{days})$, making it difficult to run fitting tests. This means that the fit must be significantly simplified to make in-depth fit studies feasible in the future.

An increase in data should reduce the ambiguity in the fit, as well as the background reduction to be achieved with the use of the D_{Xbb} tagger, and event selection studies. Strategies of non-parametric QCD background descriptions should also be investigated, as a fully binned-template fit would simplify the fitting procedure, mitigating the need for the software fix. However, due to difficulties in QCD modelling, this would be a challenging undertaking.

Physics Interpretations

As this study has originated from an BSM resonance search [4], the measurement could be re-interpreted to set limits for a low-mass BSM resonance decays to two b -quarks. More information on possible BSM models can be found in [152].

As mentioned earlier in the thesis, the measurement of Higgs production cross-section through ggF could be particularly sensitive to BSM enhancements, so a ggF only measurement is expected in the future. Significant interest within the Higgs boson analysis group was also seen for a VH interpretation, where the recoil jet

⁷ Introduced in section 5.7.1.

could be tagged as a hadronic V boson decay. This topology could in the future be further interpreted as a search for heavy BSM resonances decaying to a weak boson and a Higgs $V' \rightarrow VH$ [151].

9.7 Summary of the Results

The Higgs boson production at high transverse momentum in the $H \rightarrow b\bar{b}$ channel was measured in three regimes. An **inclusive measurement** of the Higgs boson signal strength across the entire candidate jet p_T spectra was performed and found to be

$$\mu_H = 0.8 \pm 2.5(\text{stat}) \pm 2.0(\text{syst}),$$

which is consistent with the SM expectation of $\mu_H = 1$.

A **fiducial measurement** of the Higgs boson production cross-section for Higgs bosons with $p_T > 450$ GeV and $|y_H| < 2$, was also made. As no Higgs signal was measured in this regime, an upper limit at 95% CL_s was found to be

$$\sigma_H(p_T^H > 450 \text{ GeV}) < 115 \text{ fb}.$$

Upper limits on Higgs boson production cross-sections in bins of Higgs boson p_T were set by a **differential measurement**, which is a more sensitive probe of possible p_T -dependent BSM enhancements to the Higgs boson production cross-section. This included an upper limit on the Higgs boson cross-section in an ultra-high $p_T^H > 1$ TeV regime. All results were seen to agree well with expectations. A summary of all measurement results produced by this analysis is given in table 9.8.

Table 9.8: A summary of results delivered by the study of Higgs boson production at high transverse momentum in the $H \rightarrow b\bar{b}$ decay channel [5].

Inclusive Measurement			
p_T^{jet} [GeV]	μ_H		
SRL > 450	0.8 $\pm$ 2.5 (stat) $\pm$ 2.0 (syst)		
SRS > 250			

Fiducial Measurement			
p_T^H [GeV]	μ_H		95% CLs limit
> 450	−0.1 $\pm$ 2.6 (stat) $\pm$ 2.3 (syst)		< 115 fb

Differential Measurements			
p_T^Z [GeV]	μ_Z		
300 – 450	1.16 $\pm$ 0.84 (stat) $\pm$ 0.66 (syst)		
450 – 650	1.37 $\pm$ 0.21 (stat) $\pm$ 0.09 (syst)		
650 – 1000	1.25 $\pm$ 0.33 (stat) $\pm$ 0.15 (syst)		
> 1000	2.06 $\pm$ 1.56 (stat) $\pm$ 0.63 (syst)		

p_T^H [GeV]	μ_H		95% CLs limit
300 – 450	−6 $\pm$ 16 (stat)	$\pm$ 7 (syst)	< 2.9 pb
450 – 650	−3 $\pm$ 3 (stat)	$\pm$ 4 (syst)	< 89 fb
650 – 1000	5 $\pm$ 6 (stat)	$\pm$ 3 (syst)	< 39 fb
> 1000	18 $\pm$ 30 (stat)	$\pm$ 10 (syst)	< 9.6 fb

Conclusions

This thesis presented Higgs boson production measurements in $H \rightarrow b\bar{b}$ decays with a large Higgs boson transverse momentum boost. The Higgs boson signal was probed inclusively for Higgs boson candidate jets with $p_T^{\text{jet}} > 250$ GeV and found to be $\mu_H = 0.8 \pm 2.5(\text{stat}) \pm 2.0(\text{syst})$, equivalent to a 0.25σ signal sensitivity.

The Higgs boson production cross-section was probed in a fiducial region defined by truth-level Higgs boson $p_T^H > 450$ GeV, and in differential bins with $p_T^H > 250$ GeV, $250 - 450$ GeV, $450 - 650$ GeV, $650 - 1000$ GeV, and > 1 TeV. The statistical significance of the measurements were $< 3\sigma$, so 95% CL_s limits were set in all cases:

$$\begin{aligned}\sigma_H(p_T^H > 450 \text{ GeV}) &< 115 \text{ fb;} \\ \sigma_H(300 < p_T^H < 450 \text{ GeV}) &< 2.9 \text{ pb;} \\ \sigma_H(450 < p_T^H < 650 \text{ GeV}) &< 89 \text{ fb;} \\ \sigma_H(650 < p_T^H < 1000 \text{ GeV}) &< 39 \text{ fb;} \\ \sigma_H(p_T^H > 1000 \text{ GeV}) &< 9.6 \text{ fb.}\end{aligned}$$

All results showed good agreement with the Standard Model. Particular focus in this thesis was given to the development of the measurement fit model, the treatment of signal and background processes within it, and its validation.

This analysis was the first SM Higgs Boson study at ATLAS to probe the *inclusive* Higgs boson production through $H \rightarrow b\bar{b}$ decays. It was also the first ATLAS analysis to target the Higgs boson production cross-sections at $p_T^H > 650$ GeV and

$p_T^H > 1$ TeV. This analysis is the first step towards a Higgs boson observation in a regime with great sensitivity to BSM physics, and the versatility of this final state topology will allow various other SM and BSM interpretations.

This thesis described the work produced by the author, without which these measurements could not have been made. A crucial contribution was the writing of the fitting framework, which has enabled the work of many people both in and outside the $H(\rightarrow b\bar{b}) + j$ analysis group. She has also contributed many key pieces of fit development, regarding the treatment of signals, backgrounds and systematic uncertainties. Furthermore, the many validation studies produced by the author were key to delivering a robust analysis with reliable results, and her contributions to the calibration of the boosted double- b tagging efficiency will aid this and similar analyses in the future.

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Appendix A

Double b -tagging Calibration

Figure A.1 shows the p_T distributions for j_μ^{trk} and $j_{\text{non-}\mu}^{\text{trk}}$ after flavour correction and double b -tagging, as described in section 4.2, but with the use of fixed-radius $R = 0.2$ track jets, instead of VR track jets. The data and MC agreement in the same distributions from studies produced with VR track jets show a deterioration in agreement at high track jet momentum. This was hypothesised to be the result of the MV2 algorithm being trained and calibrated using fixed-radius track jets at the time. At high p_T , the VR track jet cone becomes much smaller than $R = 0.2$, and fewer tracks might be contained within the small cone making the algorithm less effective. This hypothesis is supported by the observation, that such data-to-MC discrepancies are not apparent in the track jet p_T distributions produced with fixed-radius jets, shown in figure A.1.

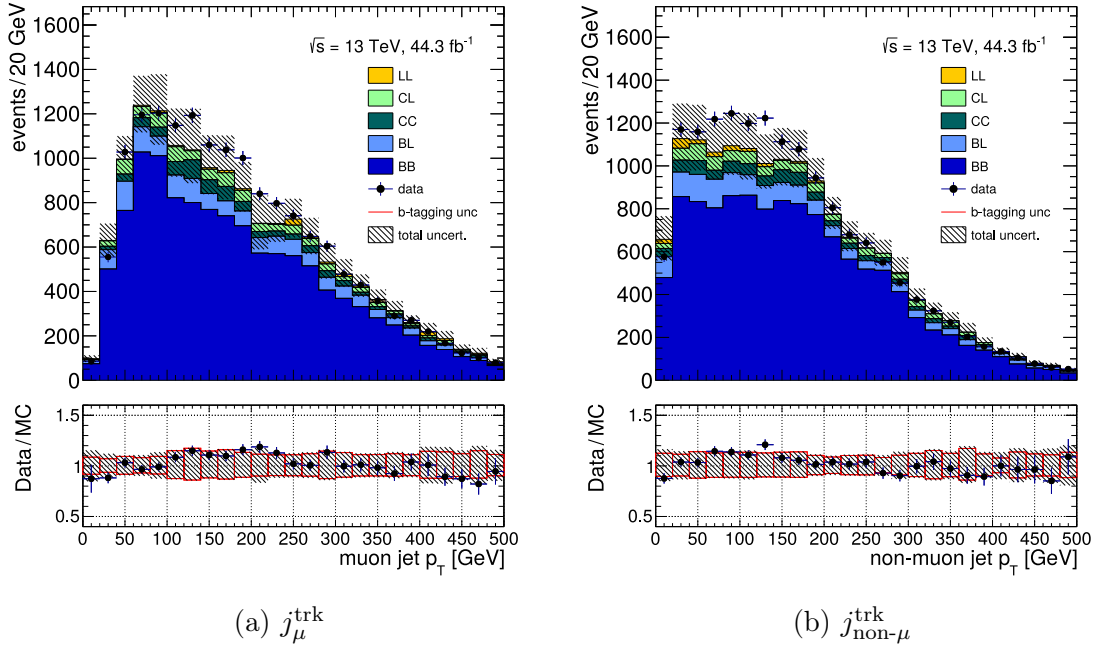


Figure A.1: Transverse momentum distributions for (a) j_{μ}^{trk} and (b) $j_{\text{non-}\mu}^{\text{trk}}$ after double b -tagging ($2 \times \text{MV2}$ tags at 70% WP) with *fixed radius* $R = 0.2$ track jets. In both cases the MC flavour composition is corrected before tagging (as described in 4.2.6).

Appendix B

Additional $H(\rightarrow b\bar{b}) + j$ Analysis Details

B.1 Muon-in-Jet Correction¹

Heavy quarks decay into lighter quarks through weak interaction involving a W boson, which in turn can decay semileptonically into a charged lepton and a neutrino ($W \rightarrow l\nu$). Muons and neutrinos escape the calorimeter, resulting in energy unaccounted in jet mass and p_T calculations and calibrations. This can lead to an underestimate of jet mass or p_T , and a deterioration of the mass resolution. Good mass resolution was particularly important for the $H(\rightarrow b\bar{b}) + j$ analysis, as the resonance shape distinguishes the signal from an overwhelming QCD background.

Figure B.1 shows the mass distributions of large- R jets which had a ghost-matched truth¹ Higgs boson in simulated ggF Higgs boson events. The component events containing semileptonic decays, and purely hadronic decays are shown. The mass distribution of events with semileptonic decays had a lower mean and a wider spread than the distribution of the events with purely hadronic decay chains, which was expected considering the jet energy loss through leptons and neutrinos.

The ATLAS $H \rightarrow b\bar{b}$ analysis focusing on VH Higgs boson production [107, 153] had developed a procedure to correct for the jet energy loss through muons.

¹ This section describes the work of other analysis members and was written with the help of [73] (internal).

¹ truth-level particle in simulation record, introduced in section 3.1

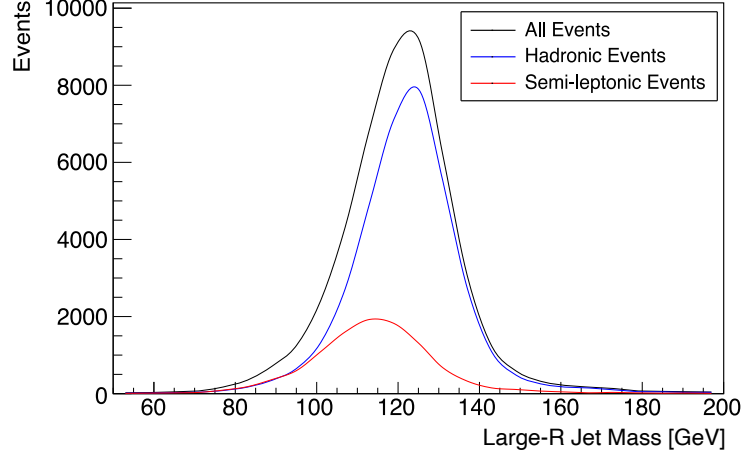


Figure B.1: Mass distribution of large- R jets matched with truth Higgs bosons in simulated Higgs boson events produced through ggF . Events with fully hadronic and semileptonic decay chains are shown in blue and red, respectively [73] (internal).

At the time of development, no satisfactory procedure to account for energy loss through neutrinos had been developed within ATLAS. Muons were associated to the candidate jet, and their four-momentum was added to the four-momentum of the large- R jet. The muon contribution to the calorimeter deposit was subtracted such that it was not double counted. The procedure was optimised by other members of the $H(\rightarrow b\bar{b}) + j$ analysis team using simulated Higgs boson ggF events.

The muons were required to be within the acceptance of the tracking system $|\eta_\mu| < 2.4$, and have $p_T^\mu > 10$ GeV – a selection optimised for the $H(\rightarrow b\bar{b}) + j$ analysis, presented in the following appendix. The muons were matched with b -tagged track jets (j_b) within the candidate large- R jet, such that

$$\Delta R(\mu, j_b) < \min \left[0.4, 0.04 + \frac{10}{p_T^\mu} \right]. \quad (\text{B.1})$$

If multiple muons were matched to a single track jet, the muon with the smallest ΔR separation was used. It was allowed for both of the b -tagged track jets within a candidate to have such associated muons, in which case two corrections were applied.

The effect on candidate large- R jet mass matched with a truth Higgs boson in simulated ggF events is shown in figure B.2. An improvement in sharpness of the

peak and spread of the resonance was seen in both SRL and SRS. The effect is much stronger when the candidate is the subleading jet. This is because the loss of energy in a semileptonic decay can cause the Higgs boson to become the subleading p_T jet in the event. The impact on p_T is shown in figure B.3. In both SRL and SRS, a reduction in the momentum difference $(p_T^H - p_T^{\text{jet}})$ was seen when the correction is applied. A significantly larger contribution from semileptonic decays was seen in the SRS as compared to the SRL.

Applying this correction after event selection ensured that semileptonic decays were mostly contained in the SRS region. This was advantageous, as the two signal regions were fit simultaneously with many fit parameters correlated between them, which could be constrained using the more sensitive SRL region.

B.1.1 Muon-in-Jet Correction Optimisation

This section describes the work of other analysis members and was written with the help of [73] (internal). The optimisation study used Higgs boson ggF MC samples. The candidate jet has to be ghost-matched with a truth Higgs boson, and have two b -tagged track jets. The study compared the correction performance for different values of muon transverse momentum (p_T^μ).

Two investigated indicators of correction performance were: the *correction rate*, which is the fraction of corrected candidate jets out of all candidate jets, and the *misidentification rate*, which quantifies the fraction of candidates which are corrected when the truth-level b -quark decay chain does not contain a muon. Such jets were said to be *mistagged*. The results are shown in figure B.4.

As p_T^μ increases, fewer muons pass the selection criteria resulting in a drop of total corrected jets, however a larger threshold helps identify muons from semileptonic decays. The misidentification rate drops sharply if $p_T^\mu > 10$ GeV, without a large effect on the overall correction rate. Therefore a $p_T^\mu > 10$ GeV threshold was chosen.

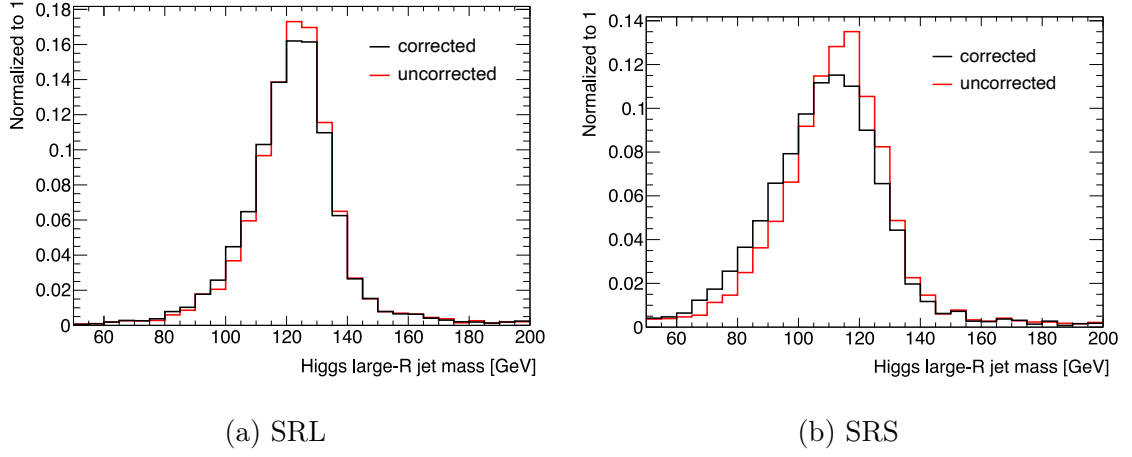


Figure B.2: Mass distributions of (a) SRL and (b) SRS candidate jets matched with Higgs bosons from the simulation record in simulated Higgs boson events produced through ggF before and after correction [73] (internal).

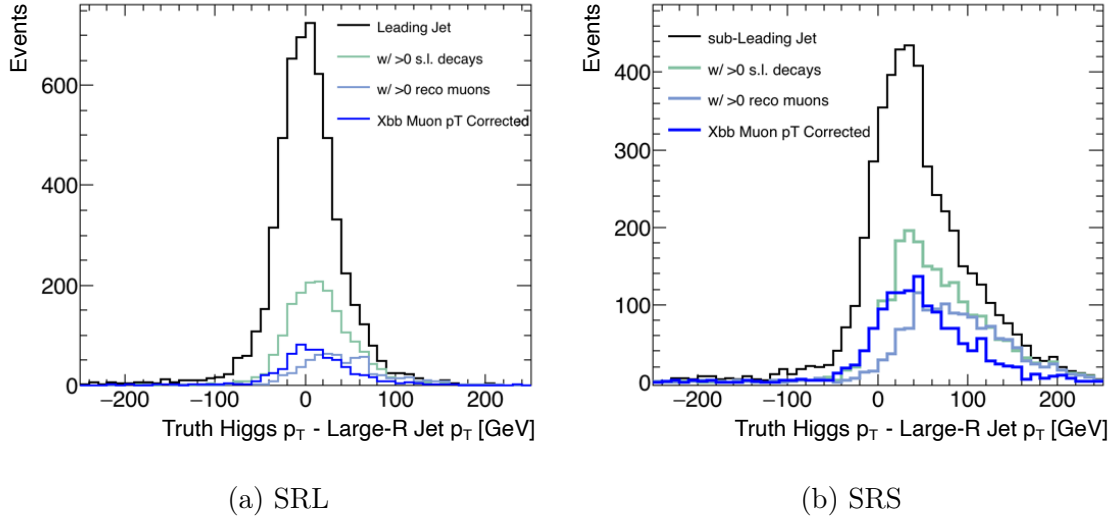


Figure B.3: Distributions of the p_T difference between truth-record Higgs bosons and candidate jets matched with truth-record Higgs bosons in (a) SRL and (b) SRS simulated Higgs boson ggF events. Four cases are shown: all events passing selection, a subset containing semileptonic b -hadron decays, a subset with a reconstructed muon, and a subset with a muon-based mass and p_T correction applied [73] (internal).

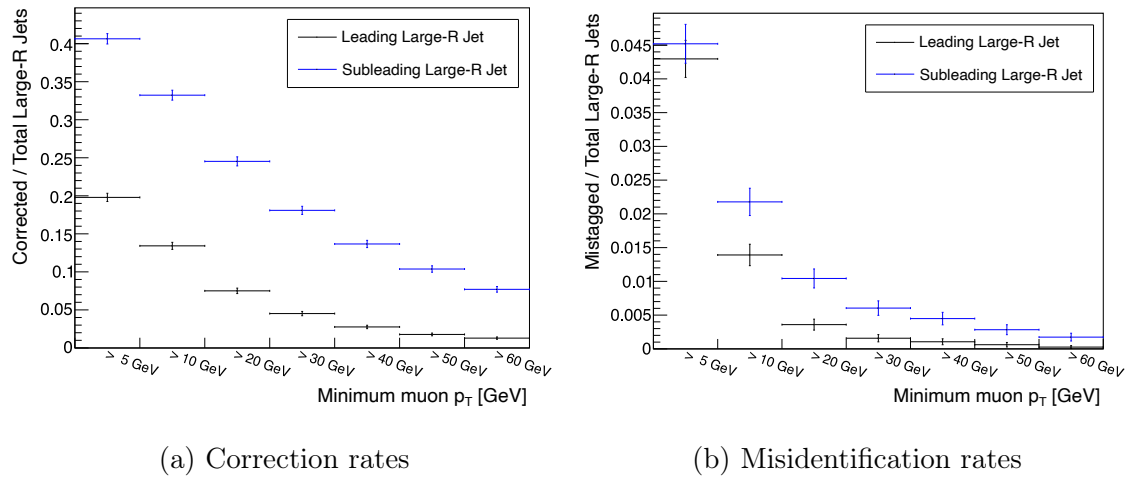


Figure B.4: (a) Correction and (b) misidentification rates for candidate jets associated with truth-level Higgs bosons in simulated Higgs boson ggF events with varied p_T^μ cuts [73] (internal).

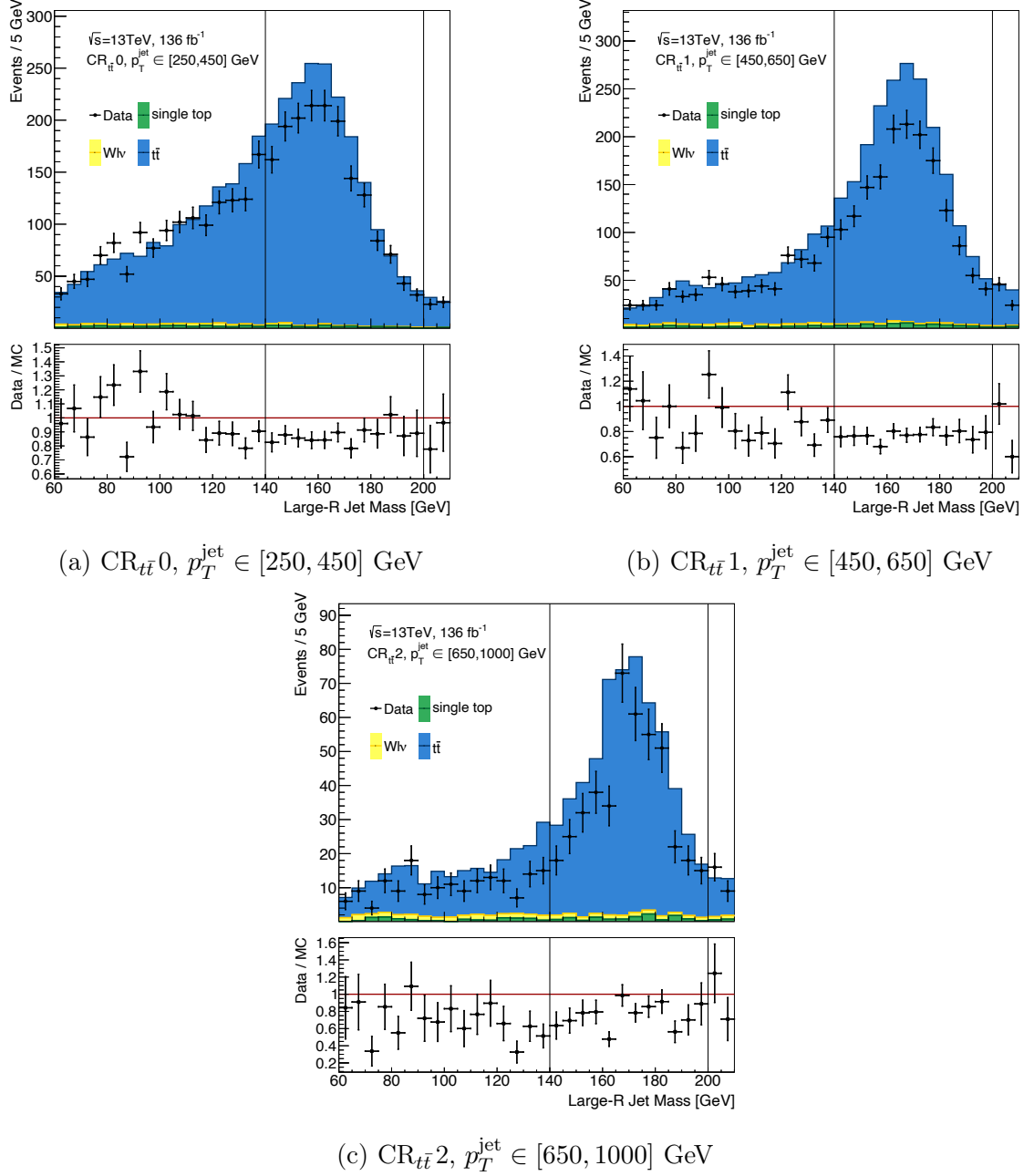
B.2 Mass Distributions in Differential p_T^{jet} Binning

Figure B.5: Stacked $\text{CR}_{t\bar{t}}$ candidate jet mass (m_{jet}) distributions of data and simulations of considered component processes in differential measurement p_T^{jet} bins. A wider range of the m_{jet} is shown, and the vertical lines indicate the fit range.

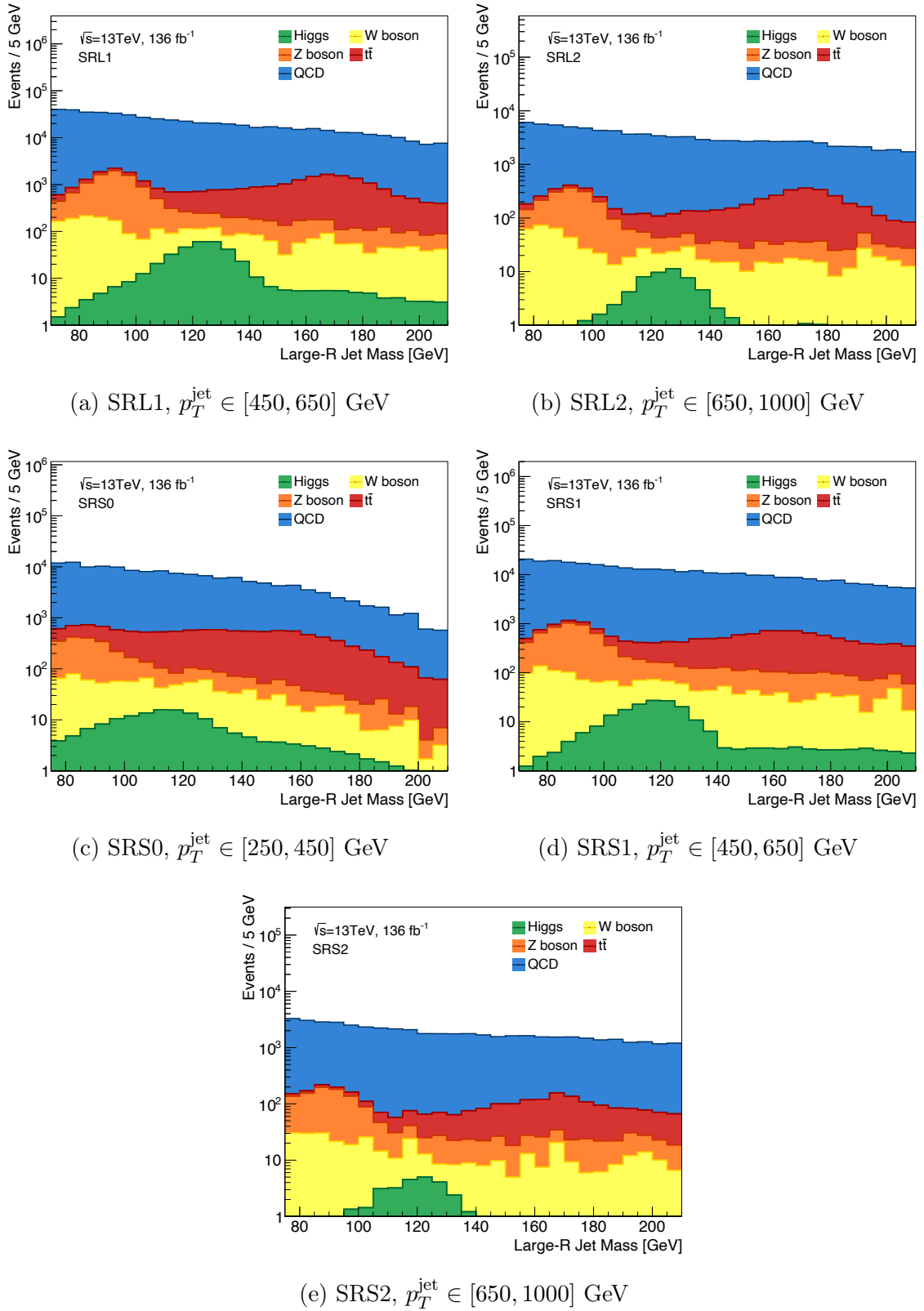


Figure B.6: Stacked SR candidate jet mass (m_{jet}) distributions of data and simulations of considered component processes in differential measurement p_T^{jet} bins. Components with larger yields are stacked on top of components with smaller yields.

B.3 Range of the Candidate Jet Mass Spectra

This analysis makes the Higgs and Z boson measurements using the candidate jet mass (m_{jet}) spectra. The high boundary of the spectra in all signal regions was chosen to be 210 GeV, as it was sufficient to encompass the full $t\bar{t}$ resonance.

The lower boundary of the mass spectrum was limited by several effects which shaped the mass spectra at low masses. Firstly the muon-based mass correction in combination with $m_{\text{jet}} > 60$ GeV threshold in the event selection created a turn-on effect. The mass correction was applied after the event selection. Some of the candidate jet masses at the low end of the mass spectra were shifted to higher values, but there were no events with $m_{\text{jet}} < 60$ GeV to be shifted up to replace them.

Furthermore, low mass candidate jets which passed the event selection were highly boosted, and therefore highly collimated. When jets are highly collimated and dense, the track association to track jets can become ambiguous, reducing the double b -tagging efficiency. This effect was seen in figure 4.1 of section 4.1 on double b -tagging. The mass correction, and b -tagging efficiency effects were studied by the group, and the lower mass boundaries have been determined for each region individually. These boundaries are given in table B.1. The same boundaries were used in signal and validation regions.

Table B.1: The lower boundaries of the m_{jet} mass spectra used in the signal regions for the inclusive and differential measurements, as well as in corresponding validation regions. Fiducial measurement boundaries were the same as those for the inclusive measurement. The upper boundary in all cases was 210 GeV.

Candidate	Inclusive	Differential Bins		
		SR*0	SR*1	SR*2
Leading Jet	70 GeV	–	70 GeV	75 GeV
Subleading Jet	75 GeV	75 GeV	70 GeV	75 GeV

Appendix C

Fitting Framework Validation Study

The $H(\rightarrow b\bar{b}) + j$ analysis presented in this thesis was a continuation of the BSM resonance search in the same final state ($X(\rightarrow b\bar{b}) + j$), in which the results were also interpreted as a Higgs boson search [4]. One of the most consequential departures from the previous analysis setup was the use of a new fitting framework, which enabled a parametric treatment of the QCD background. The author was the main contributor to the set-up of this framework, and conducted validation and performance studies, presented in this chapter.

The studies were conducted by replicating the results of the Higgs boson interpretation of the BSM search (later “BSM search”) using the new framework, and comparing them. They were performed in the first stages of the $H(\rightarrow b\bar{b}) + j$ analysis and were vital for its progression. The studies showed a significant improvement in the treatment of the QCD background using the new framework, signifying the importance of this work.

The development of the new framework and the conducted studies formed a basis for the current $H(\rightarrow b\bar{b}) + j$ measurements, and any other studies requiring complex fits in the analysis development. The presented studies gave confidence in the validity of the $H(\rightarrow b\bar{b}) + j$ measurement strategy, and showcased the improvement in the treatment of the QCD background – the most prolific background in the signal regions.

C.1 Analysis Set-up

Many components of the experimental setup of the BSM search were similar to the current $H(\rightarrow b\bar{b}) + j$ analysis. This section gives a brief description of the setup.

Data and Simulated Samples

This study used the same data and simulated samples as the BSM search [4]. The pp collision data were collected at the ATLAS Experiment in 2015, 2016 and 2017 at 13 TeV centre-of-mass energy. The events used were collected using a single large- R jet trigger with p_T thresholds ranging between 360 GeV and 460 GeV, and amounted to 80.5 fb^{-1} of data. The simulated samples were produced using MC simulations. The details of the MC generators used are given in [4].

Event Selection

The event selection used in the BSM search and this study was very similar to the one used in the current $H(\rightarrow b\bar{b}) + j$ analysis. The event selection of the current analysis is presented in section 5.4. The differences between the selection used in this study and the $H(\rightarrow b\bar{b}) + j$ analysis are summarised in the following.

Firstly, only the leading large- R jet in the event was considered as the Higgs boson candidate, which is analogous to the leading signal region (SRL) used in the current analysis. The kinematic selection differences between the current analysis are summarised in table C.1 and were primarily due to different trigger requirements.

As in the current analysis, the candidate large- R jets were required to have at least two associated track jets. The events were divided into *three* regions of interest: the **Signal Region** (SR), which was made up of events with two b -tags; a **Validation Region** (VR)¹ used for the data-driven QCD background shape parametrisation, made up of events with zero b -tags; and the dedicated **$t\bar{t}$ Control Region**

¹ In the documentation of the previous BSM analysis [4], the validation region was called *the QCD Control Region* (CR_{QCD}).

Table C.1: A summary of event selection differences between the $H(\rightarrow b\bar{b}) + j$ analysis presented in this thesis, and the event selection used in this study and the BSM search [4]. Where relevant the comparison is in reference to the leading-jet signal region (SRL) of the current analysis. The *recoil jet* was the sub-leading p_T large- R jet in the event. b -tagging requirements are given in terms of the efficiency working points (WP) of the MV2 b -tagging algorithm. * – requirement imposed for full trigger efficiency in the selection, as some triggers used to collect data had minimum jet mass thresholds.

Region	Quantity	$H(\rightarrow b\bar{b}) + j$	Past [4] / This Study
SR/VR	Candidate jet p_T	> 450 GeV	> 470 GeV
	Candidate jet mass	> 60 GeV*	–
	Recoil jet p_T	> 200 GeV	> 250 GeV
	SR b -tagging	$2\times$ at 77% WP	$2\times$ at 77% WP
	VR b -tagging	$0\times$ at 77% WP	$0\times$ at 85% WP
$\text{CR}_{t\bar{t}}$	Candidate jet p_T	> 250 GeV	> 470 GeV
	Muon p_T	> 40 GeV	> 52.5 GeV

$(\text{CR}_{t\bar{t}})$, constructed in the same way as the $\text{CR}_{t\bar{t}}$ in the current analysis.

As all the data were collected using the same triggers, the SR and VR events containing a muon with $p_T^\mu > 40$ GeV opposite to the candidate jet ($\Delta\phi > 2\pi/3$) were removed to make the regions orthogonal to $\text{CR}_{t\bar{t}}$. More detailed information on the event selection can be found in [4].

Systematic Uncertainties

The considered sources of systematic uncertainties were largely the same as those included in the current analysis fit model: flavour tagging uncertainties, large- R jet uncertainties and modelling uncertainties.

All uncertainties were based on ATLAS recommendations available at the time (2018). The flavour tagging and jet uncertainties were derived using the same cal-

Table C.2: A summary of systematic uncertainties used in this study and the BSM resonance search [4]. The “Effect” column indicates whether the uncertainty acts on the normalisation (N) and/or the m_{jet} template shape (S) of the process. * – see JMS uncertainty description in section 7.2.1 for more information. $\circ$ – uncertainties produced using alternative MC generators.

Uncertainty	Effect	Reference
Flavour tagging uncertainties		
b -jet b -tag SF	N	[91]
c -jet mistag SF	N	[89]
Light-jet mistag SF	N	[90]
Large- R jet uncertainties		
Jet Mass Resolution	N+S	[75]
	Baseline*	N+S
Jet Mass and Energy Scale	Modelling*	N+S
	Tracking*	N+S
	TotalStat*	N+S
Modelling uncertainties		
V +jets	N+S	$\circ$
$t\bar{t}$	N+S	$\circ$

ibration methods as those used in the current analysis. However, in all cases, simplified estimates or correlation schemes were used. The modelling uncertainties for both V +jets and $t\bar{t}$ processes were derived using alternative MC generators. All systematic uncertainties are summarised in table C.2.

Note: The results produced with the new framework did not include luminosity and alternative QCD function uncertainties, which were present in the BSM search results. Both were seen to have a small impact on the results (2% – 4%) [4], and would not have significantly impacted the results.

C.2 Fit Set-up

The study compares measurements performed using likelihood models built using the framework used in the BSM search, and the new framework, in large part developed by the author. In the following they will be called the *previous framework* (or *model*) and *new framework* (or *model*), respectively. This section describes the measurement set-up, and outlines any differences between the two compared models.

The SR Measurement

As in the current analysis the fit was used to measure the Higgs boson signal strength, μ . The combined Z and W boson signal strength μ_V was also measured simultaneously. The signal region also included $t\bar{t}$ and QCD backgrounds. The measurement was done in a slightly wider mass range: $m_{\text{jet}} \in [70, 230]$ GeV.

All resonant processes were modelled using MC simulations, and smoothed using parametric fitting, as described in the second part of appendix F.1. The QCD background was modelled using the same polynomial exponential form as in the current analysis (equation 6.1), with $N = 4$ parameters².

The $\text{CR}_{t\bar{t}}$ Fit

The previous framework did not have the capability to perform simultaneous fits. The $t\bar{t}$ scale factor ($\text{SF}_{t\bar{t}}$) was measured in $\text{CR}_{t\bar{t}}$ separately, and included as a Gaussian prior on the $t\bar{t}$ yield in the SR. The method of including external $t\bar{t}$ constraints was discussed previously in section 8.2.

The $\text{SF}_{t\bar{t}}$ measured using both frameworks are given in table C.3. The results showed good agreement between the two frameworks, and also agreed with the $\text{CR}_{t\bar{t}}$ measurements made with the 136 fb^{-1} dataset using the current analysis setup, given previously, in table 6.5.

² Due to a different mass range, the x in eq. 6.1 was defined as $x = (m_{\text{jet}} - 150 \text{ GeV}) / 80 \text{ GeV}$.

Table C.3: Scale factors and uncertainties for the $t\bar{t}$ yield found in $\text{CR}_{t\bar{t}}$ by the BSM search (previous), and the new fitting framework. The combined statistical and systematic uncertainties are quoted.

Framework	Scale Factor	Uncertainty
Previous	0.84	0.11
New	0.83	0.11

The ability to perform simultaneous SR and $\text{CR}_{t\bar{t}}$ fits was seen as another major advantage of the new framework, and led to improvements in the measurements.

C.2.1 Model Differences

This section describes the differences between the fit models used in the previous study (the BSM search) and the new framework, which are important to contextualise the results in the following section.

Software: The previous framework was based on the *Bayesian Analysis Toolkit* (BAT) [154], whereas the new framework utilises *XML Analytic Workspace Builder* and *QuickFit* packages based on *RooFit* [139] fitting software.

Treatment of QCD Parameters

In both models the same QCD background definition (f_{QCD}) was used: a 4th order exponential polynomial with a normalisation parameter (5 parameters in total). However, the previous framework did not have an ability to fit parametric functions and binned templates (which the analysis used for resonant processes) simultaneously. Therefore the QCD background estimate had to be included in the likelihood as a binned template.

In order to use a parametric description for the QCD background and input it as a binned template, these steps were taken:

1. other software was used to run a simple statistics-only SR fit (no systematic uncertainties), with a parametric QCD description;
2. a nominal QCD template was constructed by sampling the f_{QCD} with best-fit parameter values from the statistics-only fit;
3. QCD parameter uncertainty templates were constructed using f_{QCD} parameter uncertainties derived from the statistics-only, as described below.

The nominal template was constructed by sampling the QCD function with best-fit parameters: $\{\hat{\theta}_0, \hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3, \hat{\theta}_4\}$. The uncertainties on the QCD parameters in the SR fit were defined as templates constructed using $\pm 1\sigma$ variations of a corresponding best-fit parameter, e.g. the template describing the $+1\sigma$ uncertainty on θ_1 , was constructed by sampling the f_{QCD} function with parameters: $\{\hat{\theta}_0, (\hat{\theta}_1 + 1\sigma), \hat{\theta}_2, \hat{\theta}_3, \hat{\theta}_4\}$.

The described treatment constrains the QCD parameters to stay within the range of the statistical uncertainties, penalising deviations from the nominal shape, and restricting the correlations of QCD parameters with the other processes in the fit. As initial QCD parameters and their uncertainties were derived from a statistics-only fit, this treatment could bias the final fit towards the nominal descriptions of the resonant processes.

The new framework allowed the use of parametric functions and binned templates simultaneously. Hence, the QCD parameters could be included in the likelihood description directly, and could correlate with all nuisance parameters in the fit without any restrictions. This treatment does not artificially constrain the QCD description, therefore improving the treatment of the QCD background and, by extension, the treatment of all of the processes in the fit.

C.3 Results

All results said to be produced with the *previous* framework were taken from the BSM resonance search results [4] or associated internal documentation [155].

The SR data and post-fit expectations of the processes found using the new framework are shown in figure C.1. The top panel shows the data and all the post-fit SR components. The fit was seen to describe the data well. The middle panel shows the V +jets and Higgs boson post-fit estimates, and data with the QCD and $t\bar{t}$ components subtracted. In this panel the estimated contribution of the Higgs boson became more apparent. The bottom panel shows the Higgs boson estimate and data with all estimated background processes subtracted. The small excess was visible by eye and was modelled well by the Higgs boson estimate with the measured signal strength.

The best-fit values found using both fitting frameworks are given in table C.4. Both fits found the measured μ_H and μ_V to be within 2σ of the SM prediction ($\mu = 1$). In both cases the μ_H measurement significance was under 2σ . The V +jets signal significance measured with the previous framework was 5σ , whereas, due to larger uncertainties, the V +jets signal significance with the new framework only amounted to 2σ . The following studies and discussion will provide some insight into this behaviour.

The new framework was also tested using Asimov fits³, which were not performed by the previous analysis and were not available for comparison. The uncertainty on μ_V was reduced by 45% in the Asimov fit, suggesting that the large uncertainty could have been caused by tension between the data and the new fit model. It was also notable that the Asimov fit returned SM values for μ_H and μ_V indicating that there were no technical issues affecting the signal strength determination in the fit. This was an important observation at the time, validating the technical quality of the analysis software.

³ Asimov data is an idealised dataset, built from the model itself, providing the expected results and sensitivity of the measurement. Described in section 5.7.2.

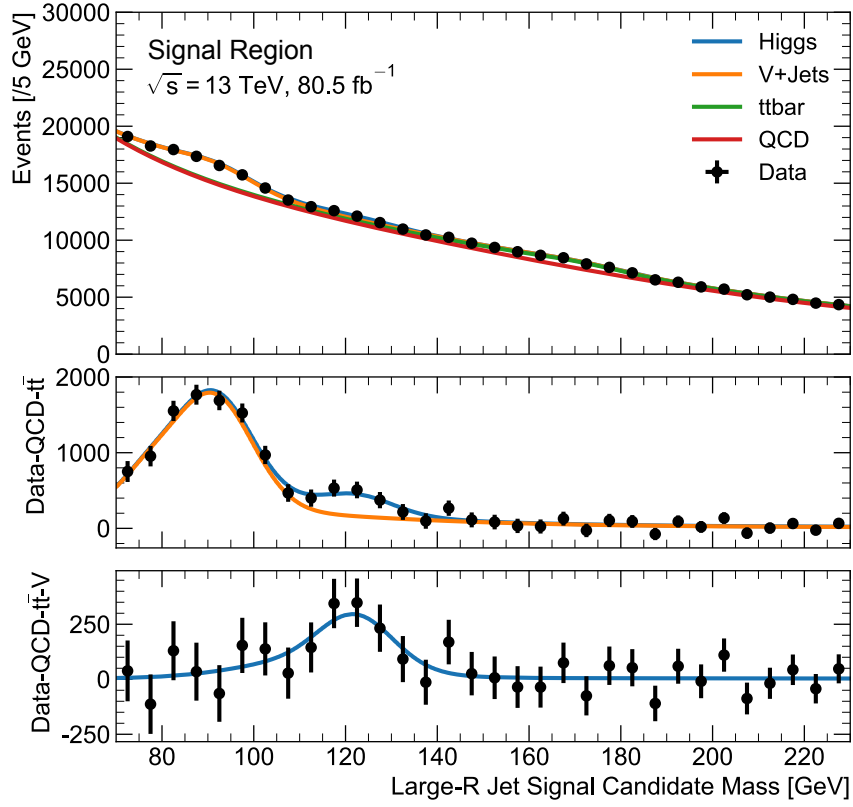


Figure C.1: SR data and the post-fit estimates of Higgs boson, V +jets, $t\bar{t}$ and QCD processes found using the new fitting framework. $\mu_H = 7.4 \pm 6.5$ and $\mu_V = 1.4 \pm 0.6$. Top: all SR components; middle: data with the QCD and $t\bar{t}$ predictions subtracted; bottom: data with all background components subtracted, such that the Higgs boson estimate is visible.

Table C.4: Fit results from the BSM study (*previous*) [4] and fits using the new framework in real and Asimov data. μ - signal strength, σ - uncertainty, Z - significance in units of standard deviations. SM values of μ_H and μ_V are 1.

Fit	μ_H	$\sigma(\mu_H)$	$Z(\mu_H)$	μ_V	$\sigma(\mu_V)$	$Z(\mu_V)$
Previous, Data	5.8	3.6	1.6	1.5	$^{+0.4}_{-0.3}$	5.0
New, Data	7.4	6.5	1.2	1.4	0.6	2.2
New, Asimov	1.0	4.6	0.2	1.0	0.4	2.8

Correlation Scheme Improvement

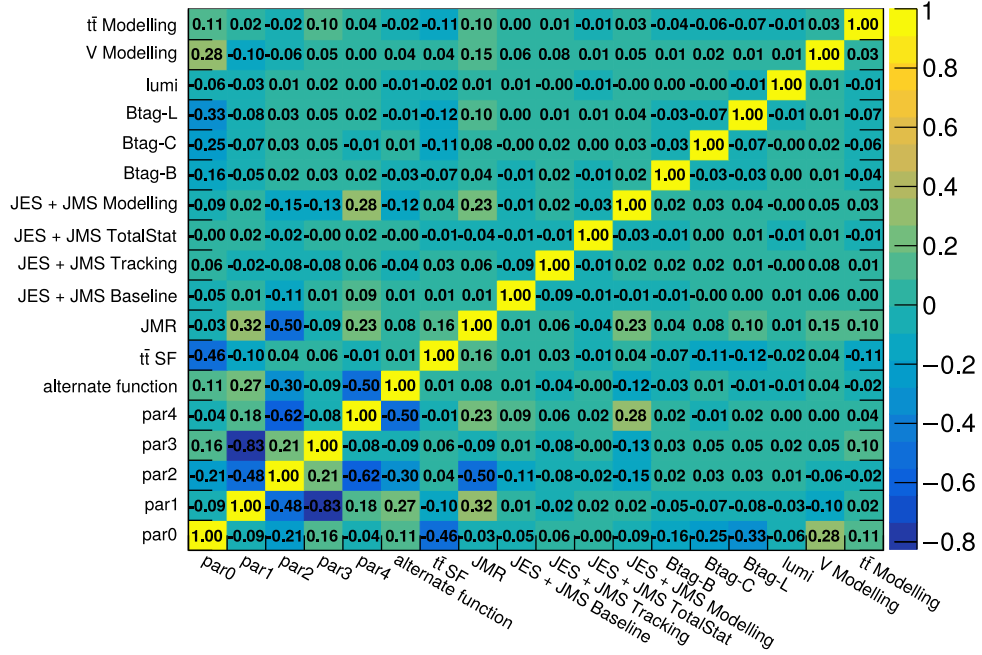
Differences between the two models were strikingly apparent when comparing their fit parameter correlations. The correlation plots from the Higgs interpretation in the BSM measurement [4], and the new fit to data are shown in figures C.2a and C.2b, respectively.

The correlations between the QCD parameters were generally much stronger in the new fit. For example, all of the QCD parameters (including the yield) had (anti)correlations larger than 50%. This was the case in only two out of ten parameter combinations in the previous fit. As the QCD parameter treatment was understood to be more legitimate in the new fit setup, the increased correlations were evidence of a significant improvement in the model description and a clear advantage of the new framework.

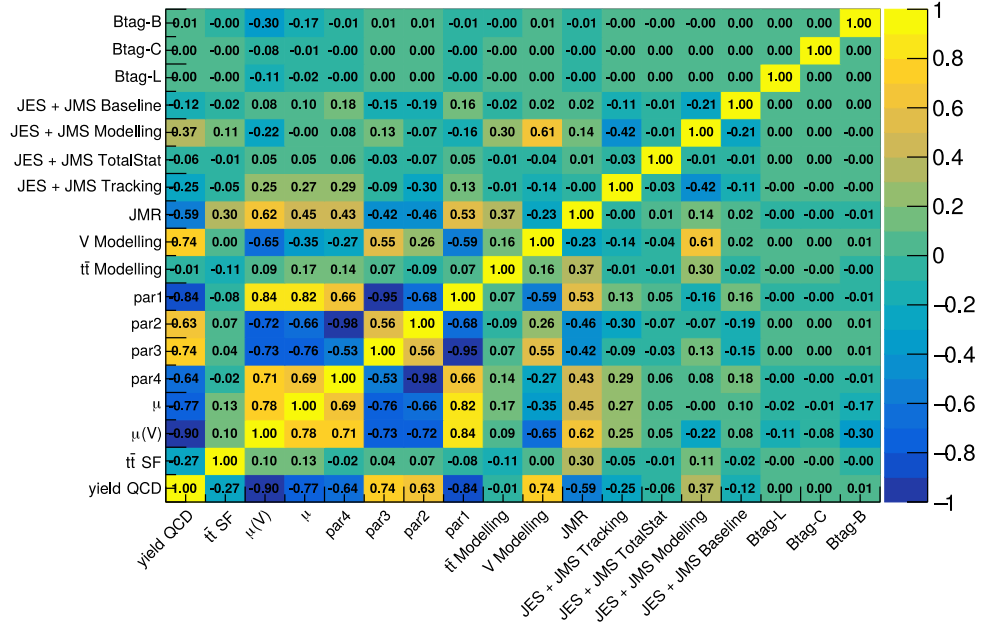
Much more prominent correlations were also seen for the V +jets MC modelling and the JMR uncertainties with the rest of the fit parameters. These correlations were reduced in the Asimov data fit, indicating that the JMR and V +jets modelling uncertainties played a large role in adapting the fit model to the data, and had a strong influence on the behaviour of the fit. These important correlations were clearly neglected in the previous fit configuration. The rigidity imposed on the QCD background with the previous treatment made it unable to adapt to changes in other nuisance parameters, and therefore constrained the fit.

Uncertainty Pull Comparison

To gain more insight into the nuisance parameter (NP) behaviour, the NP pulls from both fits were compared, shown in figure C.3. The effects agreed for all but three cases: the JMR, $t\bar{t}$ modelling, and V +jets modelling uncertainties, where the former two were less constrained, and the latter was more constrained in the new fit. Generally, the effects could be explained by a larger freedom in the model introduced by the more flexible QCD description. All uncertainties in question showed stronger



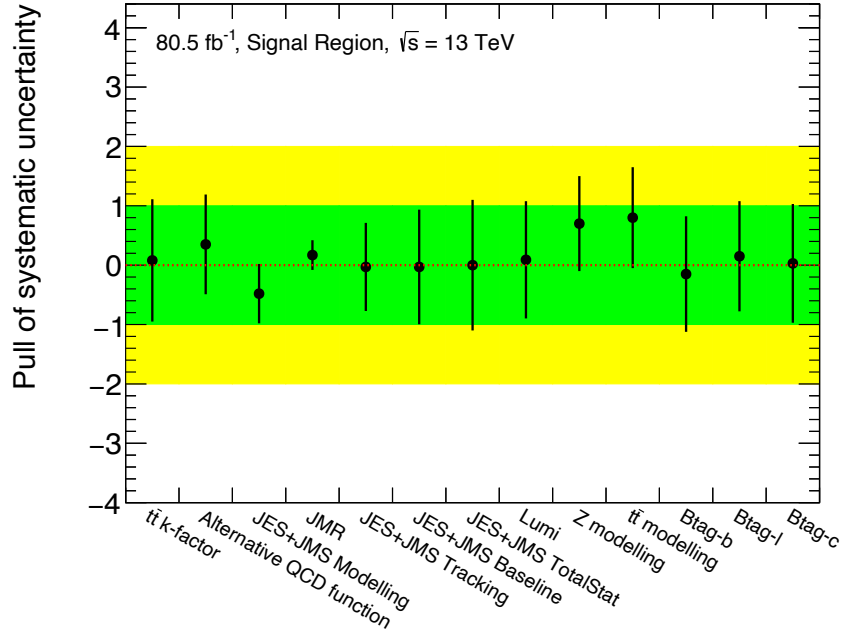
(a) Higgs boson measurement in the BSM Search [155] (internal)



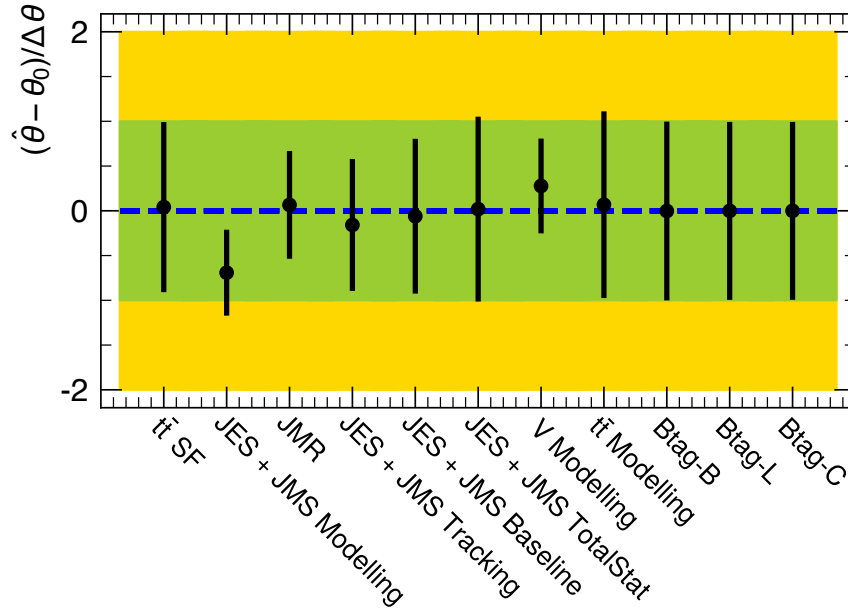
(b) New Framework

Figure C.2: The correlation plots from the Higgs boson measurement fits of the (a) nuisance parameters found using the previous fit framework [155] (internal); and (b) all fit parameters using the new fitting framework. par0–4 correspond to QCD parameters $\theta_{0\dots 4}$, and the yield QCD parameter in (b) is equivalent to par0 in (a).

The yield QCD parameter is the QCD yield, and par0 is the multiplier in front of the exponential in the QCD parametric description



(a) Higgs boson measurement in the BSM Search [155] (internal)



(b) New Framework

Figure C.3: Uncertainty pull plots from the (a) the Higgs boson interpretation of the BSM resonance search [155] (internal); and (b) the SR data fit using the new fitting framework. *Note:* the alternative QCD function and luminosity uncertainties were not included in the new framework, but are not expected to affect the results due to small, 2% – 4% impact [4].

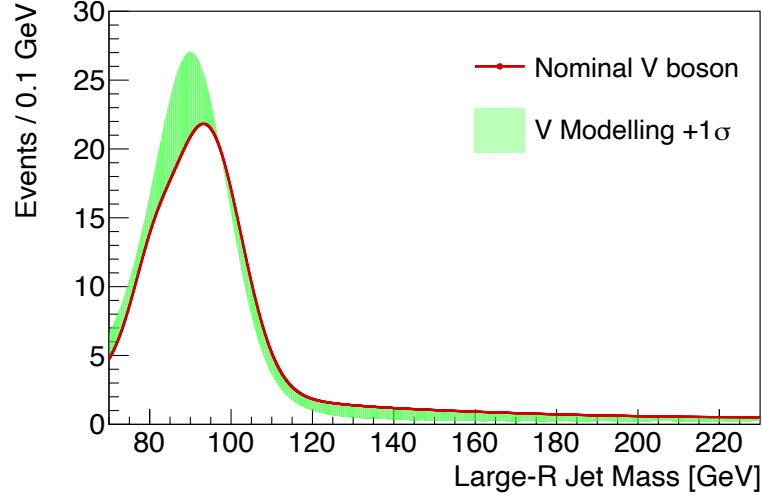


Figure C.4: The nominal V +jets estimate in MC, and the V +jets modelling uncertainty derived using an alternative generator, showing that the uncertainty shifted the V boson resonance peak to lower masses and made it larger.

interactions with the QCD parameters in the new model, as seen comparing the correlations in figures C.2a and C.2b.

The JMR and $t\bar{t}$ modelling uncertainties were significantly less constrained in the new fit, which was understandable with a more flexible model. Insight into the slightly stronger constraints seen on the V +jets modelling uncertainties could be gained by observing the effects of this uncertainty shown in figure C.4. The V +jets modelling uncertainty was one of the largest uncertainties on this process, and the only uncertainty which shifted the V boson resonance peak to lower values and made it larger. The previous, less flexible model, could have relied on having larger V +jets modelling uncertainties to describe the shape of the data, in that particular region. However, the more flexible model would have been able to interact more freely with other processes to adapt to the data, and could constrain the large uncertainty.

The previous fit model also showed larger post-fit pulls of the MC modelling uncertainties, which also could be explained by a lack of flexibility in the previous model. If the QCD background has a poorer ability to shape itself to data, the

differences between the data and model will be accounted for by pulling the nuisance parameters of the other contributing processes.

The NP pull comparison also gave some insight into the large uncertainty differences between the fit results found with the previous and the new model. The JMR uncertainty was the largest pre-fit uncertainty in the model, hence a reduced ability to constrain this uncertainty was likely to reflect in the uncertainties on the parameters of interest, μ_H and μ_V . In fact, if the JMR uncertainty was removed from the fit, the uncertainties on μ_H and μ_V were reduced by 27% and 35% (to $\sigma_H = 4.7$ and $\sigma_V = 0.4$), respectively.

Profile Likelihoods and Uncertainties

The increase in uncertainty on $\mu_{H/V}$ in the new fit results had to be understood before the framework could be used for the new analysis. Further insight into the measurement was gained by observing the 2-dimensional profile likelihood distribution of μ_H and μ_V . A close-up of the minimum⁴ is shown in figure C.5a.

In fact, two nearby minima were observed. Complex fits can have several minima, but in this case the global minimum (at $\mu_H = 9.0$, $\mu_V = 1.6$) does not correspond to the minimum chosen as the “best-fit” by the fitting framework ($\mu_H = 7.3$, $\mu_V = 1.4$)⁵. It was a cause of some concern, however it was noteworthy that the two minima were well within the uncertainties on the measurement.

The double peak structure was not observed in the fit to the Asimov dataset shown in figure C.5b, suggesting that the discontinuity in the probability distribution was caused by differences between the data and the model. The situation in data was improved in a test fit wherein the uncertainties with the highest correlations with the SR processes: JMR and MC modelling, were removed, shown in figure C.5c. A double minima structure was still seen, but now the distance between the

⁴ The minimum of $-2 \ln \lambda$ corresponds to the most likely values of the parameters of interest.

⁵ These values ($\mu_H = 7.3$, $\mu_V = 1.4$) also correspond to the best-fit values of μ_H and μ_V in a statistics-only fit.

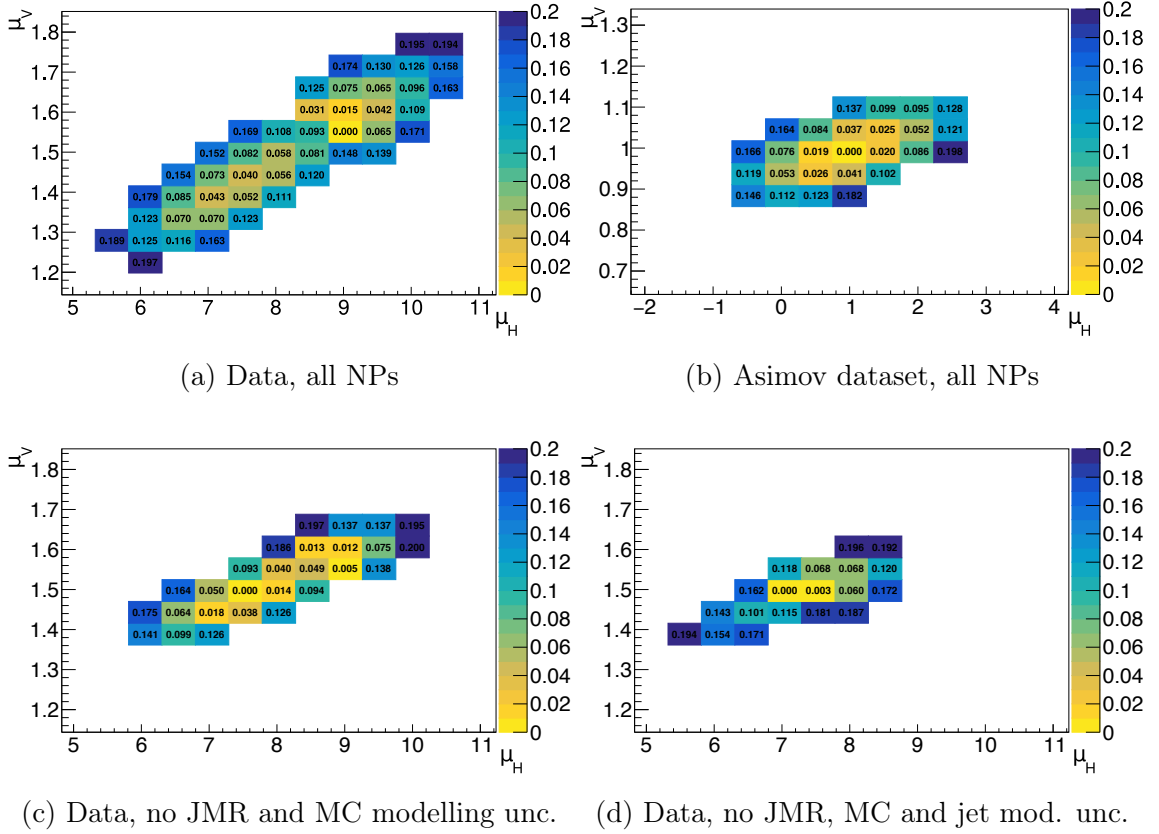


Figure C.5: Profile likelihood distributions ($-2 \ln \lambda$, where λ is the Wilk's test statistic [140]) for the signal hypothesis as found with the new fit framework in fits to (a) data, including all systematic uncertainties; (b) SR Asimov data, including all systematic uncertainties; (c) data, without including JMR and MC modelling uncertainties; and (d) data, without including JMR, MC modelling and jet modelling uncertainties. With the removal of large uncertainty descriptions the model becomes less flexible, reducing the width of the profile likelihood. No multiple minimas were seen in the Asimov fit.

two minima was reduced and the lower value was the global minima, making the fit results and the profile likelihood distribution consistent. Furthermore, when the jet modelling uncertainty (also showing larger correlations) was removed, the two minima structure was mitigated completely, as shown in figure C.5d.

The strong impact these uncertainties had on the results was unsurprising as these uncertainties were large and displayed increased correlations compared to the previous model. The increased flexibility of the QCD description had less ability to

constrain particularly large uncertainties such as JMR and $t\bar{t}$ modelling, which lead to an even greater flexibility in the model, such that it was able to have multiple acceptable descriptions of the data. This reflected in the broad likelihoods and second minima. At the time of these studies, it was known that the treatment of the uncertainties in question will be improved: new, more precise, uncertainty recommendations were available, a more precise correlation scheme for jet uncertainties was to be employed.

The primary aim of this study was to validate the framework for use in the analysis. The observed “issues” with the measurement were understood to be the consequences of a more accurate treatment of the fit parameters, and not due to technical issues with the framework. This was further supported by the fit to Asimov data, seen to be without issue. Therefore the framework was deemed to be ready for use in the analysis.

All of the expected improvements in uncertainty treatment were expected to improve the constraints and stability of the fit. Indeed, no such issues were encountered by the $H(\rightarrow b\bar{b}) + j$ analysis regarding the MC modelling or jet modelling uncertainties. However, the expected improved derivation for the JMR uncertainties was not developed in time to be used in this analysis, and the large conservative estimates for the JMR uncertainty were used. As discussed, previously in section 7.7, due to the additional flexibility in the model introduced by this large uncertainty, the model was able to have multiple acceptable descriptions of the data, making the fit unreliable. This had to be rectified by developing constraints for the JMR uncertainty using external datasets (CR_W and VR).

Profile Likelihood Comparison Between Frameworks

To visualise the impact the new fit set-up, and, in particular, the new QCD parameter treatment had on the parameters of interest, the combined profile likelihood distributions of μ_H and μ_V were compared in figures C.6a and C.6b. The former shows the result from the Higgs boson interpretation of the BSM search [4], and the

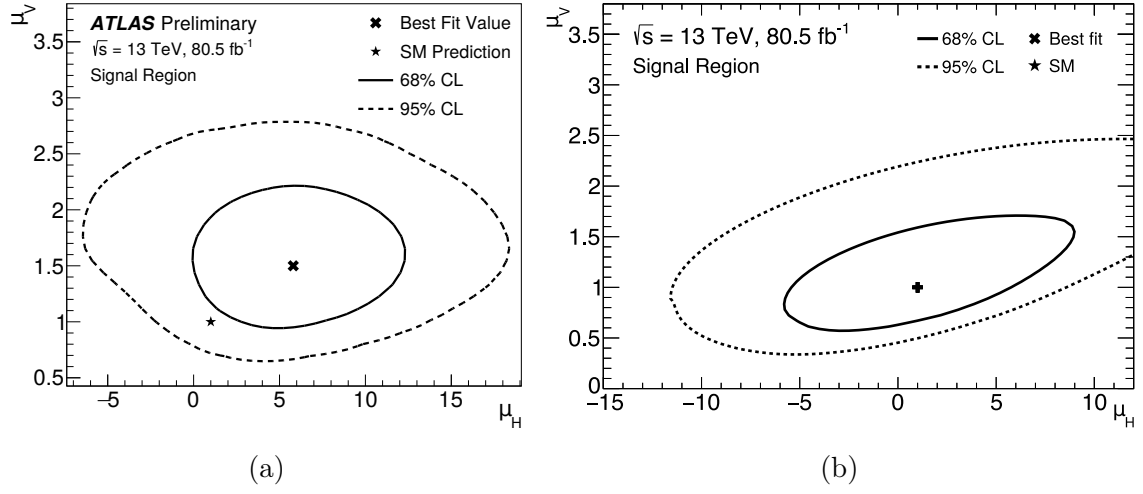


Figure C.6: Combined profile likelihood distributions of μ_H and μ_V as found by the (a) Higgs boson interpretation of the BSM search [4], and (b) a fit to SR Asimov data using the new framework. Note, the best-fit point in an Asimov fit is $\mu_H = \mu_V = 1$, coinciding with the SM point.

latter - the new fit on the Asimov dataset.

In the previous result, μ_H and μ_V did not appear to be correlated, whereas in the new fits (both in figure C.5 and C.6b) a strong correlation was seen. The correlation plot shown in figure C.2 confirmed this, showing a 71% correlation between μ_H and μ_V in the new model.

Such interaction between these parameters was almost certainly due to the improved treatment of the QCD parameters in the new set-up, which introduced more flexibility in the fit. As either μ_H or μ_V was increased by the fit, the QCD estimate had to reduce due to an increased amount of signal in the region, as was evident by the large anti-correlations between $\mu_{H/V}$ and the QCD yield. As this happened, the other resonance had to compensate for the reduction of background and had to increase to describe the data. Therefore, the increased positive correlation between the signal strengths of these two resonances was a consequence of the more complete and flexible QCD fit treatment.

C.4 Chapter Overview

Implementing a new fitting framework based on common Higgs measurement tools within ATLAS was one of the key hurdles for this analysis. This section has presented the validation studies of the new framework permitting its use in the $H(\rightarrow b\bar{b}) + j$ analysis; and compared it to the previously used framework in the Higgs boson interpretation of the BSM resonance search [4].

The studies used the experimental setup of the Higgs interpretation of the BSM search, to have good grounds for comparison. The key components of the experimental setup were introduced, and the main differences between the two frameworks were outlined.

The key difference between the two frameworks was that the new framework had the ability to include parametric functions and binned templates in the likelihood description. This was not possible with the previous framework, where the QCD estimate had to be converted to a set of binned templates for the Higgs boson measurement fit. This treatment limited the flexibility of the QCD estimate function, restricting the possible correlations between fit parameters. The new fit setup was a considerable improvement upon the previous one, as the treatment of the QCD parameters did not involve artificial restrictions, and therefore was more appropriate.

A better treatment of the QCD background lead to a more flexible model which was had less ability to constrain large JMR, and $t\bar{t}$ modelling uncertainties. The overall increased flexibility in the fit, and increased correlations between the processes and large uncertainties lead to a broadening of the likelihood distribution and a formation of a second minima in the likelihood. Overall, the issues were understood to have arisen from a more sophisticated QCD description and large uncertainty descriptions, and were not introduced artificially. As significant improvements in the uncertainty treatment were expected, no concerns were raised going forward.

Greater fit description flexibility was also seen to result in correlations between the signal strengths of the Higgs and V boson resonances, which was not apparent in the previous fit, which constrained the description of the QCD background. This was seen as evidence of an improvement in the signal region modelling, as the greater flexibility in the QCD shape allowed more complete interplay between the signal resonances and the QCD background.

In all, the new fit framework and the model built using it was seen to be an improvement upon the previous framework, and was determined to be ready for use in the $H(\rightarrow b\bar{b}) + j$ analysis. The implementation of the new fitting framework and new fit setup, its maintenance, and the validation studies presented in this section were a major contribution to the analysis by the author.

Appendix D

Signal and Background Modelling

D.1 Higgs Boson Resonance Composition

Table D.1: Yields of simulated Higgs boson events from different production modes overall (“All”), and within the Higgs boson resonance peak ($m_{\text{jet}} \in [105, 140]$ GeV, “In Res.”), for inclusive and differential signal regions. The percentages listed in the “In Res.” column depict the fraction of total yield in the resonance. Binning for differential measurement: bin 0: $p_T^{\text{jet}} \in [250, 450]$ GeV; bin 1: $p_T^{\text{jet}} \in [450, 650]$ GeV; bin 2: $p_T^{\text{jet}} \in [650, 1000]$ GeV.

Mode		Differential Bins							
		Inclusive		SR*0		SR*1		SR*2	
		All	In Res.	All	In Res.	All	In Res.	All	In Res.
SRL	ggF	226	186 (82%)	—	—	196	160 (82%)	29	25 (86%)
	VBF	65	56 (86%)	—	—	56	48 (86%)	9	8 (89%)
	VH	70	48 (69%)	—	—	59	40 (68%)	11	7 (64%)
	$t\bar{t}H$	150	45 (30%)	—	—	117	37 (32%)	30	8 (27%)
	Total	513	335 (65%)	—	—	428	285 (67%)	79	47 (59%)
SRS	ggF	139	94 (68%)	47	23 (49%)	81	61 (75%)	11	10 (91%)
	VBF	47	35 (74%)	10	5 (50%)	32	24 (75%)	5	5 (100%)
	VH	97	59 (61%)	43	21 (49%)	44	31 (70%)	8	6 (75%)
	$t\bar{t}H$	163	49 (30%)	82	32 (39%)	62	15 (24%)	17	2 (11%)
	Total	448	237 (53%)	183	81 (44%)	220	132 (60%)	41	24 (59%)

Table D.2: Fraction of signal contribution of each Higgs boson production mode within the Higgs boson resonance peak ($m_{\text{jet}} \in [105, 140]$ GeV) for inclusive and differential signal regions [73] (internal). Binning for differential measurement: bin 0: $p_T^{\text{jet}} \in [250, 450]$ GeV; bin 1: $p_T^{\text{jet}} \in [450, 650]$ GeV; bin 2: $p_T^{\text{jet}} \in [650, 1000]$ GeV.

Region	Production Mode	Inclusive	Differential Bins		
			SR*0	SR*1	SR*2
SRL	ggF	0.55	–	0.56	0.52
	VBF	0.17	–	0.17	0.17
	VH	0.14	–	0.14	0.15
	$t\bar{t}H$	0.14	–	0.13	0.16
SRS	ggF	0.40	0.28	0.46	0.43
	VBF	0.15	0.07	0.19	0.21
	VH	0.25	0.26	0.24	0.26
	$t\bar{t}H$	0.21	0.39	0.11	0.10

D.2 Z Boson Templates In Differential Measurement Bins

Table D.3: State of systematic uncertainty inclusion for truth p_T^Z templates in the differential measurement signal regions. To reduce the complexity of the fits, systematic uncertainties were not included for templates with small overall yields, and relative yields in the resonance region ($m_{\text{jet}} \in [70, 110]$ GeV). FS – full systematic uncertainty description, *nominal only* – systematic uncertainties not included in the model. Entries in bold (e.g. **FS**) are shown for bins with corresponding p_T^{jet} and p_T^Z . Template distributions, and relative yields in the resonance region are shown in figure D.1.

		Differential Bins, [GeV]			
		SR*0	SR*1	SR*2	
	μ	p_T^Z , [GeV]	$p_T^{\text{jet}} \in [250, 450]$	$p_T^{\text{jet}} \in [450, 650]$	$p_T^{\text{jet}} \in [650, 1000]$
SRL	$\mu_{Z,\text{out}}$	[300, 450]	–	FS	nominal only
	$\mu_{Z,0}$	[450, 650]	–	FS	FS
	$\mu_{Z,1}$	[650, 1000]	–	nominal only	FS
SRS	$\mu_{Z,\text{out}}$	[300, 450]	FS	FS	nominal only
	$\mu_{Z,0}$	[450, 650]	FS	FS	FS
	$\mu_{Z,1}$	> 650	not in fit	FS	FS

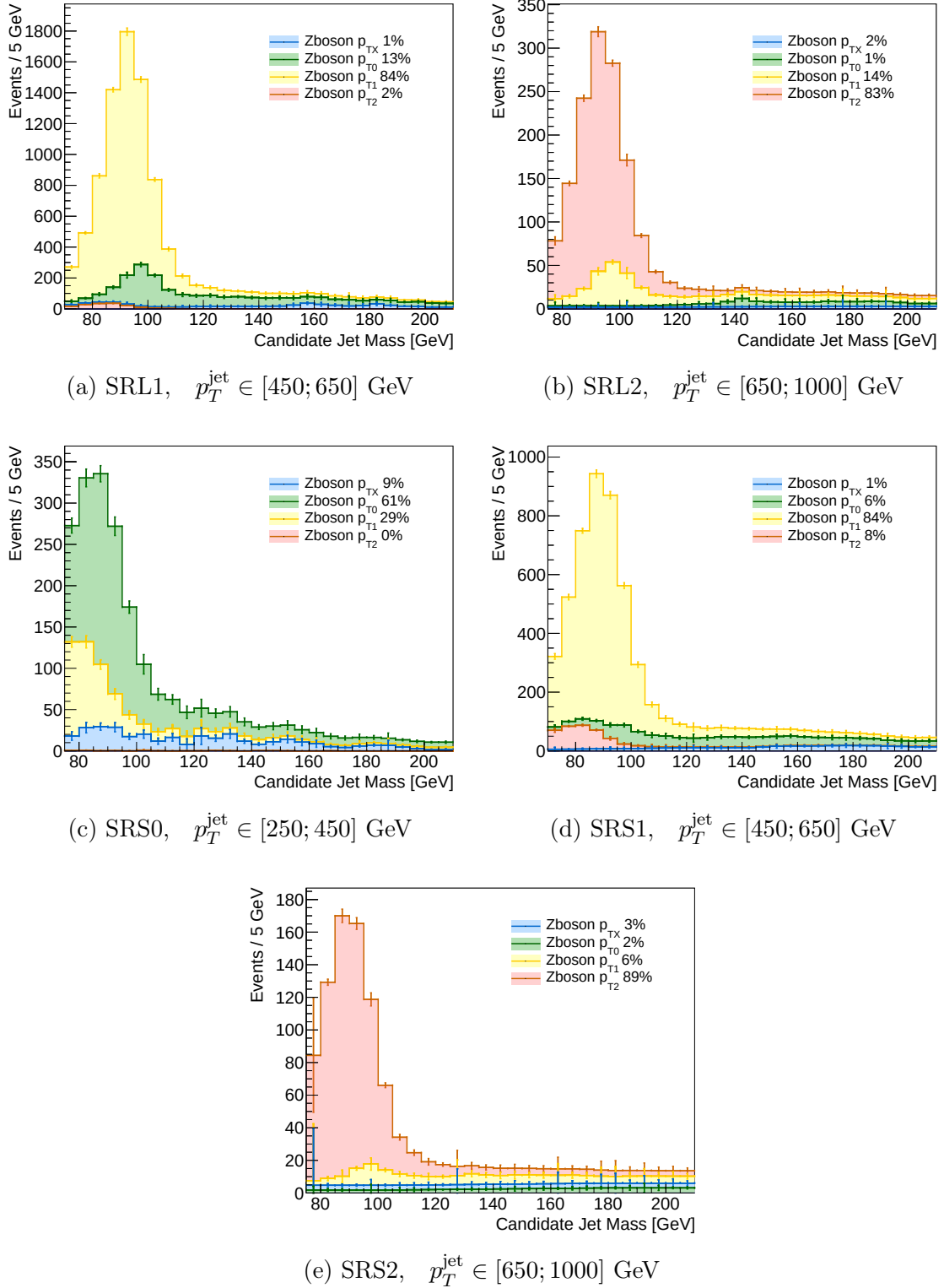


Figure D.1: Stacked histograms of simulated Z boson events in truth p_T^H bins in differential measurement signal regions. The percentage of yield each template contributes within $m_{\text{jet}} \in [70, 110]$ GeV is shown in the legend. The p_T^H momentum bins are: $250 \text{ GeV} < p_{T,X}^Z < 300 \text{ GeV} < p_{T,0}^Z < 450 \text{ GeV} < p_{T,1}^Z < 650 \text{ GeV} < p_{T,2}^Z$.

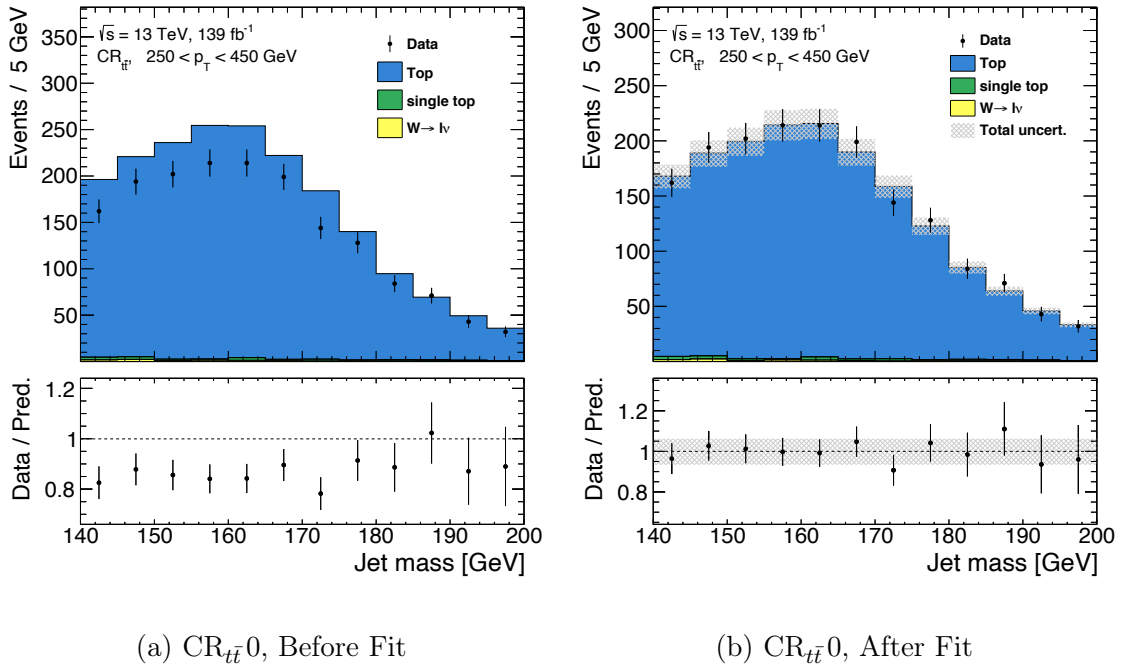
D.3 Plots: Standalone $\text{CR}_{t\bar{t}}$ Fits in Differential p_T^{jet} Bins

Figure D.2: The $\text{CR}_{t\bar{t}}0$ ($p_T^{\text{jet}} \in [250, 450]$ GeV) data and model m_{jet} distributions (a) before and (b) after a standalone likelihood fit of the $\text{CR}_{t\bar{t}}0$ region. The measured $t\bar{t}$ scale factors was $\text{SF}_{t\bar{t},0} = 0.86 \pm 0.02$ (stat) $^{+0.06}_{-0.06}$ (syst). The single-top and $W(\ell\nu)$ backgrounds were fixed to the SM predictions in the fits.

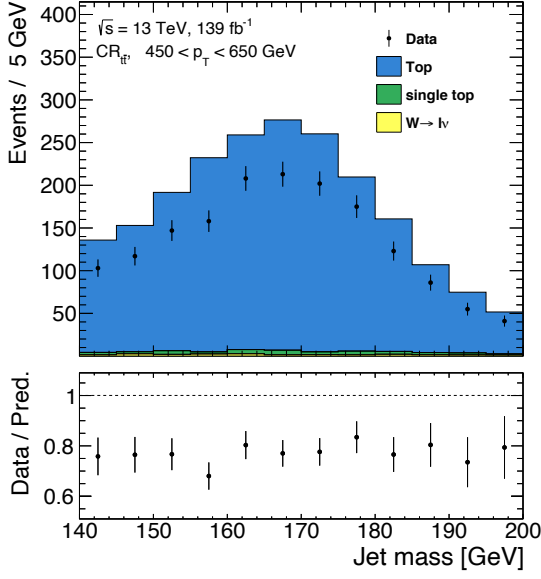
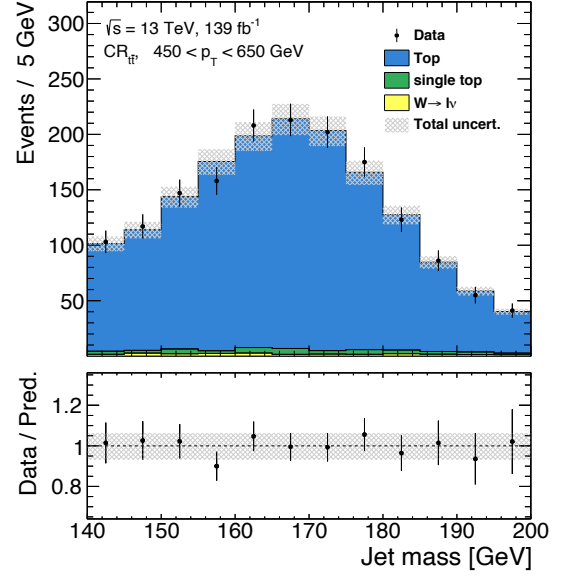
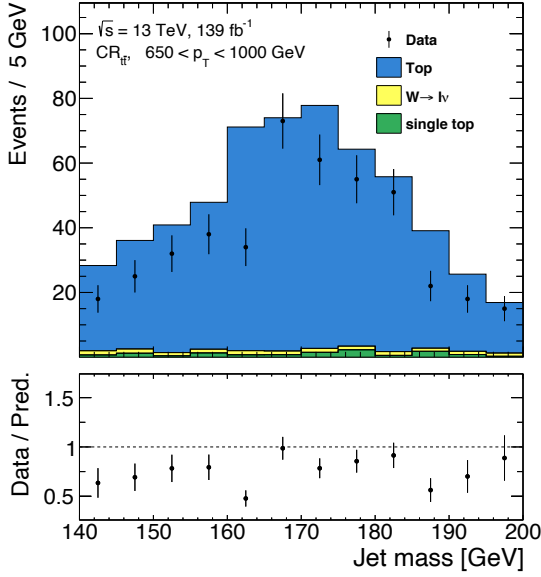
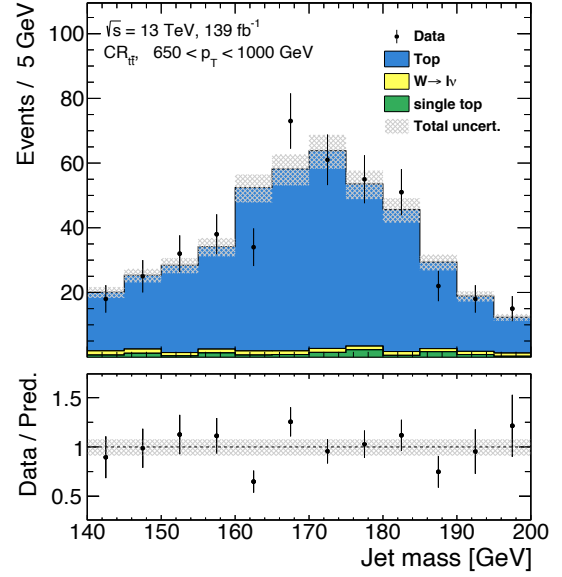
(a) $\text{CR}_{t\bar{t}}1$, Before Fit(b) $\text{CR}_{t\bar{t}}1$, After Fit(c) $\text{CR}_{t\bar{t}}2$, Before Fit(d) $\text{CR}_{t\bar{t}}2$, After Fit

Figure D.3: The (top) $\text{CR}_{t\bar{t}}1$ ($p_T^{\text{jet}} \in [450, 650]$ GeV) and (bottom) $\text{CR}_{t\bar{t}}2$ ($p_T^{\text{jet}} \in [650, 1000]$ GeV) data and model m_{jet} distributions (left) before and (right) after a standalone fits to said region. The measured $t\bar{t}$ scale factors were $\text{SF}_{t\bar{t},1} = 0.76 \pm 0.02$ (stat) $^{+0.07}_{-0.07}$ (syst), and $\text{SF}_{t\bar{t},2} = 0.73 \pm 0.04$ (stat) $^{+0.08}_{-0.07}$ (syst). The single-top and $W(\ell\nu)$ backgrounds were fixed to the SM predictions in the fits.

Appendix E

Nominal V +jets Template Smoothing

E.1 V +jets Template Smoothing Procedure

The V +jets samples available to use in this analysis were statistically limited. In some cases this resulted in relatively “unsmooth” mass templates used for Z +jets and W +jets estimates in the signal regions. Particularly this effected the mass templates with small yields, such as W +jets, and the off-diagonal Z +jets templates¹ used in the differential Z boson measurement. Examples of these templates can be seen in figures E.1a, showing W +jets events in the SRS inclusive region, and E.1b, showing Z +jets events with $p_T^Z \in [350, 450]$ GeV in SRS1 (defined by $p_T^{\text{jet}} \in [450, 650]$ GeV).

Throughout most of the analysis development, the effect was even more severe. The available MC samples were 10 times smaller, and a finer 0.5 GeV binning was used². The fluctuations were evident in all V +jets signal region templates, including the Z +jets templates in the inclusive signal regions, shown in figures E.1c and E.1d.

Large statistical fluctuations in the model of a process can impact the ability of the fit to measure that process. This effect was studied using validation region data

¹ The differential measurement signal regions were binned in candidate jet p_T . The mass templates describing the signal (in this case Z +jets process) in each p_T^{jet} -binned signal region were split into truth-level p_T^Z bins, such that the signal strength $\mu_{Z,i}$ defined in a $p_T^{Z,i}$ bin was measured separately, as described in section 5.5. Off-diagonal components, are jet mass templates of the signal process with truth-level $p_T^{Z,i}$ bin not aligned to the $p_{T,j}^{\text{jet}}$ of the differential measurement signal region ($i \neq j$). The concept was introduced in section 6.3.3.

² See section 5.7.1 for more details on the binning.

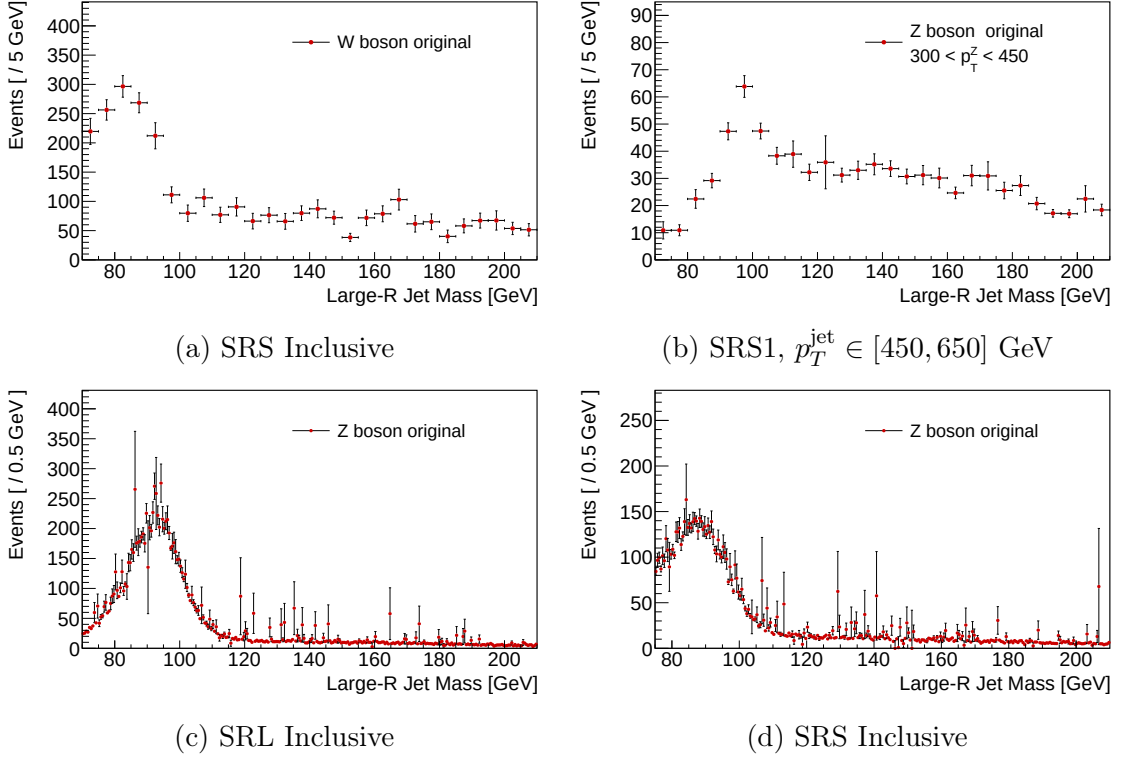


Figure E.1: The original (non-smoothed) templates of simulated W +jets and Z +jets events in the signal regions, with evident large statistical fluctuations. The top figures, are examples with the latest MC samples in 5 GeV binning used in the current set-up. The bottom plots show examples from samples used when the smoothing procedure was initially designed, which were 10 times smaller, and 0.5 GeV binning was used in the fit.

(in 0.5 GeV binning, with the smaller V +jets samples). Proxies to the signal regions were created from VR data slices, by subtracting the resonant VR backgrounds, and adding SR resonant background expectations derived from MC simulations:

$$\text{VR}_{\text{proxy}}^i = (\text{VR}^i - V_{\text{VR}} - t\bar{t}_{\text{VR}}) + Z_{\text{SR}}^{\text{smoothed}} + t\bar{t}_{\text{SR}}, \quad (\text{E.1})$$

similarly to the VR_{hyb} creation described in the previous section. The added Z +jets templates were smoothed in order to emulate the effects of the distributions being different in data. The test was done with VR proxies of both leading and subleading inclusive signal regions. The smoothed Z +jets mass templates ($Z_{\text{SR}}^{\text{smoothed}}$) for each region were created by fitting the simulated Z +jets distributions with a sum of a

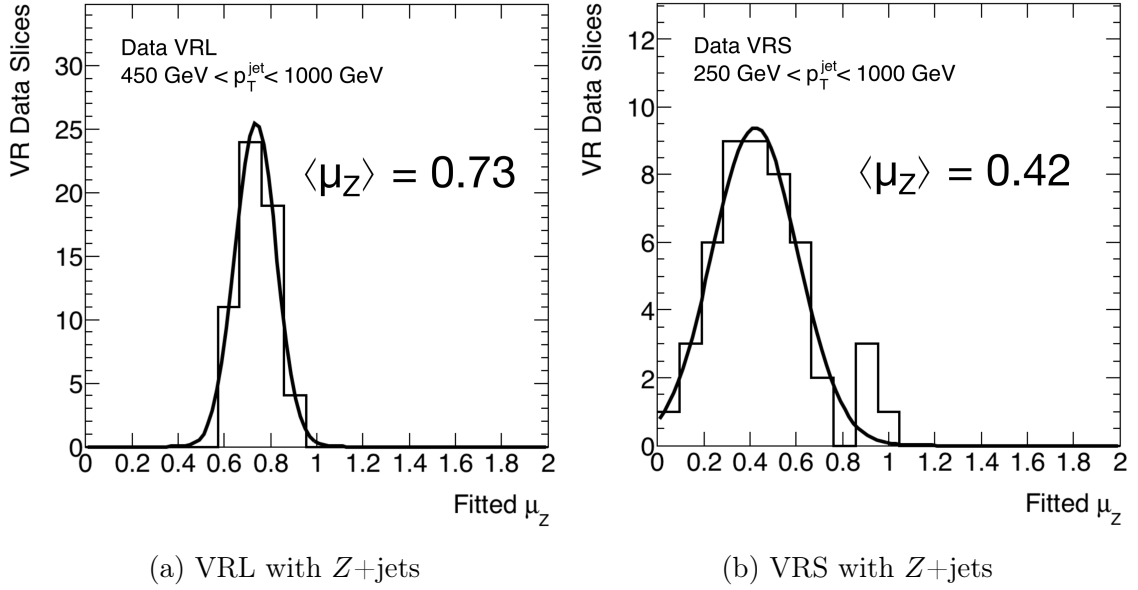


Figure E.2: The distributions of extracted Z +jets signal strengths (μ_Z) from fits to modified (a) VRL and (b) VRS data slices, described in equation E.1, with added smooth Z +jets signal ($\mu_Z^{\text{in}} = 1$) [73] (internal). The fit models use original non-smooth Z +jets MC templates. The $\langle \mu_Z \rangle$ values were found through Gaussian fits to the distributions. The model used 0.5 GeV binning and $10\times$ smaller MC samples than available during in the final measurement.

Gaussian function ($Z \rightarrow b\bar{b}$ candidates) and a parametric QCD background estimate (recoiling jet candidates), and sampling from the resulting distributions.

The $\text{VR}_{\text{proxy}}^i$ slices were fit with the parametric QCD, $t\bar{t}$ and original (non-smooth) Z +jets estimates. The distributions of the extracted Z +jets signal strength (μ_Z) in VRL and VRS are shown in figures E.2a and E.2b, respectively. The mean extracted values were found to be $\langle \mu_Z \rangle = 0.73$ in VRL and $\langle \mu_Z \rangle = 0.42$ in VRS, indicating that this model was unable to efficiently recover the Z boson signal.

The Solution: Template Smoothing

The fit bias caused by the fluctuating MC templates could have possibly been remedied by including the MC statistical uncertainties in the fit, which would have given the fit the required additional freedom to account for the differences between the

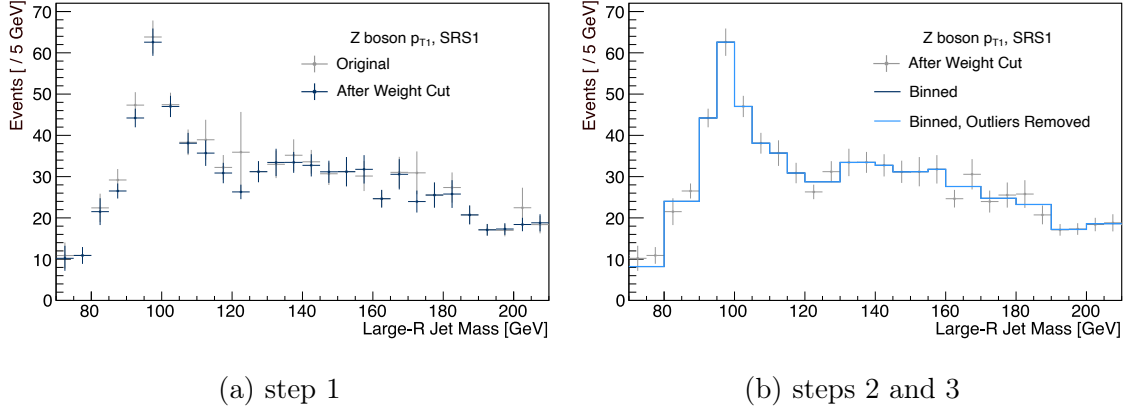


Figure E.3: Z +jets template with $p_T^Z \in [300, 450]$ GeV in the SRS1 differential measurement region, defined by $p_T^{\text{jet}} \in [450, 650]$ GeV, (a) before and after removal of events with large MC generator weights (step 1, using p_T^Z dependent cut discussed later in the section); and (b) after variable binning (step 2) and outlier removal (step 3). The outlier removal does not have any effect in this example.

model and the true distributions. However, each bin of each template would have needed an independent parameter describing the MC statistical uncertainty in it. This would have added a large number of nuisance parameters (up to 685 in 5 GeV binning)³, which would have been extremely computationally costly.

Another approach is to smooth the templates, addressing the issue without additional nuisance parameters. With high statistics these distributions would have been naturally smooth, and the aim was to develop an intelligent procedure which could recover this smoothness, without removing physical features. The approach consisted of these steps:

1. Apply a cut removing events with large MC generator weights;
2. Rebin the template into variable-size bins, with a minimum $\frac{\text{entries}}{\text{bin}}$ condition;
3. Recalculate bin values by removing outlying bin contributions;
4. Use linear interpolation to create a smooth template shape;
5. Generate a template with desirable binning from the smooth shape;

³ Calculated from a differential Z measurement set-up: $[4 \times Z + 1 \times W \text{ templates}] \times [3 \text{ regions} \times 27 \text{ bins} + 2 \text{ regions} \times 28 \text{ bins}]$.

6. Rescale the new template to the integral of the original template.

The MC generator weight cut will be discussed in detail in the following section. With a 5 GeV binning the outlier removal very rarely had any effect, and in the cases where there was an effect, the effect was very small. More information on outlier removal can be found in appendix E.3.

An example of an off-diagonal Z boson template used in the differential momentum bin before and after the weight cut (step 1) is shown in figure E.3a. Figure E.3b shows the same template after the binning into variable size bins, and after outlier removal (steps 2 and 3). These, and later examples of the smoothing procedure in figures E.4 and E.5, are from the final fit set-up, which used 5 GeV binning and larger MC samples.

W +jets samples had a large fraction of candidates from recoiling jets, thus a *hybrid* smoothing approach was taken. After the weight cuts were applied (step 1), the sample was split depending on whether the candidate jet had an associated truth-level boson or not. The events with associated truth-level bosons went through the previously outlined smoothing procedure. The events without the association, likely came from a recoiling jet, and therefore were fit with, and sampled from a QCD background estimate function. The two separately smoothed components were finally combined to make a smooth W +jets template.

Figure E.4 illustrates the hybrid smoothing procedure of W +jets templates in inclusive SRL and SRS regions. The original and smoothed templates were shown, as well as the components without a truth-level boson association and QCD background fits with good agreement.

Figures E.5a and E.5b show comparisons of the original and smoothed templates of the W +jets process in the inclusive SRS region, and Z +jets process with $p_T^Z \in [350, 450]$ GeV in SRS1 ($p_T^{\text{jet}} \in [450, 650]$ GeV). In both cases the templates were considerably smoother and the agreement between the smoothed and original templates was within uncertainties. The MC statistical uncertainties on the

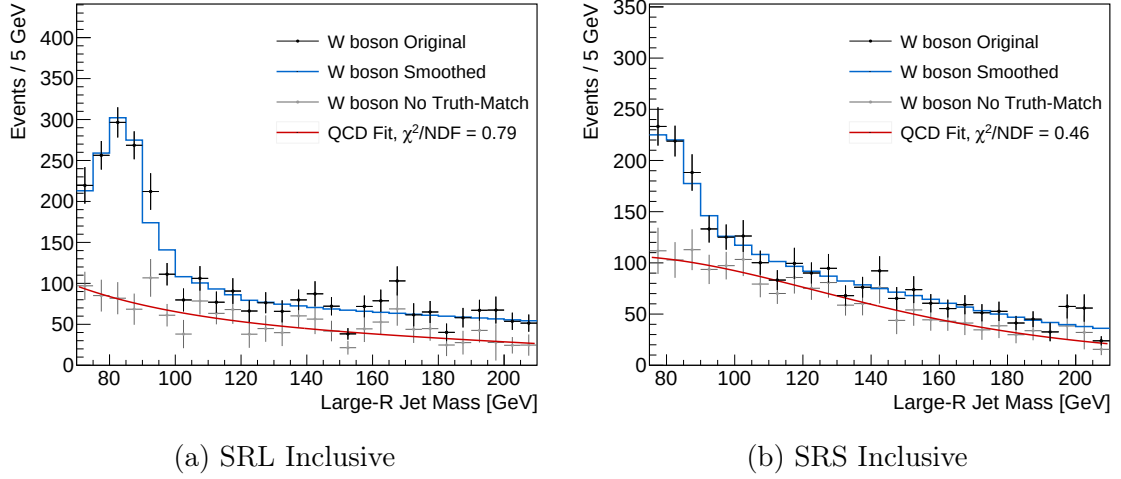


Figure E.4: W +jets template smoothing in inclusive (a) SRL and (b) SRS regions using the hybrid smoothing method. The components with candidate jets without truth boson association, and the parametric QCD background estimate fits to these events are also shown.

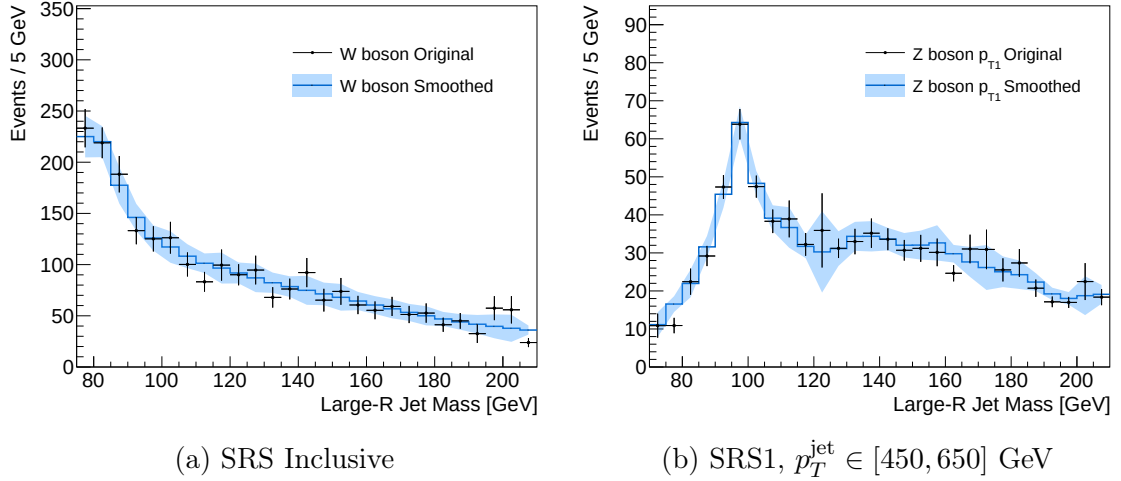


Figure E.5: Comparisons of original and smoothed templates of (a) W +jets process in inclusive SRS region, and (b) Z +jets process with $p_T^Z \in [300, 450]$ GeV in SRS1 region (defined by $p_T^{\text{jet}} \in [450, 650]$ GeV), using the described smoothing procedure.

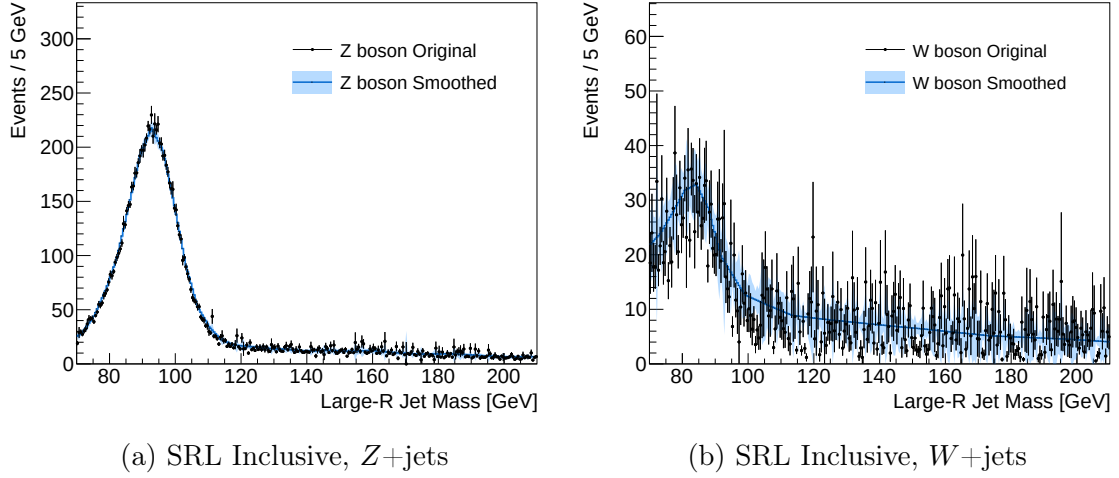


Figure E.6: Comparisons of original and smoothed templates of (a) Z +jets and (b) W +jets processes in the inclusive SRL region using the described smoothing procedure, with a former fit setup using 0.5 GeV binning and smaller MC samples.

smoothed templates were taken from the original templates and adjusted to take into account the distance between the values in the smoothed and original bin.

The importance and impact of the smoothing was particularly evident in the previous fit model set-up using 0.5 GeV binning and smaller V +jets MC samples. Examples of Z +jets and W +jets templates in inclusive SRL region are shown in figure E.6.

The signal extraction test using VR data slices was repeated for models built with smoothed V +jets templates. The pseudo-data slices were constructed as described previously in equation E.1. The VR slices were fit with a models using smoothed Z +jets templates. As previously, the test was conducted with the former fit set-up using 0.5 GeV binning, and smaller MC samples. The distributions of measured signal strengths in inclusive VRL and VRS regions are shown in figures E.7b and E.7b, and have the mean values of $\langle\mu_Z\rangle = 0.95$ and $\langle\mu_Z\rangle = 1.10$, respectively. The test showed that models built with the smoothed Z +jets templates were considerably better at recovering the original signal and did not bias the fit.

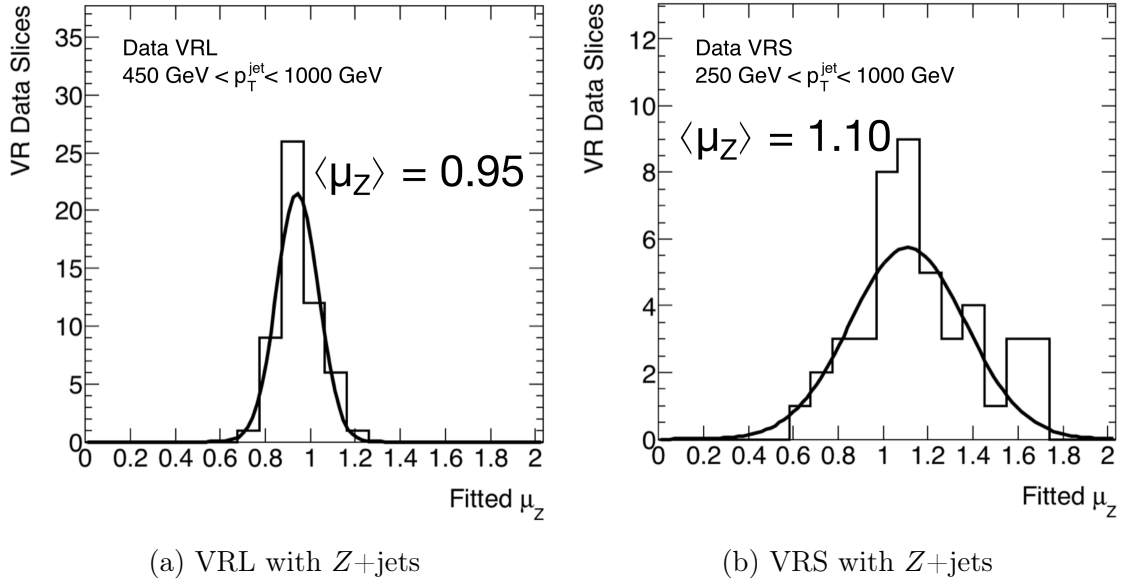


Figure E.7: The distributions of extracted Z +jets signal strengths (μ_Z) from fits to modified (a) VRL and (b) VRS data slices, described in equation E.1, with added smooth Z +jets signal ($\mu_Z^{\text{in}} = 1$) [73] (internal). The fit models use Z +jets MC templates smoothed using the described smoothing procedure. The $\langle \mu_Z \rangle$ values were found through Gaussian fits to the distributions, and show that the original signal is recovered. The model used 0.5 GeV binning and $10\times$ smaller MC samples than available during in the final measurement. These distributions can be compared to equivalent distributions in figure E.7, showing significant bias in the measurements when the smoothing procedure for Z +jets templates is not used.

E.2 Validation of the Smoothing Procedure

This section presents validations studies for the event weight cut choice used in the smoothing procedure, produced by the author. The findings of these studies highlighted sculpting effects on m_{jet} and p_T^{jet} distributions caused by the in the initial procedure, and lead to its refinement. Note that the author highlighted the issues which were present in the initial procedure, and validated the final procedure, but the improvements were designed by other members of the analysis team.

Event Weights

Event simulation is a time and resource consuming process, especially if high modelling precision is required. Users can input biases in the matrix element simulation process, to enhance the production of events in the desired phase-spaces. To return the events to true distributions, the generator provides weights for each event, called *MC event weights* (α).

As well as phase-space corrections, multiple other corrections need to be applied to simulated events before use. Simulated events are produced in (usually round) numbers determined by computing capabilities, and need to be scaled to the correct luminosity before use to represent data collected by the ATLAS detectors. Pileup simulation corrections, and mismodelling scale factors from object reconstruction also need to be applied to the simulated events, such that they would be as close of an estimate of data as possible. The products of all weights to be applied to each event (including α) are called *event weights* (w).

The Validation Study

Large fluctuations in the V +jets MC templates were often caused by simulated events with large event weights (w) in the tails of the distribution. The initial approach in the smoothing procedure used a flat cut ($|w| < 5$) on large event weights. As the W +jets template was highly uneven, a tight weight cut was selected. For example, the weight cut choice in the inclusive SRL removed around 20% of the raw⁴ events in the W +jets sample, which made up 73% of the yield of the template. Also, at the time there was no hybrid approach used for W +jets events.

Figures E.8a and E.8b show the m_{jet} distributions of the W +jets process in inclusive SRL and SRS regions with different weight cuts applied. The flat weight cuts were seen to disproportionately affect events in the high mass tails. As the templates were rescaled to the original integral at the end of the smoothing procedure, the re-

⁴ *Raw events* are the number of entries in the sample, not scaled by event weights.

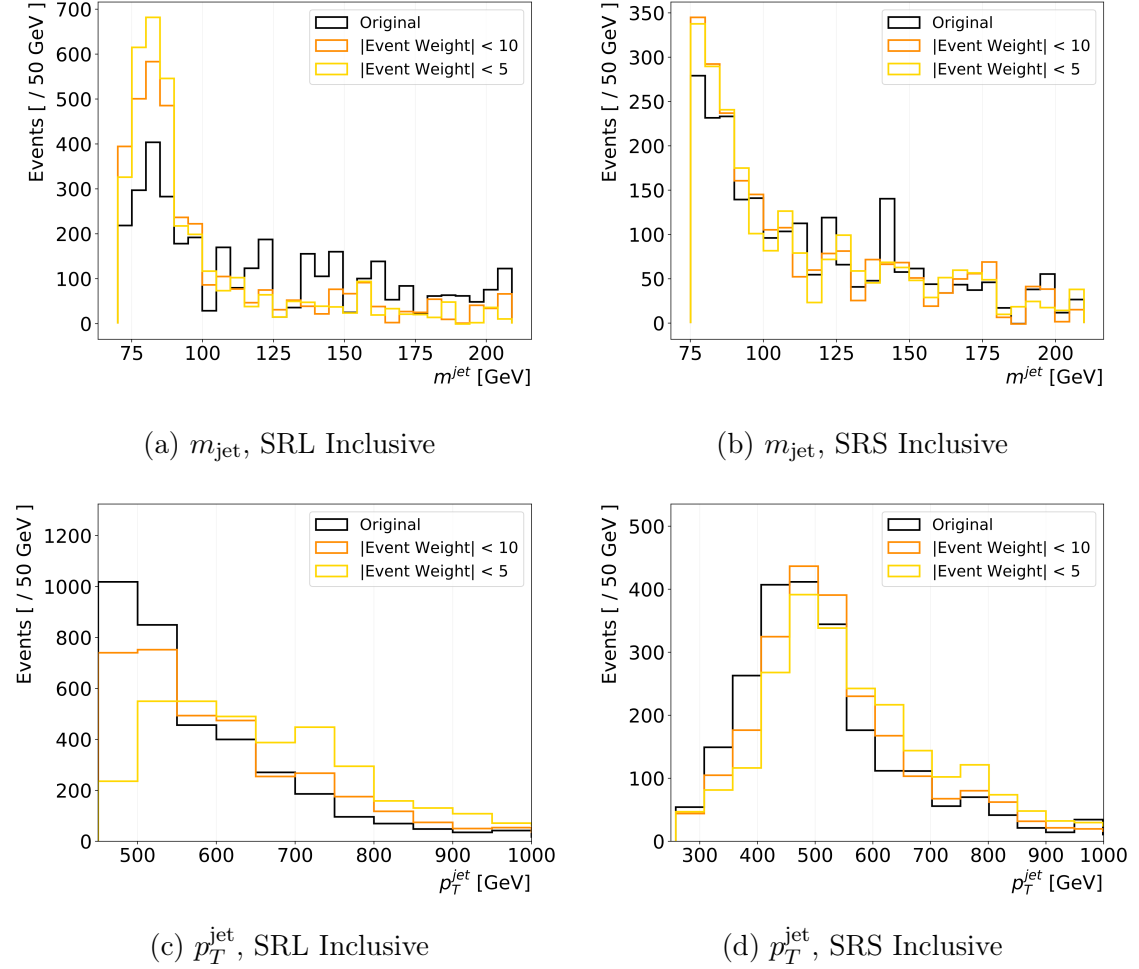


Figure E.8: Candidate jet (top) mass and (bottom) p_T^{jet} distributions of W +jets simulated events in inclusive (left) SRL and (right) SRS regions with different event weight (w) cuts. $|w| < 5$ threshold was used in the smoothing procedure at the time of the study.

removal of events in the tails resulted in a shift of events to the resonance, artificially inflating it. Furthermore, a sculpting effect was also seen in the p_T^{jet} spectra, with yields shifting to higher values of p_T^{jet} in both inclusive SRS and SRL regions, as shown in figures E.8c and E.8d.

The V +jets MC samples were generated with flat p_T^{truth} spectra, to achieve sufficient events in the high momentum regions this analysis was interested in. The generated events were produced with associated *generator weights* (α) used to reweight

the events to the exponentially falling p_T spectrum expected for this process.

The generator weights were included in the event weights (w), meaning that on average events with low momentum, will have larger event weights. This tendency was clear in the distributions of event weights against candidate p_T^{jet} shown later in figure E.10. Thus, a flat cut on large event weights caused a disproportionate reduction of events with low p_T^{jet} , and sculpted the p_T^{jet} spectrum by shifting it to higher values.

In light of this finding, the fixed event weight cut was replaced with a p_T^{truth} -dependent cut on the generator weights (α), with a passing condition defined as:

$$\frac{|\alpha - \hat{\alpha}(p_T^{\text{truth}})|}{\hat{\alpha}(p_T^{\text{truth}})} < \text{threshold}, \quad (\text{E.2})$$

where $\hat{\alpha}$ was the expected average generator weight for a given p_T^{truth} , found by fitting average generator weights with a second order polynomial exponential

$$f(p_T^{\text{truth}}|\theta_0) = \theta_0 \exp \left[\theta_1 p_T^{\text{truth}} + \theta_2 (p_T^{\text{truth}})^2 \right]. \quad (\text{E.3})$$

The average generator weights were expected to follow this distribution up to 1 TeV, as determined by the generator settings. Above 1 TeV the average weights were expected to be constant at the value of $\hat{\alpha}(p_T^{\text{truth}} = 1 \text{ TeV})$. Figure E.9 shows the distributions of the generator weights, α , as functions of p_T^{truth} of the W +jets and Z +jets samples in the inclusive SRL region. The average generator weights and the parametric fit used for the p_T^{truth} -dependent cut are also shown, as well as the events removed with the flat event weight cut ($|w| < 5$), and the p_T^{truth} -based cut.

For both W +jets and Z +jets, the fixed cut on w removed events at the low ends of the spectra, whereas the p_T^{truth} -based cut on α resulted in a uniform removal of events across the spectra. This effect also translated to event weight, w , distributions as functions of p_T^{jet} , shown in figure E.10. The majority of events removed by the flat weight cut were concentrated at the low end of the p_T^{jet} spectra, whereas the p_T^{truth} -based cut provided a uniform removal of events. The distributions shown in figures E.9 and E.10 displayed the same behaviour in SRS.

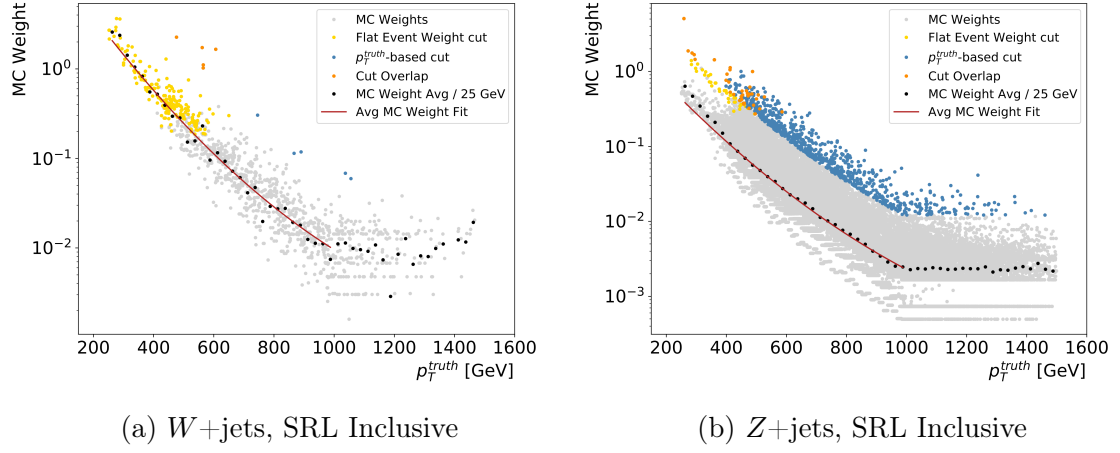


Figure E.9: Generator weight, α , (here, “MC Weight”) distributions of raw MC events as functions of p_T^{truth} for (a) W +jets and (b) Z +jets processes in the inclusive SRL region. Events removed with a flat event weight cut, $|w| < 5$, and the p_T^{truth} -dependent cut are indicated, as well as average α values and the parametric fit used in the p_T^{truth} -based cut. The distributions are displayed on a logarithmic scale for visibility, hence some entries with negative weights are not shown.

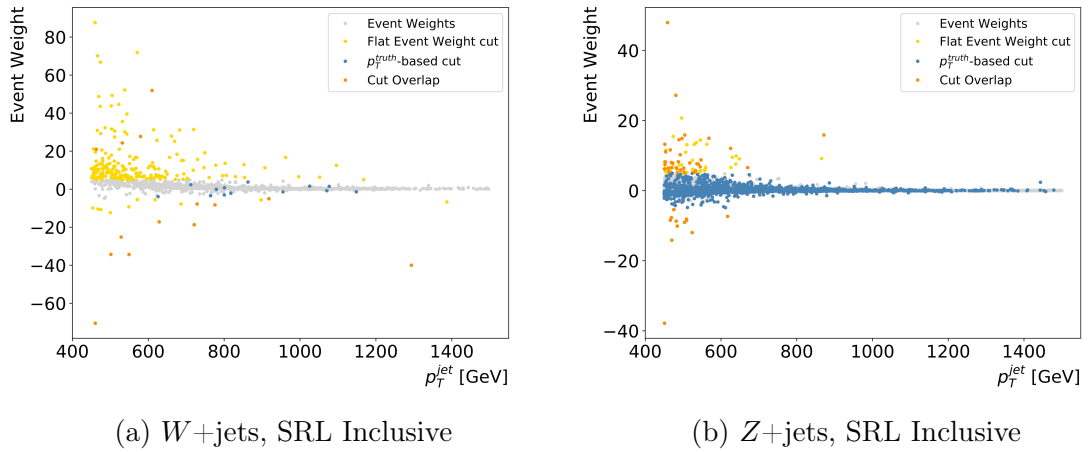


Figure E.10: Event weight, w , distributions of raw MC events as functions of p_T^{jet} for (a) W +jets and (b) Z +jets processes in the inclusive SRL region. Events removed with a flat event weight cut, $|w| < 5$, and the p_T^{truth} -dependent cut are shown.

It was also evident that the removal of W +jets events was much less harsh. The p_T^{truth} -dependent cuts only removed 1% of raw events from the samples, as opposed to 20% and 14% removed with the fixed w cut in SRL and SRS regions, respectively.

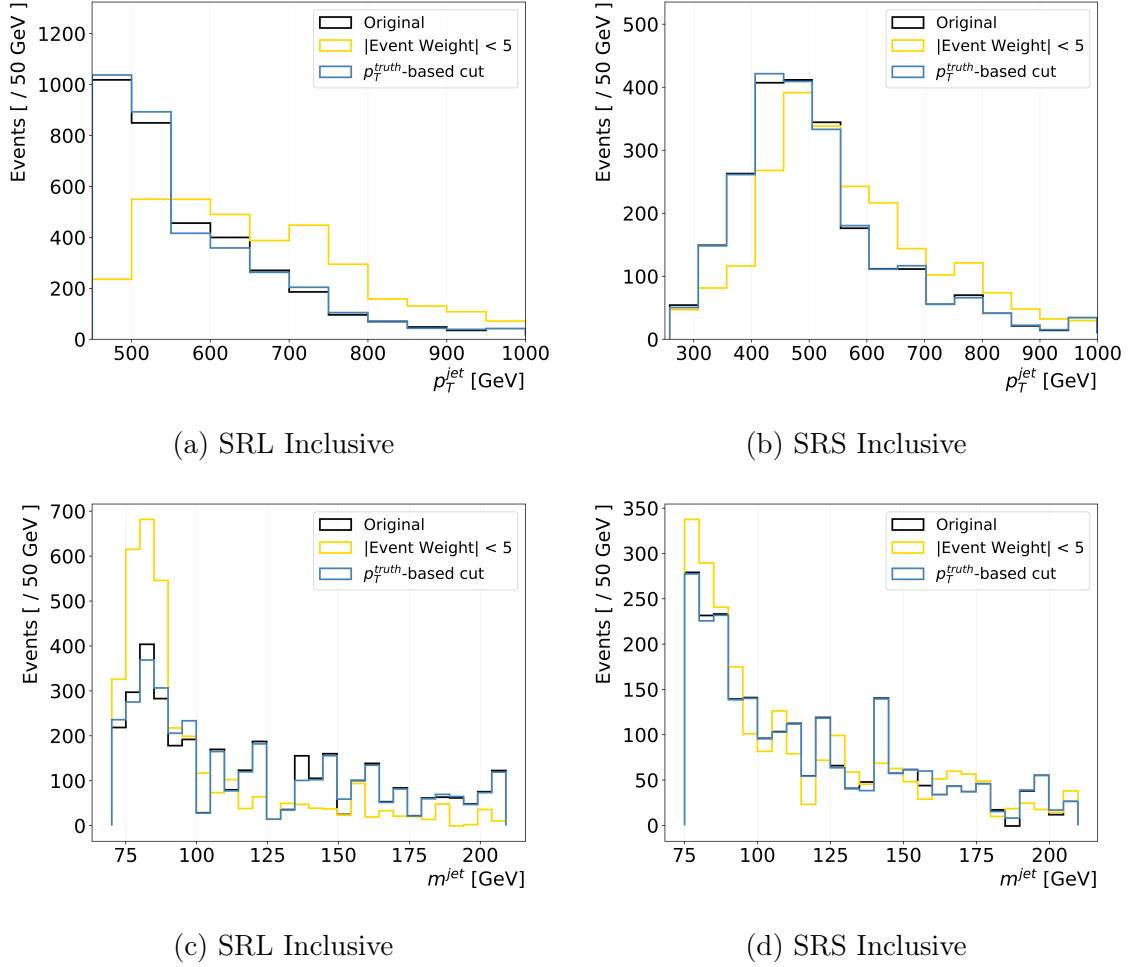


Figure E.11: Candidate jet (top) mass and (bottom) p_T^{jet} distributions of W +jets simulated events in inclusive (left) SRL and (right) SRS regions without weight cuts, with a flat event weight $|w| < 5$ cut, and a p_T^{truth} -dependent cut.

The extent of Z +jets event removal was slightly increased from $> 0.5\%$ of raw events removed with the fixed cut, to around 1% in both regions.

Figure E.11 shows the p_T^{jet} (top) and m_{jet} (bottom) distributions of W +jets events in inclusive SRL (left) and SRS (right) regions, with and without investigated weight cuts. It was seen that a p_T^{truth} -dependent cut mitigated the sculpting effects, which were observed with a flat cut on event weight w . As the p_T -dependent cut removed significantly fewer events from W +jets templates than the flat cut on w , the same distributions were observed with a four times smaller threshold ($\frac{\text{threshold}}{4}$), such

that if present, any sculpting effects would have been enhanced, however significant sculpting effects were observed. The distributions are shown in appendix E.4.

For Z +jets templates sculpting effects were not apparent with either types of cuts (shown in appendix E.5), as the samples had higher statistics in the signal regions. However, using weight cuts robust against momentum bias is good practice, and protects against possible unwanted effects that could occur when separating Z +jets templates into momentum bins for the differential measurements.

The hybrid method of smoothing W +jets samples was also introduced to address the dual nature of the candidates (QCD and W boson) in these samples. The flat weight cuts were seen to artificially shift the bulk of the W +jets template yield to the resonance, effectively removing the QCD component. This effect was remedied by applying p_T^{truth} based cuts, and smoothing the W +jets templates using the hybrid method, which treated the boson and recoil-jet candidates separately.

This kinematic variable and event weight distribution study had lead to improvements of the V +jets template treatment in the fit models. In light of these studies a flat cut on total event weights w was replaced by a p_T^{truth} -dependent cut on the MC event weights α , and a hybrid method was introduced to treat the relatively large QCD component in W +jets events separately, which mitigated unwanted sculpting effects on important kinematic variables.

E.3 Outlier Removal

This section describes the outlier removal sub-procedure. For more information on the V +jets smoothing refer to appendix E.1.

The values in the variable-bins (y_{var}) were averages of the “fine” bins (y_{fine}) of the templates after weight cuts were applied. The outlier removal procedure consisted of: recalculating the values of the variable bins such that if the values of the “fine”

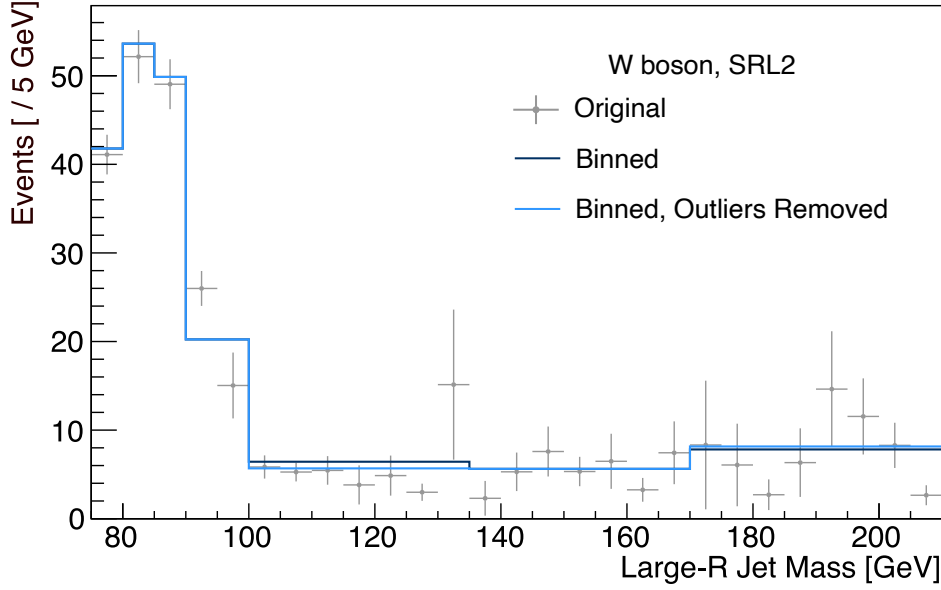


Figure E.12: Example of the effect of outlier removal on a W +jets template in a SRL1 differential measurement bin defined by $p_T^{\text{jet}} \in [650, 1000]$.

bins within the variable bin pass

$$\frac{|y_{\text{fine}} - y_{\text{var}}|}{y_{\text{var}}} > \text{threshold}, \quad (\text{E.4})$$

i.e. if y_{fine} is relatively far from the y_{var} , then, the contribution of that bin is replaced with the value of the variable bin. For example if $y_{\text{var, old}} = y_1 + y_2 + y_3$, and y_2 does not pass the condition, the variable bin value will be $y_{\text{var, new}} = y_1 + y_{\text{var, old}} + y_3$.

With 5 GeV binning the outlier removal very rarely had any effect. Figure E.12 shows an example of outlier removal having effect on a W boson template in a high momentum differential measurement signal region bin (SRL2). Very minor effect was seen, which was the case in all templates where any effect was seen.

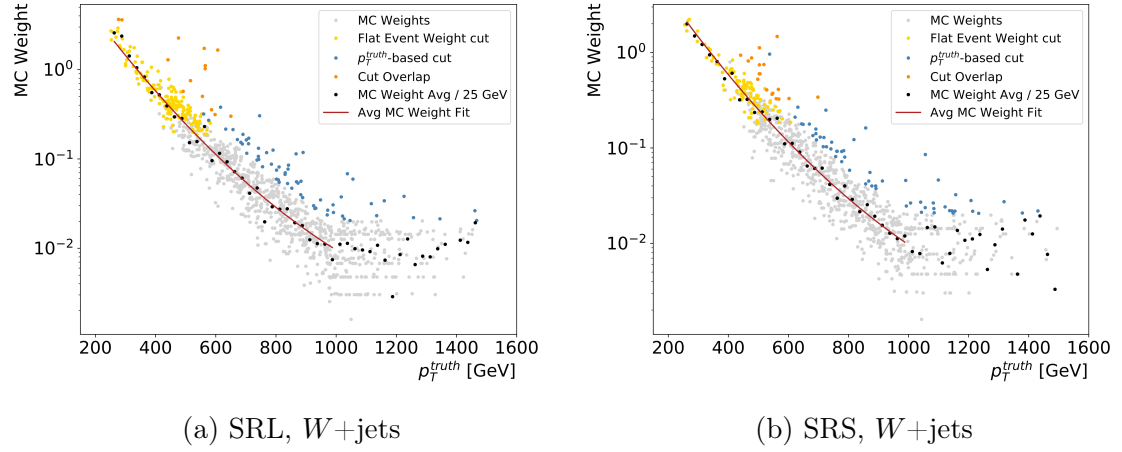
E.4 Plots: W +jets with Tighter p_T^{truth} -based Weight Cuts

Figure E.13: Generator weight, α , (here, “MC Weight”) distributions of raw MC events as functions of p_T^{truth} for W +jets process in (a) SRL and (b) SRS regions. Events removed with a flat event weight cut, $|w| < 5$, and the p_T^{truth} -dependent cut are indicated, as well as average α values and the parametric fit used in the p_T^{truth} -based cut. The p_T^{truth} -dependent cut shown here has a $\times 4$ tighter threshold than the one used in the analysis. The distributions are displayed on a logarithmic scale for visibility, hence some entries with negative weights are not shown.

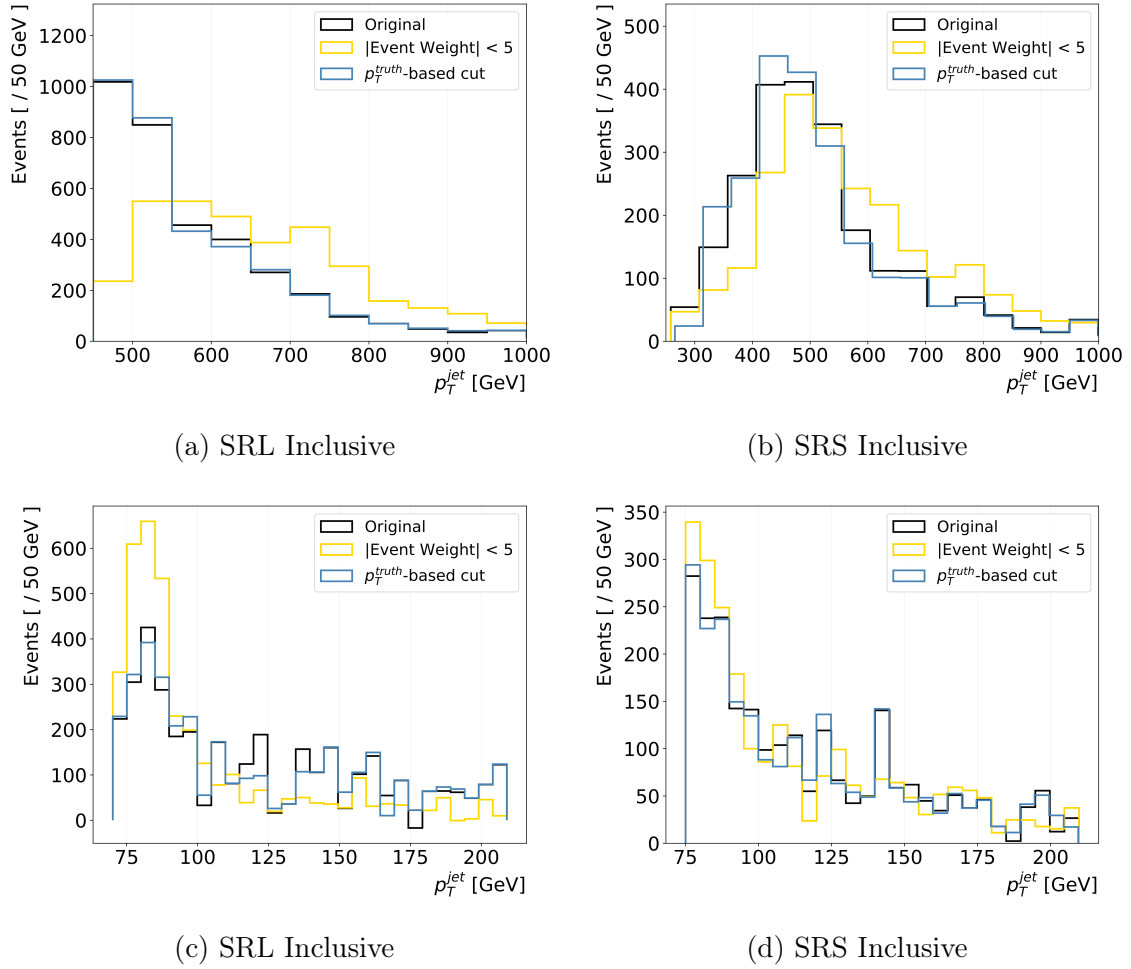


Figure E.14: Candidate jet (top) mass and (bottom) p_T^{jet} distributions of W +jets simulated events in inclusive (left) SRL and (right) SRS regions without weight cuts, with a flat event weight $|w| < 5$ cut, and a p_T^{truth} -dependent cut with a 4 times smaller threshold than the one used in the smoothing procedure.

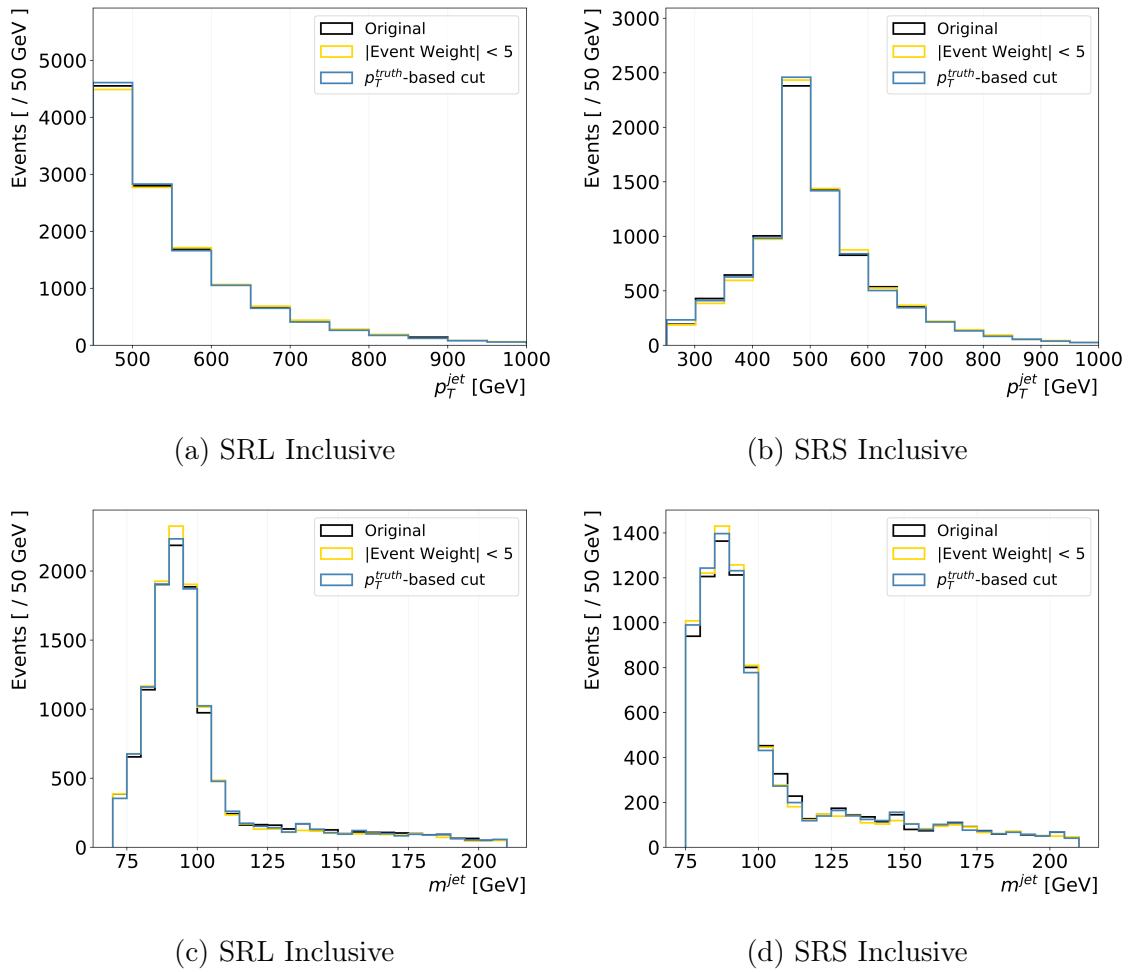
E.5 Plots: Z +jets Distributions with Weight Cuts

Figure E.15: Candidate jet (top) mass and (bottom) p_T^{jet} distributions of Z +jets simulated events in inclusive (left) SRL and (right) SRS regions without weight cuts, with a flat event weight $|w| < 5$ cut, and a p_T^{truth} -dependent cut.

Appendix F

Parametric Treatment of Resonances

F.1 Parametric Treatment of Resonance

In the early stages of the analysis, the author conducted a brief study to investigate the feasibility of modelling resonances using parametric descriptions. The ability to describe the resonances and related uncertainties as parametric functions would allow for a fully parametric treatment of the measurement fits, as the QCD background estimate was also modelled by a parametric function. A fully parametric treatment would bypass the fitting bias issue in the *RooFit* fitting software, arising when the model contains both parametric and binned template descriptions, which led to the use of 0.5 GeV binning throughout most of the analysis development.

Double-sided Crystal Ball (DSCB) functions were used to model the resonances empirically. A DSCB function consists of a central Gaussian part with two power-law tails on either side, and is defined as:

$$f_{\text{CB}} = N \cdot \begin{cases} e^{-\frac{1}{2}t^2} & \text{if } -\alpha_- \leq t \leq \alpha_+ \\ e^{-\frac{1}{2}\alpha_-^2} \left(\frac{n_-}{\alpha_-}\right)^{n_-} \left(\frac{n_-}{\alpha_-} - \alpha_- - t\right)^{-n_-} & \text{if } t < -\alpha_- \\ e^{-\frac{1}{2}\alpha_+^2} \left(\frac{n_+}{\alpha_+}\right)^{n_+} \left(\frac{n_+}{\alpha_+} - \alpha_+ - t\right)^{-n_+} & \text{if } t > \alpha_+ \end{cases} \quad (\text{F.1})$$

where $t = (m_{\text{jet}} - \mu_{\text{CB}}) / \sigma_{\text{CB}}$, μ_{CB} and σ_{CB} are the mean and the width of the Gaussian distribution, $\alpha_{\pm}$ parameterise the points in the spectra where the distribution becomes a power-law distribution, and $n_{\pm}$ are the exponents of the power-law distribution. The “−” and “+” signs indicate the parameters of the power-law distributions below and above the mean, respectively. $\alpha_{\pm}$ and $n_{\pm}$ have to be positive.

DSCB functions are commonly used in high energy physics experiments to model resonances. For example, a fully parametric approach using DSCB functions to model resonances had been successfully used by the ATLAS $H \rightarrow \gamma\gamma$ measurement [156], which used the same fitting software as this analysis.

The MC templates of the resonant processes in the inclusive signal regions were fit with DSCB functions. The fitting was done in an extended mass range of $m_{\text{jet}} \in [60, 250]$ GeV, such that the upward slopes of the Z and W boson resonances could be contained. The study used early V +jets samples with smaller statistics compared to the final version. Examples of the DSCB fits of the templates, as well as the corresponding reduced χ^2 values are shown in figure F.1.

It was clear that most of the resonances were not well described, resulting in large reduced χ^2 values. In Higgs boson events, the DSCB function did not have an ability to describe the relative abundance of events in the upper tail caused by a top-quark contamination from $t\bar{t}H$ events. Similarly, the DSCB function could not describe the irregularities in the $t\bar{t}$ template shape caused by top-quark decays which were not fully contained within the candidate jet.

In Z +jets events some difficulty was seen in describing the tail of the resonance, known to contain candidates from the recoil jet. In fact, using MC samples with higher statistics, made available after these studies were conducted, the discrepancy in the tail became more prominent, giving a reduced χ^2 value of 8.75 in the same region. Due to the large uncertainties of the W +jets templates it was unclear whether the DSCB functional fit did not remove important physical features.

Overall the resonant signal and background templates in this analysis had subtle

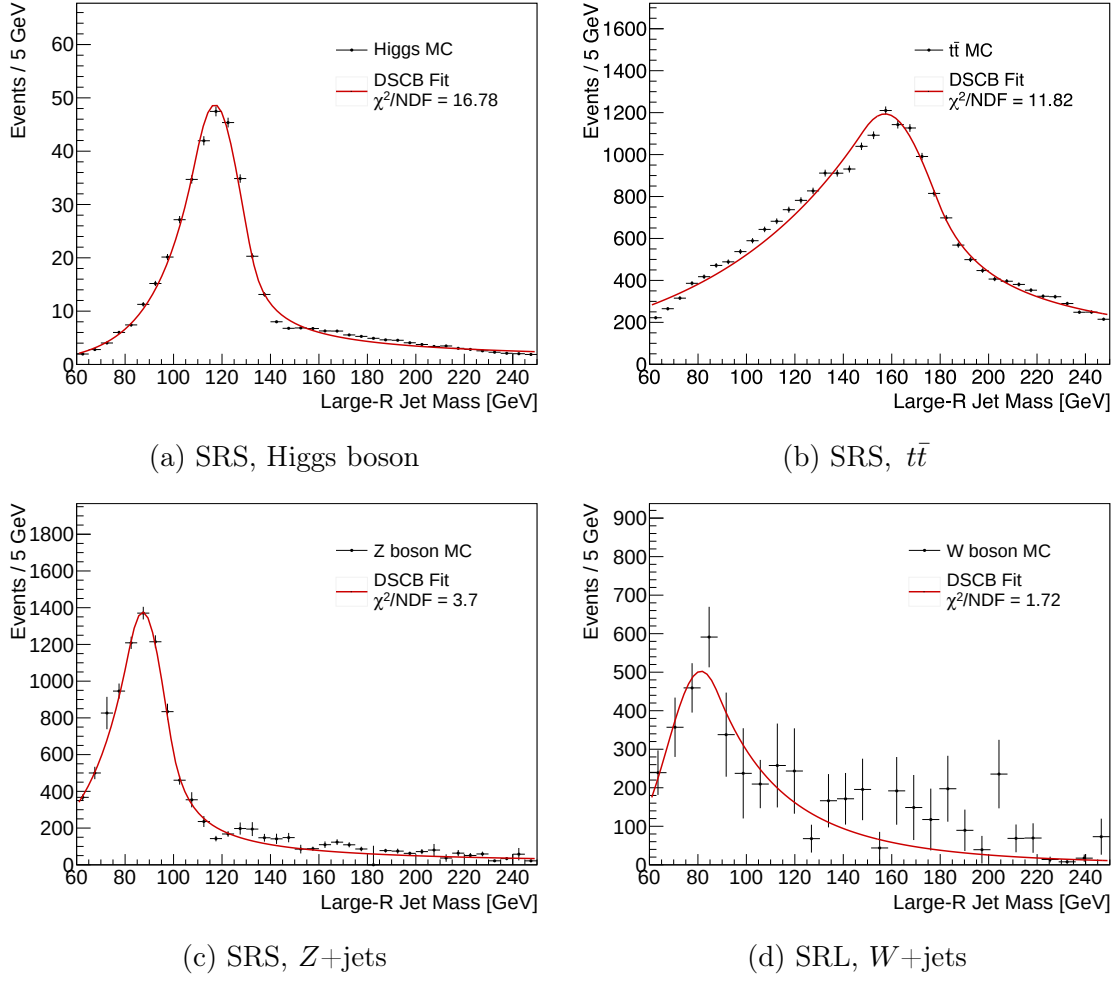


Figure F.1: Examples of DSCB fits to the simulated resonant processes in the inclusive signal regions.

complex features rising from various sources, which cannot be straightforwardly described by a DSCB functional form. In light of these findings, it was decided not to use parametric fitting to smooth the resonance mass templates.

Instead, a dedicated smoothing procedure for V +jets mass templates was developed, as the templates were particularly unsmooth due to generator properties. The smoothing procedure was discussed in appendix E. The other templates were used without smoothing.

F.2 Parametric Smoothing for Framework Validation

The BSM resonance search from which this analysis was developed [4] used parametric fitting to smooth the templates of the resonant processes and associated systematic shape uncertainties, so as not to encounter issues from low MC statistics, such as the ones described in appendix E.1.

The Higgs boson interpretation of the BSM resonance search was replicated with the new analysis framework by the author of the thesis as a starting point for the $H(\rightarrow b\bar{b}) + j$ measurement. It was also used for validation tests of the new framework, described in appendix C. This model set-up included the implementation of the parametric smoothing of resonant process templates and associated shape uncertainties.

The H , Z and W boson templates were empirically modelled with a sum of three Gaussian functions, and the $t\bar{t}$ background was modelled with a DSCB function. Originally fitting was performed in the m_{jet} range between 70 GeV and 230 GeV for all templates except W +jets, for which the lower boundary was extended to 55 GeV. In the new framework, the procedure was simplified by setting the range to $m_{\text{jet}} \in [55, 230]$ GeV for all templates. In both cases, the smooth templates were produced by sampling the parametric descriptions, and all associated systematic uncertainty templates were also smoothed using the same procedure. The machinery to fit the resonances and sample the distributions was implemented into the $H(\rightarrow b\bar{b}) + j$ fitting framework by the author.

The replicated fits are shown in figure F.2 and the reference fits from the BSM search are shown in figure F.3. A comparison of reduced χ^2 values from the fits produced by the BSM search and the replicated fits is shown in table F.1. All fits were seen to be accurately replicated, resulting in matching shapes and similar reduced χ^2 values. Slight differences seen in the comparison were likely due to small differences in sample processing and differences between fit ranges.

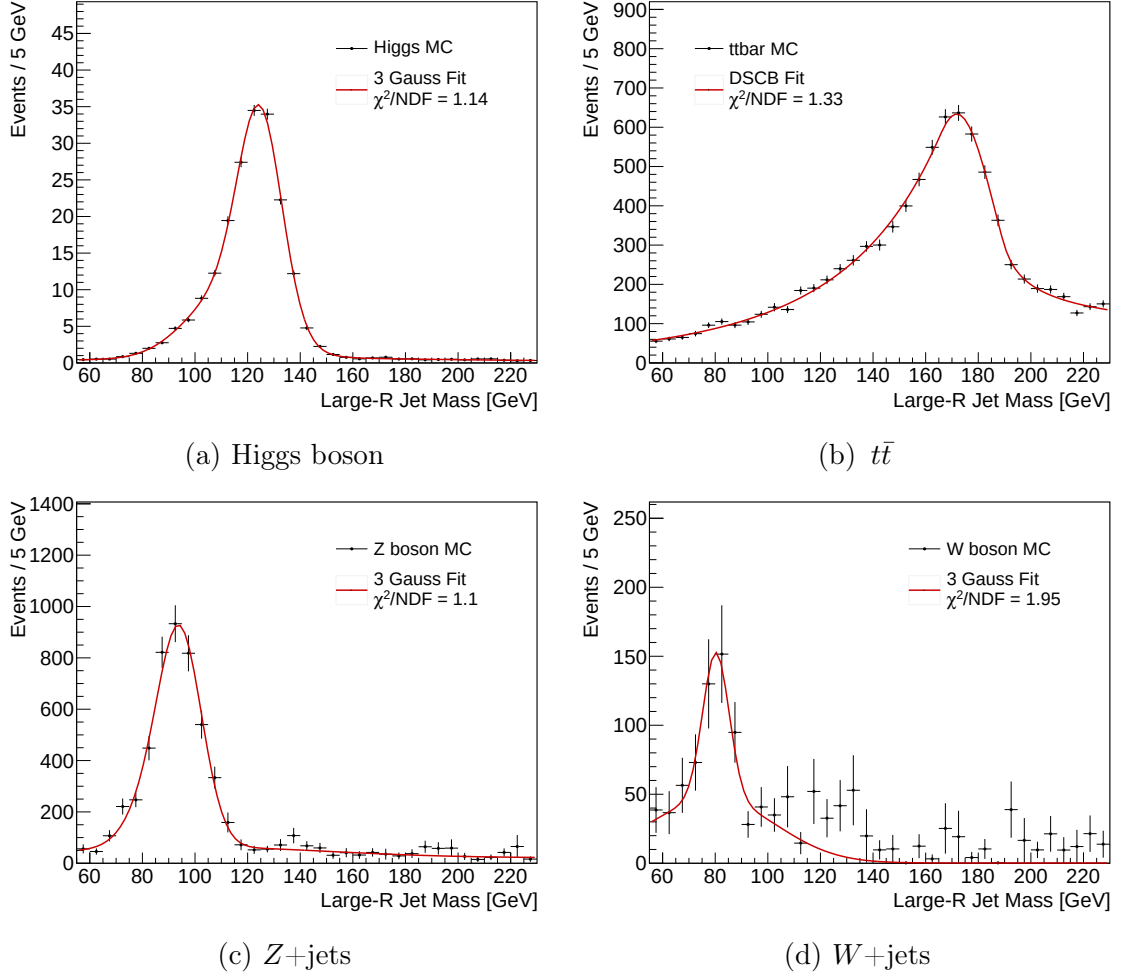


Figure F.2: Parametric fits to Higgs, Z and W boson templates with a sum of three Gaussian functions, and the $t\bar{t}$ template with a DSCB function in the signal region of the $X(\rightarrow b\bar{b}) + j$ search [4] from which the $H(\rightarrow b\bar{b}) + j$ measurement analysis was developed, replicated using the new analysis framework implementation.

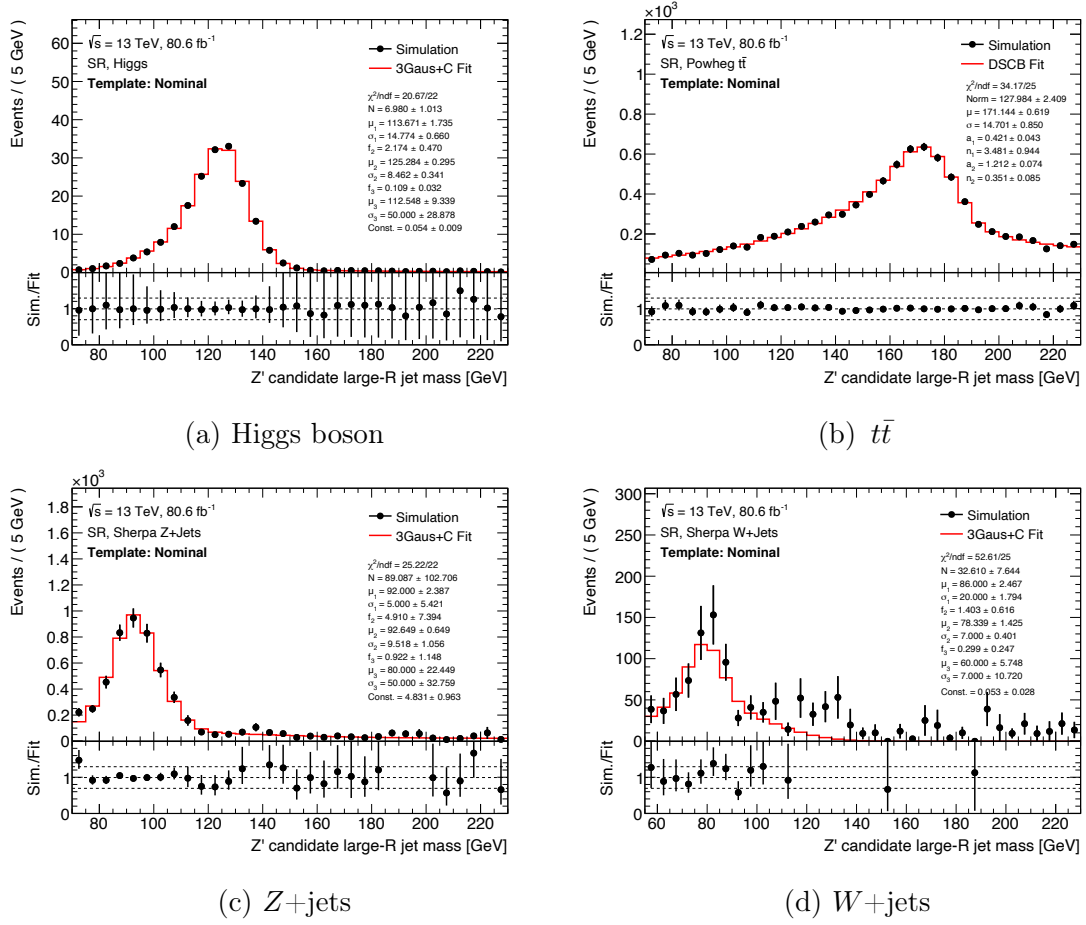


Figure F.3: Parametric fits to Higgs, Z and W boson templates with a sum of three Gaussian functions, and the $t\bar{t}$ template with a DSCB function, performed by the $X(\rightarrow b\bar{b}) + j$ search [4] from which the $H(\rightarrow b\bar{b}) + j$ measurement analysis was developed. Plots taken from the internal documentation of the search [155].

Table F.1: Reduced χ^2 values from parametric fits to signal region resonances from the BSM resonance search [4] from which this analysis was developed, and a replica of those fits fit the current analysis framework.

	χ^2 / NDF			
	H	$t\bar{t}$	Z	W
BSM Search	0.94	1.37	1.15	2.10
Replica	1.14	1.33	1.10	1.95

Appendix G

Systematic Uncertainties

G.1 Systematic Uncertainty Labels and Descriptions

This section provides the labels and sources of all uncertainties included in the $H(\rightarrow b\bar{b}) + j$ measurement fits. The uncertainties which were not included in the fits, but were added to the final result calculation (spurious signal, and Higgs boson modelling uncertainties) are not listed, more details can be found in section 7.2. Four categories of systematic uncertainties were considered:

- jet uncertainties;
- flavour tagging uncertainties;
- spurious signal uncertainties (not included in the fit);
- modelling uncertainties.

Jet Uncertainties

Jet uncertainties include standalone jet mass resolution (JMR) jet mass scale (JMS) and jet energy scale (JES) uncertainties¹. The jet mass resolution uncertainties were standalone, labelled JMR_Hbb, JMR_WZ, and JMR_Top, depending on the type of process it is applied to. Four jet mass scale uncertainties were included:

¹ Jet energy resolution (JER) uncertainties were negligible.

Jet Mass Scale (JMS) , prefix JMS_ or JET_CombMass_	
<i>Label</i>	<i>Source</i>
Baseline	– differences between data and simulation (PYTHIA 8);
Modelling	– differences between the nominal (PYTHIA 8) and alternative MC generators;
Tracking_[1-3]	– various tracking-related uncertainties;
TotalStat	– statistical uncertainty on the measurement.

The jet energy scale uncertainties were subdivided into four categories:

Jet Energy Scale (JES) , prefix JES_ or JET_	
<i>Label</i>	<i>Source</i>
EffectiveNP_R10	– central region calibration, $ \eta < 0.8$
EtaIntercalibration	– calibration extension to more forward regions, $ \eta < 2.5$
Flavor	– quark vs. gluon modelling
LargeR_TopologyUncertainty	– topology differences of q/g vs. top quarks or V bosons

The four JES uncertainty categories included these uncertainties:

Jet Energy Scale (JES), prefix JES_ or JET_	
<i>Label</i>	<i>Source</i>
JES_EffectiveNP_R10_	
Detector[1-2]	– experimental, detector uncertainties;
Mixed[1-4]	– mixed detector and modelling uncertainties;
Modelling[1-4]	– PYTHIA 8 (nominal) vs. alternative MC generators;
Statistical[1-6]	– statistical uncertainties;
JES_EtaIntercalibration_	
R10_TotalStat	– statistical uncertainties;
Modelling	– PYTHIA 8 (nominal) vs. alternative MC generators;
JES_Flavor_	
Composition	– uncertainty in quark and gluon fraction modelling;
Response	– quark and gluon jet response modelling;
JES_LargeR_TopologyUncertainty_	
top	– q/g vs. top quarks;
V	– q/g vs. V bosons.

Flavour Tagging Uncertainties

Flavour Tagging, prefix FTAG_ or FT_EFF_	
<i>Label</i>	<i>Source</i>
Eigen_B_[0-4]	- b -jet b -tagging scale factor uncertainties;
Eigen_C_[1-3]	- c -jet mistagging —“— ;
Eigen_Light_[1-3]	- light-jet mistagging —“— ;
extrap_from_charm	- τ -jet mistagging —“— ;
extrapolation	- b -jet b -tagging high p_T^{jet} extrapolation uncertainty.

Modelling Uncertainties

V+jets Modelling	
<i>Label</i>	<i>Source</i>
xsec_unc_Wboson	– W+jets cross-section and acceptance uncertainty (normalisation only)
V+jets_QCD_scale	– μ_R and μ_F (QCD) scale variation
$t\bar{t}$ Modelling	
<i>Label</i>	<i>Source</i>
ttbar_PartonShower	– PS generator: PYTHIA8 (nominal) vs. Herwig 7;
ttbar_MatrixElement	– ME calculation: POWHEG-BOX (nominal) vs. MADGRAPH5_AMC@NLO;
ttbar_ISR	– ISR modelling
ttbar_FSR	– FSR modelling

G.2 Normalisation Uncertainties in Inclusive Fits

Table G.1: The normalisation components of uncertainties on mass templates of H , Z , W and $t\bar{t}$ processes in the inclusive (a) SRL, (b) SRS and (c) $\text{CR}_{t\bar{t}}$ regions entering the inclusive measurement fit (average of $+1\sigma$ and -1σ components). Uncertainties with a $< 2\%$ extent were pruned, as described in section 7.6, and did not enter the measurement fit. * – uncertainty also has a shape component entering the fit. The uncertainties are sorted by extent with regard to H , Z , $t\bar{t}$ and W templates in sequential order (i.e. first sorting with respect to H , then, remaining with respect to Z , etc.). For an overview of all uncertainties entering the inclusive measurement fit see figure G.9. The uncertainty label descriptions are given in appendix G.1. (Continued on next page).

(a) Inclusive Leading Candidate SR (SRL)

Uncertainties, SRL	H	Z	W	$t\bar{t}$
FTAG Eigen B 0	5.6%	5.2%	2.3%	3.2%
FTAG Eigen B 1	2.5%	2.3%	–	–
JES EffectiveNP R10 Modelling 1	2.2%*	2.1%*	–	–
V+jets QCD Scale	–	5.3%*	15.4%*	–
JES LargeR TopologyUncertainty V	–	4.3%*	–	–
V+jets JMR	–	2.5%*	2.7%*	–
$t\bar{t}$ Parton Shower	–	–	–	18.0%*
$t\bar{t}$ Matrix Element	–	–	–	12.6%*
FTAG Eigen Light 0	–	–	15.8%*	5.6%*
FTAG Eigen C 1	–	–	3.3%	3.7%
FTAG Eigen C 0	–	–	2.6%	2.8%
FTAG Eigen Light 1	–	–	3.0%	–

(b) Inclusive Subleading Candidate SR (SRS)

Uncertainties, SRS	H	Z	W	$t\bar{t}$
FTAG Eigen B 0	5.0%	5.2%	3.1%	2.9%
JES EffectiveNP R10 Modelling 1	2.0%*	2.4%*	—	—
V +jets QCD Scale	—	7.6%*	13.9%*	—
V +jets JMR	—	3.4%*	—	—
JES Flavor Response	—	3.1%*	—	—
V +jets JMS Modelling	—	2.9%*	—	—
FTAG Eigen B 1	—	2.2%	—	—
JES Flavor Composition	—	2.1%*	—	—
$t\bar{t}$ Matrix Element	—	—	—	19.3%*
$t\bar{t}$ Parton Shower	—	—	—	14.5%*
FTAG Eigen Light 0	—	—	11.4%*	4.1%
FTAG Eigen C 1	—	—	2.6%	2.9%
FTAG Eigen C 0	—	—	2.1%	2.3%
JES LargeR TopologyUncertainty V	—	—	1.8%*	—

(c) Inclusive $t\bar{t}$ Control Region ($\text{CR}_{t\bar{t}}$)

Uncertainties, $\text{CR}_{t\bar{t}}$	$t\bar{t}$
$t\bar{t}$ Parton Shower	7.0%*
FTAG Eigen B 0	4.8%
JMR Top	4.0%*
JMS Modelling $t\bar{t}$	2.1%*
JES EffectiveNP R10 Modelling 1	2.0%*
FTAG Eigen B 1	2.0%
$t\bar{t}$ FSR	1.7%*

G.3 Mass Distributions of Systematic Uncertainties

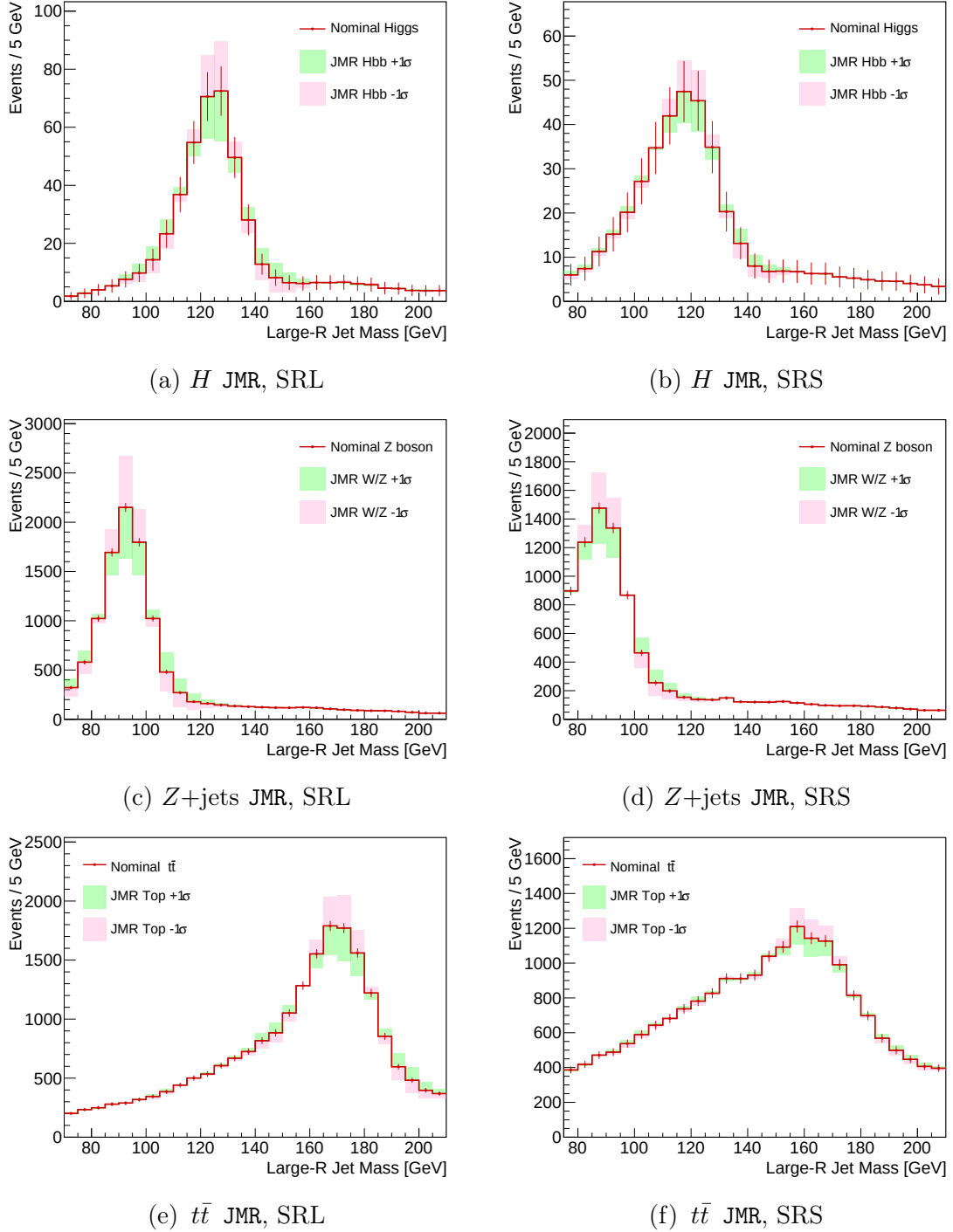


Figure G.1: Jet mass resolution (JMR) uncertainties on the (top) Higgs boson (middle) Z +jets and (bottom) $t\bar{t}$ process templates in the inclusive (left) SRL and (right) SRS regions. The uncertainties on the nominal templates are Poisson distributed.

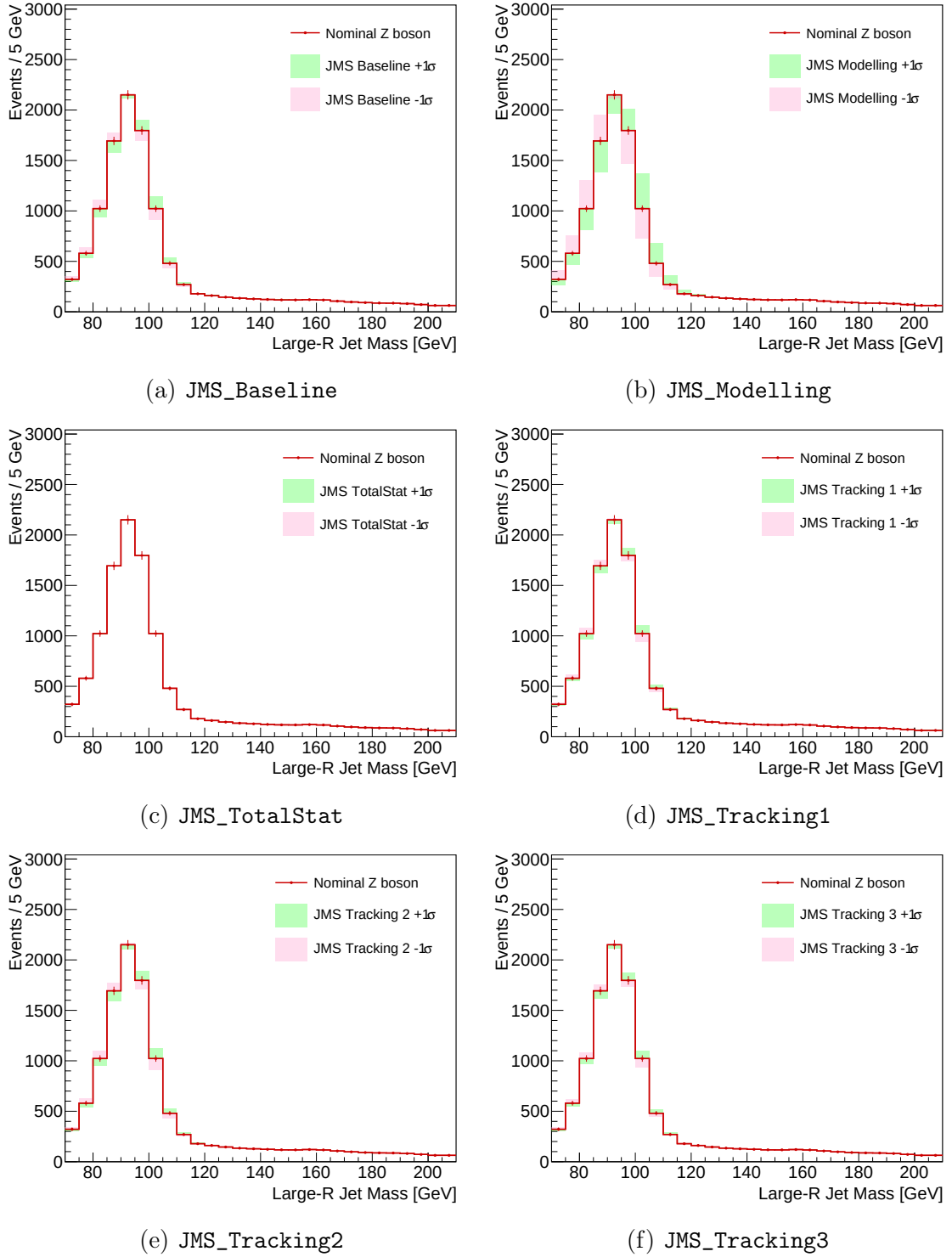


Figure G.2: Jet mass scale (JMS) uncertainties on the Z+jets template in the inclusive SRL region. The uncertainties on the nominal templates are Poisson distributed.

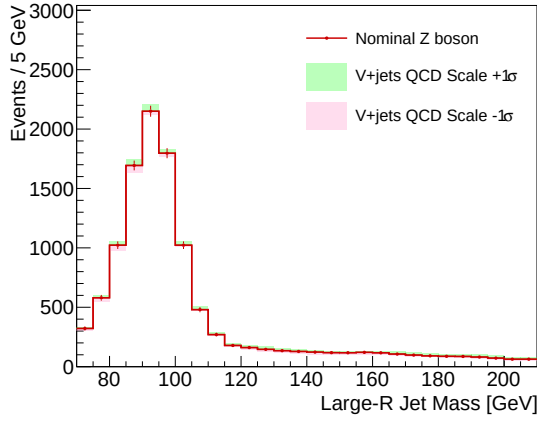
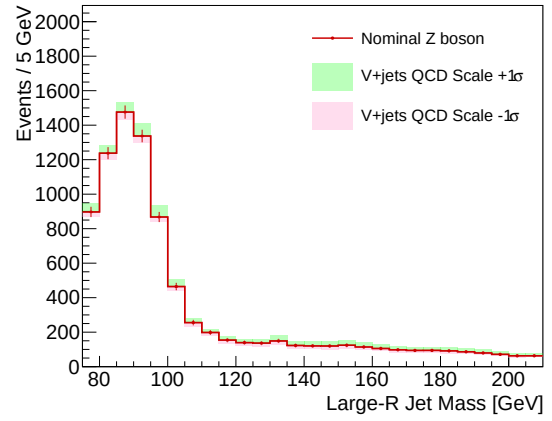
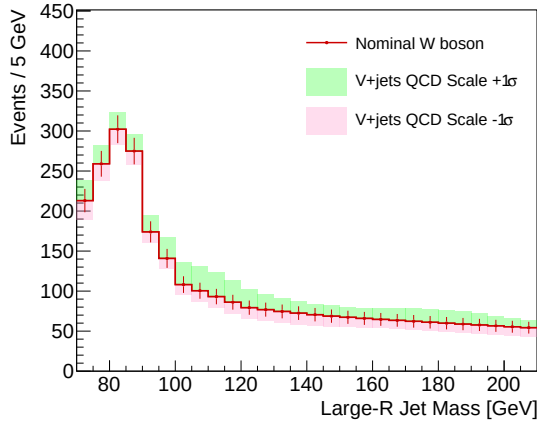
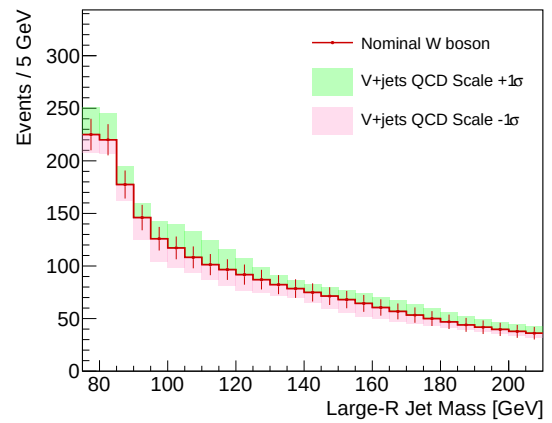
(a) Z +jets, V +jets_QCD_Scale, SRL(b) Z +jets, V +jets_QCD_Scale, SRS(c) W +jets, V +jets_QCD_Scale, SRL(d) W +jets, V +jets_QCD_Scale, SRS

Figure G.3: MC generator uncertainties on the (top) Z +jets and (bottom) W +jets templates in the inclusive (left) SRL and (right) SRS regions. The uncertainties on the nominal templates are Poisson distributed.

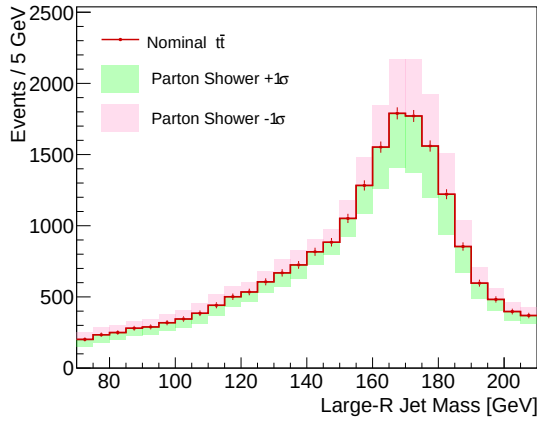
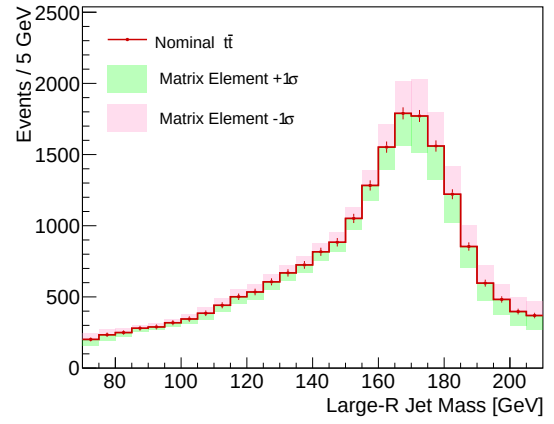
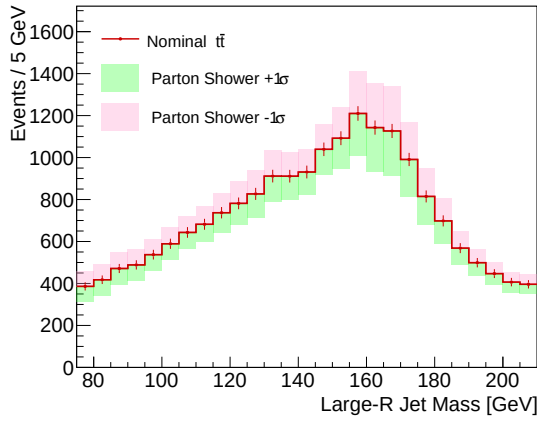
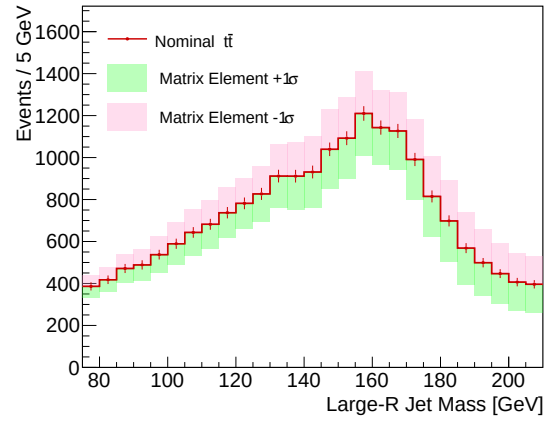
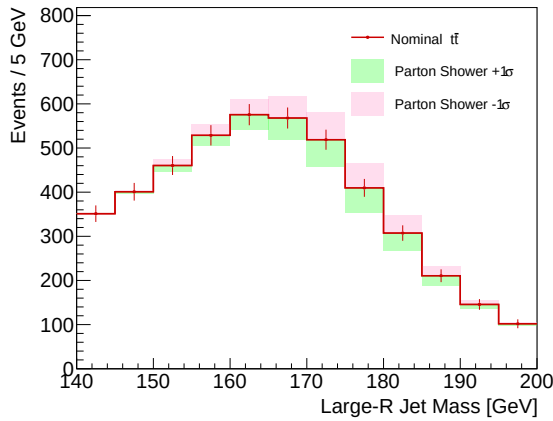
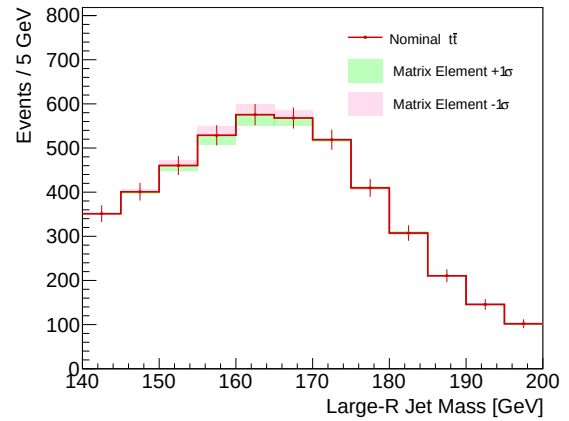
(a) $t\bar{t}$ Parton_Shower, SRL(b) $t\bar{t}$ Matrix_Element, SRL(c) $t\bar{t}$ Parton_Shower, SRS(d) $t\bar{t}$ Matrix_Element, SRS(e) $t\bar{t}$ Parton_Shower, $CR_{t\bar{t}}$ (f) $t\bar{t}$ Matrix_Element, $CR_{t\bar{t}}$

Figure G.4: The (left) parton shower, and (right) matrix element modelling uncertainties on the $t\bar{t}$ templates in the inclusive (top) SRL, (middle) SRS, and (bottom) $CR_{t\bar{t}}$ regions. The uncertainties on the nominal templates are Poisson distributed.

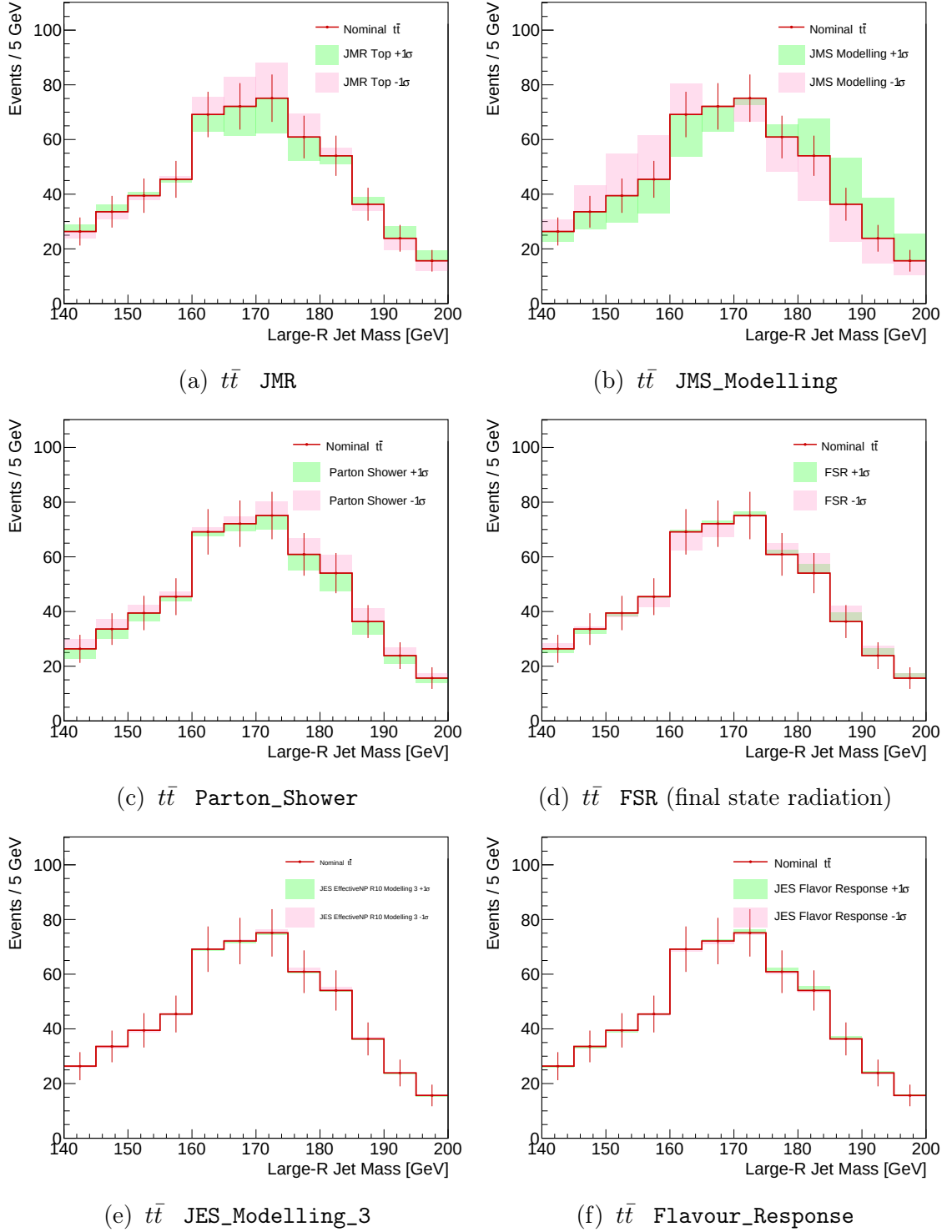


Figure G.5: Various uncertainties on the $t\bar{t}$ templates in the $CR_{t\bar{t}2}$ region ($p_T^{\text{jet}} \in [650, 1000]$ GeV) discussed throughout section 7.5.3. The uncertainties in the top 4 panels are some of the largest $t\bar{t}$ uncertainties, whereas the bottom two are examples of small, low impact uncertainties. The uncertainties on the nominal templates are Poisson distributed. The labels and descriptions of all uncertainties are given in appendix G.1.

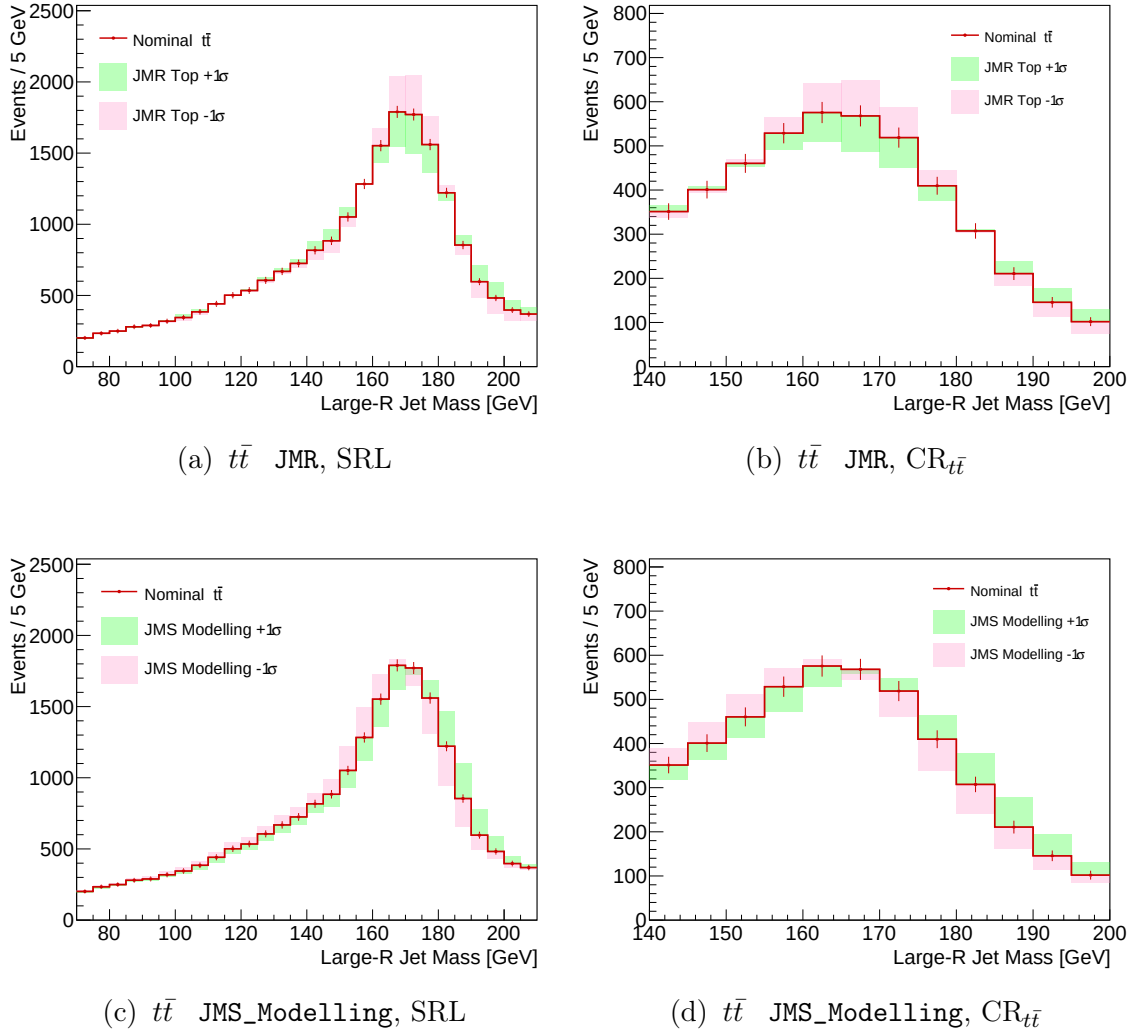


Figure G.6: The (top) jet mass resolution, and (bottom) jet mass scale modelling uncertainties on the $t\bar{t}$ candidate jet mass templates in the inclusive (left) SRL and (right) $CR_{t\bar{t}}$ regions. The uncertainties on the nominal templates are Poisson distributed.

G.4 Uncertainty Smoothing: Correlations

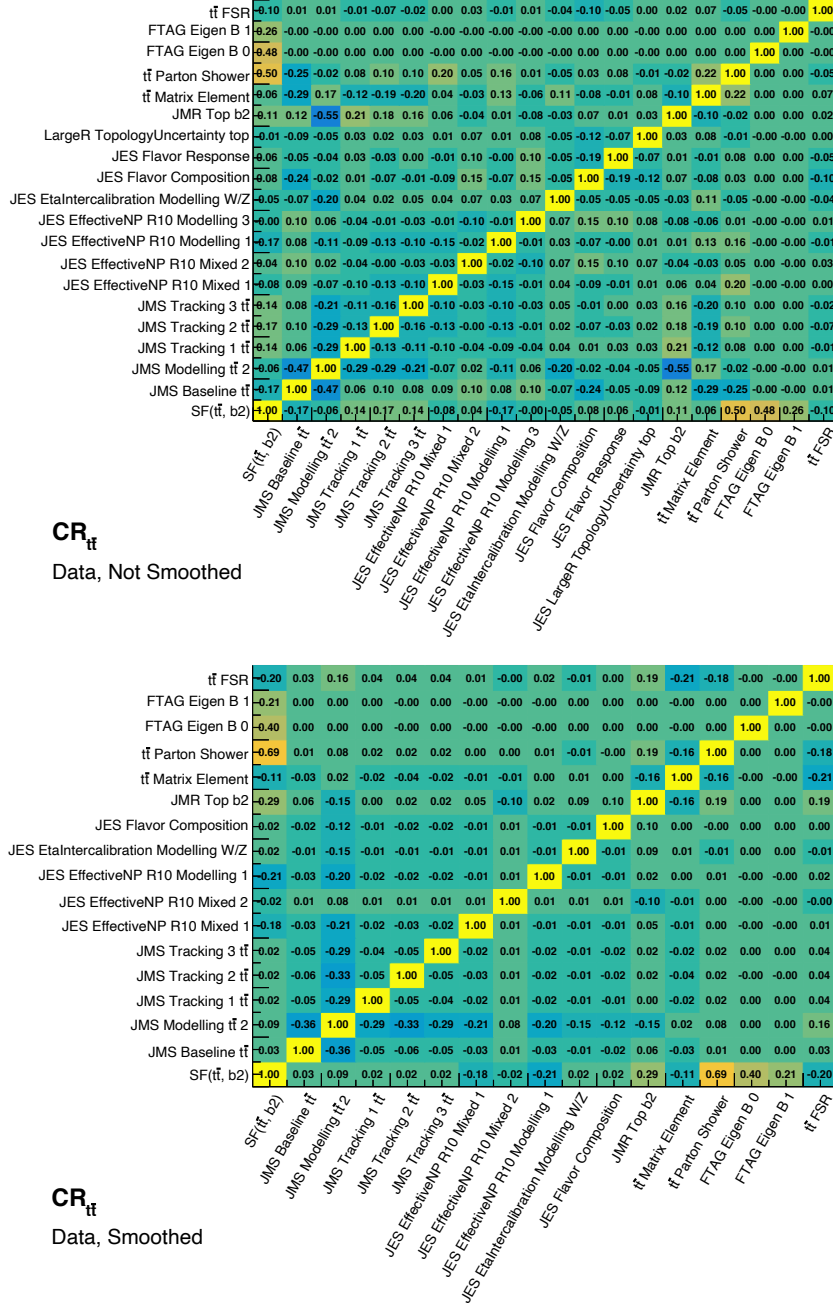


Figure G.7: Correlation plots from standalone fits to CR_{tt} data (CR_{tt} region with smallest event statistics) without (top) and with (bottom) systematic uncertainty smoothing, presented in section 7.5. Nuisance parameters with all correlation coefficients $|r| < 0.1$ are not shown. Stronger correlations are seen when no uncertainty smoothing is applied, indicating more interplay between nuisance parameters in the fit, caused by MC statistical fluctuations being treated as features by the fit.

G.5 Uncertainty Smoothing: Final Thresholds

Table G.2: Optimised systematic uncertainty smoothing statistical uncertainty threshold factors (c in $t = cN_{\text{bins}}$) for all processes with included systematic uncertainties in (a) $\text{CR}_{t\bar{t}}$ and signal regions for the (b) inclusive and (c) Higgs and Z boson differential measurements. Continued on the following page.

(a) $\text{CR}_{t\bar{t}}$ regions						
Process	Inclusive	$\text{CR}_{t\bar{t}}0$	$\text{CR}_{t\bar{t}}1$	$\text{CR}_{t\bar{t}}2$		
$t\bar{t}$	1.5%	1.5%	2%	3%		

(b) Inclusive Measurement SR			
Process	SRL	SRS	
H	2%	2.5%	
Z	2%	2%	
W	3%	5%	
$t\bar{t}$	1.5%	1%	

(c) Differential Measurement SR						
Measurement	Process	SRL1	SRL2	SRS0	SRS1	SRS2
Z	p_T^1	3.5%	—	2.5%	1.5%	—
	$Z \quad p_T^2$	2.5%	3.5%	2.5%	2%	3%
	p_T^3	—	2%	—	2.5%	4%
H	p_T^1	—	—	4%	—	—
	$H \quad p_T^2$	4.5%	—	4%	4.5%	—
	p_T^3	—	5%	—	—	5%
	Z	2%	2%	2%	2%	2%
Either	W	4%	3.5%	3%	2%	5%
	$t\bar{t}$	1.5%	2%	1.5%	1%	2%

G.6 Uncertainty Smoothing: Threshold Validation

Systematic uncertainty mass templates were smoothed following the procedure described in section 7.5. This appendix presents studies made to validate the smoothing procedure. The findings presented in this appendix are the work of the author.

The results obtained with different smoothing thresholds² were observed to ensure trust in the smoothing procedure. The impact of small $\pm 0.5\%$ variations in the threshold were observed in inclusive $\text{CR}_{t\bar{t}}$ data. Large differences in fit results between models with small changes in the smoothing scheme would have indicated that the procedure was unstable.

The optimised smoothing threshold for $t\bar{t}$ was $c = 1.5\%$. Variations of $\pm 0.5\%$ ($c = 1\%, 2\%$) were tested, and the fit result comparisons between them and the $c = 1.5\%$ model are given in table G.3. The effects on the fit results were quantified in three aspects: absolute and relative changes in total uncertainties on $\text{SF}_{t\bar{t}}$ ($\Delta\sigma$ and $\Delta\sigma/\sigma$)³, and the absolute shift in the measured $\text{SF}_{t\bar{t}}$ value in terms of significance ($|\Delta\text{SF}_{t\bar{t}}|/\sigma$). The larger threshold ($+0.5\%$), returned results very similar to the baseline, only a 0.3% change in uncertainties was seen, equivalent to an $\mathcal{O}(10^{-4})$ absolute change in uncertainty. The tighter threshold resulted in larger change in uncertainty, of around 5% , which was likely due to some uncertainty descriptions being “over-smoothed” by the procedure, as would be expected by the definition of the optimisation⁴. No significant shifts in $\text{SF}_{t\bar{t}}$ were observed in any case ($|\Delta\text{SF}_{t\bar{t}}|/\sigma \leq 0.07\sigma$). Overall, these results showed that the smoothing procedure behaves as expected, and that the optimal threshold is reliable, and supported by the results of a looser threshold.

² The “threshold” here is the constant factor c in the definition of the bin-dependent smoothing threshold $t = cN_{\text{bins}}$.

³ The differences were quoted between the optimal model $\sigma_{1.5\%}$ and the alternative models $\sigma_{\pm}$ relative to the optimal model: $\Delta\sigma/\sigma = (\sigma_{\pm} - \sigma_{1.5\%})/\sigma_{1.5\%}$

⁴ The optimal threshold was chosen to be the tightest threshold which does not cause differences between the smooth and original ratios, hence a tighter threshold was expected to be a non-ideal parameter.

Table G.3: Comparisons of $\text{SF}_{t\bar{t}}$ measurements and uncertainties found in inclusive $\text{CR}_{t\bar{t}}$ data fits with small, $\pm 0.5\%$, variations of the optimal threshold factor $c = 1.5\%$ (in $t = cN_{\text{bins}}$). Differences are shown in reference to the $c = 1.5\%$ model, e.g. $\Delta\sigma/\sigma = (\sigma_{\pm} - \sigma_{1.5\%})/\sigma_{1.5\%}$.

c	$\Delta\sigma$	$\Delta\sigma/\sigma$	$ \Delta\text{SF}_{t\bar{t}} /\sigma$
1% (-0.5%)	+0.003	+5.3%	0.03
2% ($+0.5\%$)	$+\mathcal{O}(10^{-4})$	+0.3%	0.07

Table G.4: Comparisons of $\text{SF}_{t\bar{t}}$ measurements and uncertainties found in inclusive $\text{CR}_{t\bar{t}}$ data fits with the optimised smoothing threshold factor $c = 1.5\%$, and a significantly larger threshold factor $c = 5\%$, to those found using a non-smoothed model. Differences are shown in reference to the non-smoothed model, e.g. $\Delta\sigma/\sigma = (\sigma_{\text{smooth}} - \sigma_{\text{no smooth}})/\sigma_{\text{no smooth}}$.

c	$\Delta\sigma$	$\Delta\sigma/\sigma$	$ \Delta\text{SF}_{t\bar{t}} /\sigma$
1.5% (chosen)	-0.003	-4.6%	0.49
5% ($+3.5\%$)	-0.002	-2.8%	< 0.01

The effects of a large threshold increase in a region with high statistics were also observed. For this the inclusive $\text{CR}_{t\bar{t}}$ region was used. The fit result comparisons between smoothed models with $c = 1.5\%$ and $c = 5\%$, and those found by a non-smoothed model are shown in table G.4. With a looser threshold factor (5%) the results became more similar to those in the non-smoothed model, as the smoothing condition became more flexible and retained features of statistical fluctuations.

The same behaviour was seen when comparing the uncertainty pulls and sizes, shown in figure G.4. The features seen in the looser model were closer to those shown by the non-smoothed model. These findings showed that the uncertainty smoothing procedure was needed even when relatively large samples were available. The comparison also illustrated that the observed results with a largely increased smoothing threshold displayed features expected by the design of the procedure.

G.7 Uncertainty Pruning: Additional Material

Table G.5: Comparison of $SF_{t\bar{t}}$ values and uncertainties measured in p_T^{jet} binned $CR_{t\bar{t}}$ region data, using models with different pruning thresholds. $\sigma = \sigma_{\text{total}}$, $Z = SF_{t\bar{t}}/\sigma_{\text{total}}$, NP_{rm} – number of pruned uncertainties (total - 49). All differences are shown in reference to the non-pruned models, such that the sign indicates reduction or increase in relation e.g. $\Delta\sigma/\sigma = (\sigma_{\text{prun}} - \sigma_{\text{no prun}})/\sigma_{\text{no prun}}$. The minimum accepted differences induced by the pruning were defined as: $|\Delta\sigma/\sigma| < 5\%$, $|\Delta SF_{t\bar{t}}|/\sigma < 0.5\sigma$, and $|\Delta Z| < 0.5\sigma$. The optimal thresholds for $CR_{t\bar{t}}0/1/2$ were found to be 3%, 2%, and 2%. An 2% pruning threshold was chosen in all regions for simplicity.

(a) $CR_{t\bar{t}}0$, $p_T^{\text{jet}} \in [250, 450]$ GeV

Pruning	$\Delta\sigma/\sigma$	$ \Delta SF_{t\bar{t}} /\sigma$	ΔZ	NP_{rm}
$< 1\%$	1.4%	$< 0.1\sigma$	-0.2σ	27
$< 2\%$	-1.2%	$< 0.1\sigma$	0.2σ	36
$< 3\%$	0.2%	$< 0.1\sigma$	0.0σ	38
$< 5\%$	-16.3%	$< 0.1\sigma$	2.6σ	41

(b) $CR_{t\bar{t}}1$, $p_T^{\text{jet}} \in [450, 650]$ GeV

Pruning	$\Delta\sigma/\sigma$	$ \Delta SF_{t\bar{t}} /\sigma$	ΔZ	NP_{rm}
$< 1\%$	0.0%	$< 0.1\sigma$	0.0σ	27
$< 2\%$	-1.1%	$< 0.1\sigma$	0.2σ	34
$< 3\%$	-5.2%	$< 0.1\sigma$	0.7σ	36
$< 5\%$	-32.5%	$< 0.1\sigma$	5.5σ	42

(c) $CR_{t\bar{t}}2$, $p_T^{\text{jet}} \in [650, 1000]$ GeV

Pruning	$\Delta\sigma/\sigma$	$ \Delta SF_{t\bar{t}} /\sigma$	ΔZ	NP_{rm}
$< 1\%$	0.4%	$< 0.1\sigma$	0.0σ	21
$< 2\%$	-2.0%	$< 0.1\sigma$	0.2σ	30
$< 3\%$	-10.2%	$< 0.1\sigma$	1.1σ	35
$< 5\%$	-22.4%	0.3σ	2.9σ	38

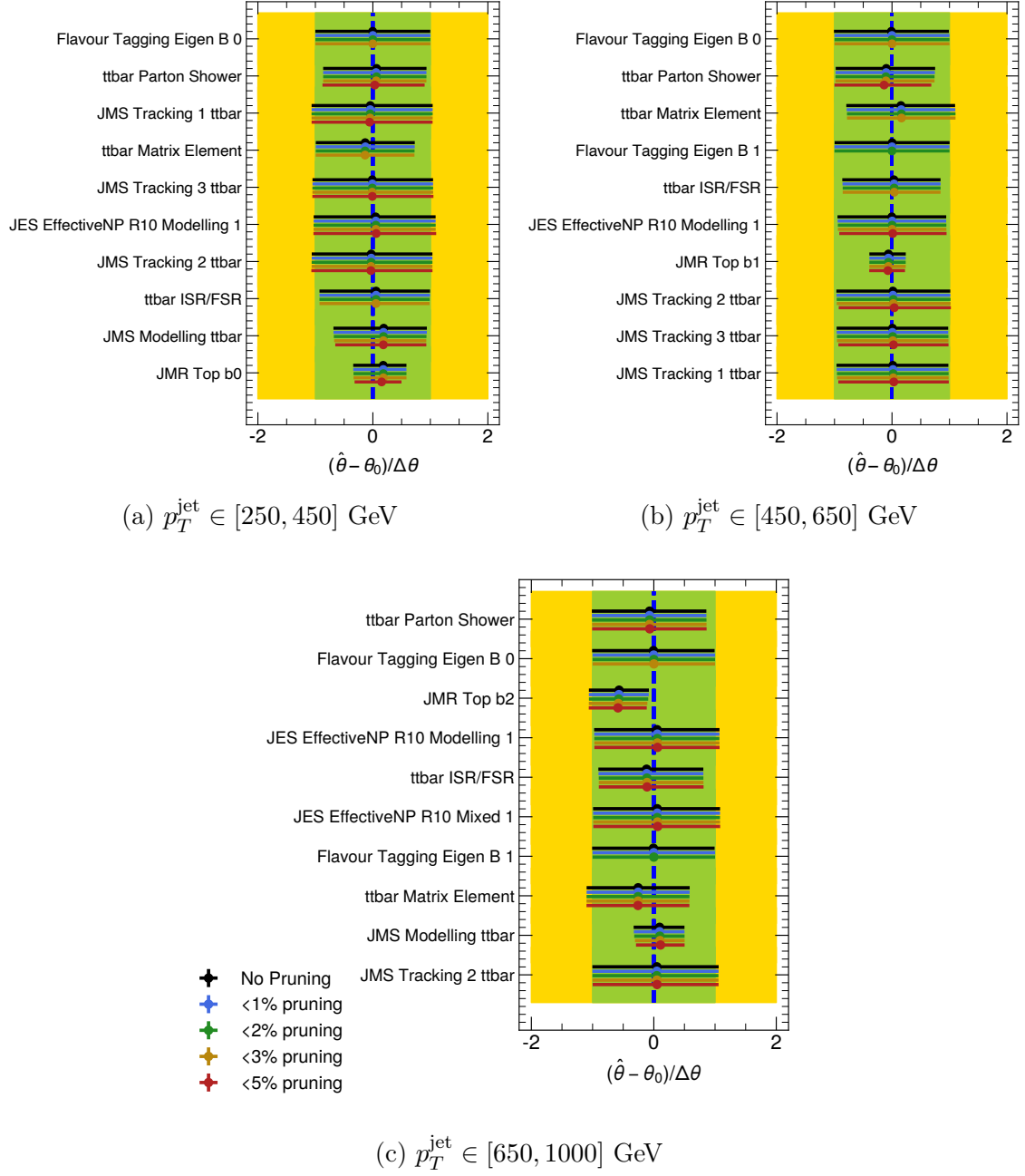


Figure G.8: Systematic uncertainty pull and width comparisons of fits to $\text{CR}_{t\bar{t}}$ data in differential measurement bins with progressively tighter systematic uncertainty pruning thresholds, for the top 10 highest impact $t\bar{t}$ uncertainties, shown in order of post-fit impact to $\text{SF}_{t\bar{t}}$: highest-to-lowest shown top-to-bottom.

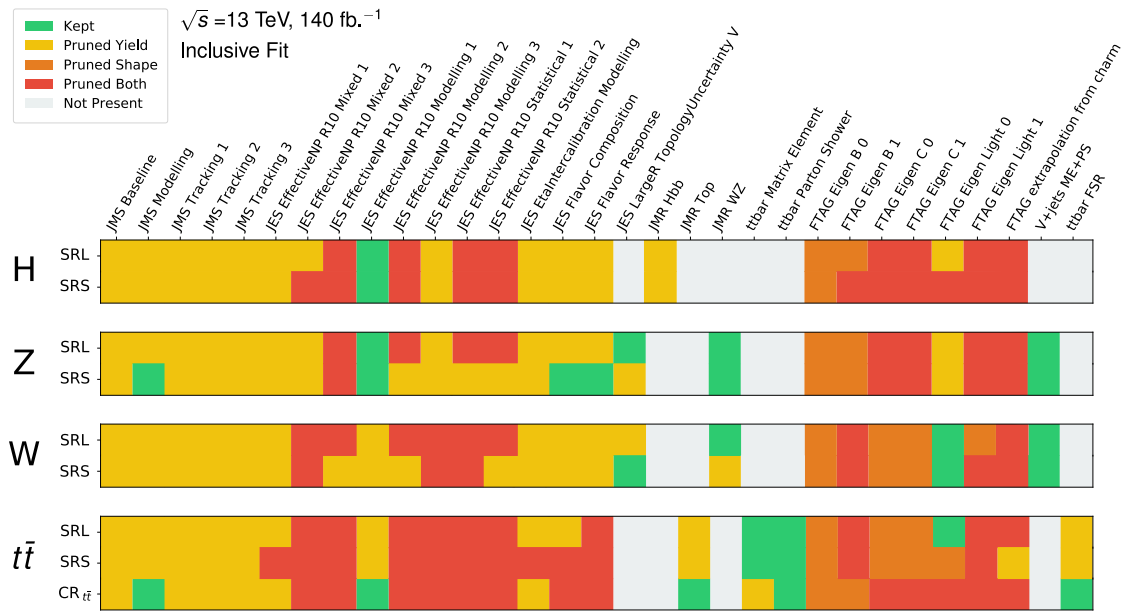


Figure G.9: An overview of systematic uncertainty descriptions with a 2% pruning threshold for all processes in all regions of the inclusive SR measurement fit. Systematic uncertainties which are fully pruned for all processes are excluded from the plot.



Figure G.10: An overview of systematic uncertainty descriptions with a 2% threshold for all processes in all regions of the differential measurement fit. (Cont.)

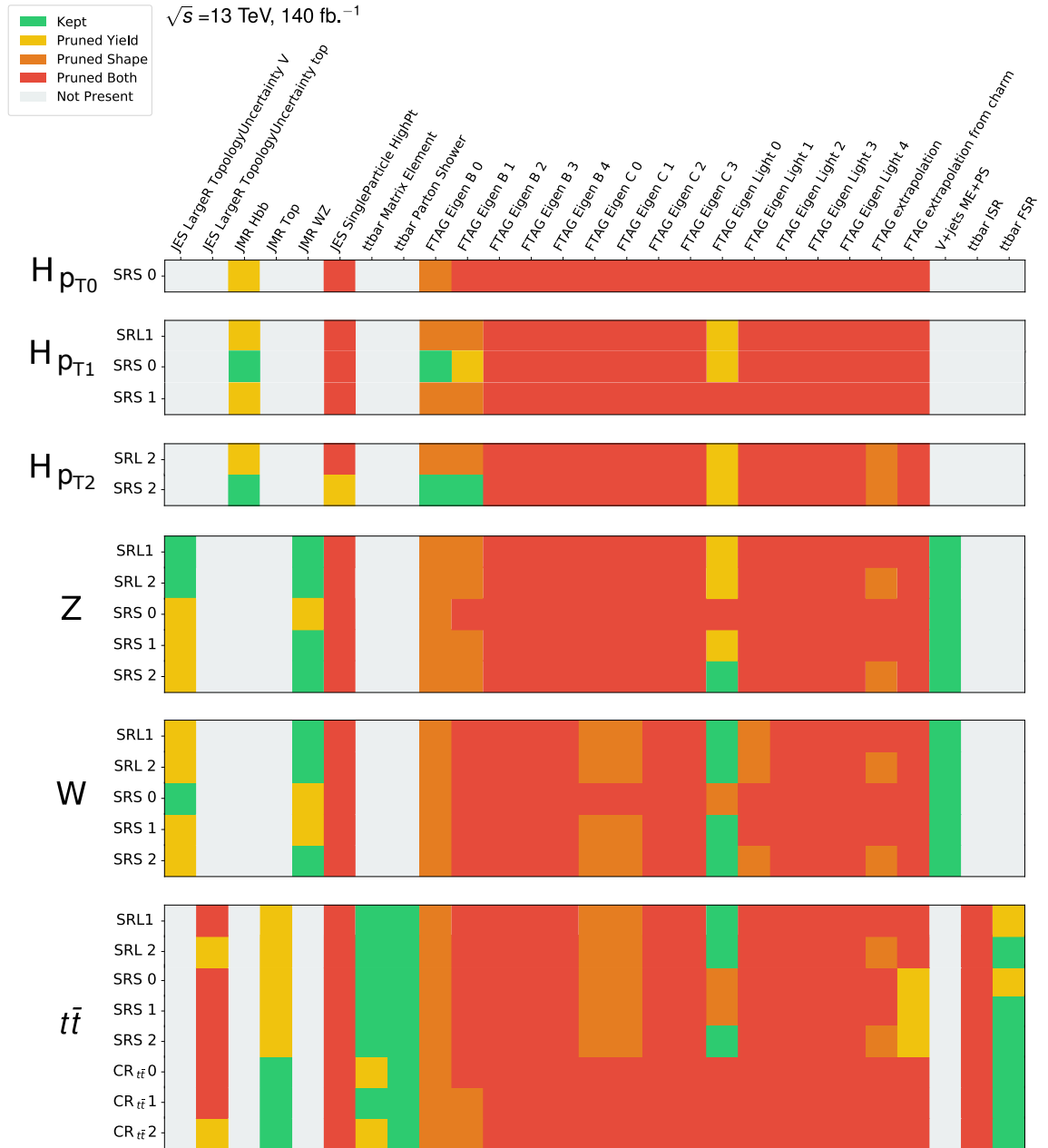


Figure G.10: (Cont.) An overview of systematic uncertainty descriptions with a 2% threshold for all processes in all regions of the differential SR measurement fit.

Appendix H

Validation of Late-stage Developments

H.1 SR Binning Comparison: 0.5 GeV vs. 5 GeV

Throughout a large part of the analysis development the signal region (SR) fits were performed in 0.5 GeV binning as opposed to a 5 GeV binning, due to an issue in the *RooFit* software discussed previously in section 5.7.1. Once the software issue was fixed, the analysis moved to a 5 GeV binning in the signal regions, however, this transition was made late in the analysis.

In order to justify the validity of studies performed using 0.5 GeV binning, the compatibility between the results produced with 5 GeV and 0.5 GeV SR binning was verified. The comparison was made by observing the inclusive measurement results in Asimov data, and in a blinded fit to real data, where the Higgs boson component was kept blind. Note that these studies were conducted before other changes described in this section were added.

Table H.1 shows the relative comparisons of expected uncertainties ($\Delta\sigma/\sigma$) found in Asimov data, as well as the shifts in measured μ_Z and $\text{SF}_{t\bar{t}}$ values in data. The results obtained with the 5 GeV binning were taken as the baseline, such that the values describe the behaviour when using 0.5 GeV binning instead of a 5 GeV binning. The differences in uncertainties on the process' yields were seen to be minor. The largest difference in the total uncertainty was shown to be a 5% relative reduc-

Table H.1: Relative differences in expected uncertainties ($\Delta\sigma/\sigma$) and measured values ($\Delta\mu/\sigma$) induced in by using a 0.5 GeV binning as opposed to a 5 GeV binning in the signal regions (SRL and SRS) of an inclusive measurement fit. Differences are shown in reference to the 5 GeV model, such that the sign indicates reduction or increase in relation to it, e.g. $\Delta\sigma/\sigma = (\sigma_{0.5 \text{ GeV}} - \sigma_{5 \text{ GeV}})/\sigma_{5 \text{ GeV}}$.

	Asimov	Data
	$\Delta\sigma/\sigma$	$ \Delta\mu /\sigma$
μ_H	-5.1%	–
μ_Z	-1.6%	0.30
SF $_{t\bar{t}}$	-0.2%	0.04

tion in the expected uncertainty on the μ_H measurement. In all cases uncertainties were seen to be reduced.

The nominal process mass templates with 0.5 GeV binning were highly uneven (an example can be seen in figure 7.4a) due to limited statistics of the MC samples. As MC statistical uncertainties on the nominal templates were not included in the model, the uneven nature of the nominal templates could have resulted in some additional constraints (similar as seen in the discussion on systematic uncertainty smoothing in section 7.5). Before the move to the 5 GeV binning this was planned to be combated by including large MC statistical uncertainties on the nominal templates as nuisance parameters. However it was not yet implemented before the transition to 5 GeV bins, and, as shown in the presented results, the impact of this effect was not large enough to require a review of the analysis methodology developed using 0.5 GeV binning in the signal regions.

The expected systematic uncertainty widths, shown in figure H.1, and fit parameter correlations, shown in figure H.2, from inclusive Asimov fits, were also compared and no significant differences were seen. Overall the differences between the results obtained with the 0.5 GeV and 5 GeV binning were seen to be moderate, with no significant impact expected for studies presented in this thesis which used

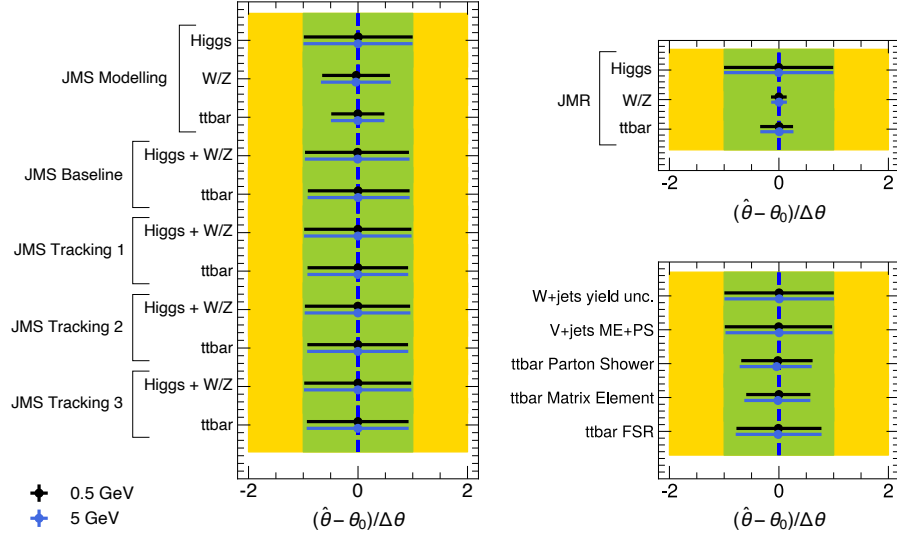


Figure H.1: Post-fit uncertainty pulls and widths from inclusive measurement fits to Asimov data with 0.5 GeV and 5 GeV binning in the signal regions. The two highest-impact uncertainty groups are shown: JMS, JMR, and modelling uncertainties, from the inclusive μ_H measurement fit. No significant differences were seen between fits using 0.5 GeV and 5 GeV binning in the signal regions.

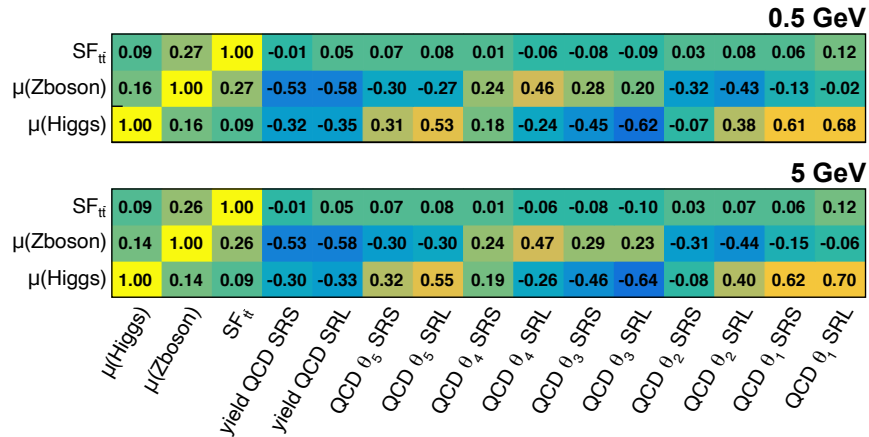


Figure H.2: The correlations between the three main parameters of interest: μ_H , μ_Z , and $SF_{t\bar{t}}$, and the rest of the parameters describing the SR processes, as found in inclusive measurement fits to Asimov data with a 0.5 GeV (top) and 5 GeV binning (bottom) in the signal regions. No significant differences were seen between fits using 0.5 GeV and 5 GeV binning in the signal regions.

0.5 GeV binning. Some more delicate studies, such as the selection of the number of parameters in the QCD estimate function, have been repeated.

H.2 Impact of Changes on the $\text{CR}_{t\bar{t}}$ Results

Some of the implemented changes also concerned the $\text{CR}_{t\bar{t}}$ region, in particular, the addition of t -channel single-top production, and the inclusion of efficiency and acceptance uncertainties on the single-top production and $W(\ell\nu)$ decays. As the thesis has a particular focus on $\text{CR}_{t\bar{t}}$ studies, it was important to observe the impact of these changes on the standalone $\text{CR}_{t\bar{t}}$ results.

The standalone $\text{CR}_{t\bar{t}}$ fit results found in data with the final fit setup are shown in table H.2. The new results are fully compatible with those presented previously in section 6.6.1, as well as behaviour seen by a dedicated ATLAS $t\bar{t}$ cross-section measurement in a similar kinematic region [133]. The largest observed differences in the total uncertainty (σ_{total}) between the two configurations were 2%, and the largest shift in the measured scale factor in terms of uncertainties was 0.2σ . Such differences are minor, and non-consequential to the studies presented in the thesis or to the results of this analysis.

Table H.2: Results from standalone $\text{CR}_{t\bar{t}}$ fits to data using the finalised fit setup.

Region	SF	σ_{stat}	σ_{syst}
Inclusive	0.78	0.01	0.06
$250 \text{ GeV} < p_T^{\text{jet}} < 450 \text{ GeV}$	0.85	0.02	0.06
$450 \text{ GeV} < p_T^{\text{jet}} < 650 \text{ GeV}$	0.75	0.02	0.06
$650 \text{ GeV} < p_T^{\text{jet}} < 1000 \text{ GeV}$	0.71	0.04	0.07
$p_T^{\text{jet}} > 1000 \text{ GeV}$	0.53	0.12	0.18

Appendix I

Results: Additional Material

Table I.1: The products of signal acceptance and selection efficiency ($A\varepsilon$) for all considered Higgs boson production modes in the fiducial measurement [5].

Process	$p_T^H > 450$ GeV
All	0.26
ggF	0.28
VBF	0.14
VH	0.28
$t\bar{t}H$	0.21

Table I.2: The products of signal acceptance and selection efficiency ($A\varepsilon$) for all considered Higgs boson production modes in the fiducial volumes of the differential Higgs boson cross-section measurements [5]. $p_T^{H,0/1/2/3/4} \equiv p_T^H < 300, 300 - 450, 450 - 650, 650 - 1000, > 1000$ GeV. All events with $p_T^{H,\text{out}}$ have $A\varepsilon < 0.1 \times 10^{-2}$.

Process	$p_T^{H,0}$	$p_T^{H,1}$	$p_T^{H,2}$	$p_T^{H,3}$
All	1.3×10^{-2}	0.23	0.31	0.23
ggF	0.7×10^{-2}	0.25	0.35	0.28
VBF	0.2×10^{-2}	0.13	0.16	0.17
VH	1.7×10^{-2}	0.26	0.30	0.20
$t\bar{t}H$	4.7×10^{-2}	0.19	0.24	0.19

Table I.3: Post-fit yields and associated uncertainties of all considered processes in inclusive SRL, SRS and $\text{CR}_{t\bar{t}}$, as found in the inclusive Higgs boson measurement fit [5]. The single top-quark production and $t\bar{t}$ process are combined as *Top*.

Process	SRL	SRS	$\text{CR}_{t\bar{t}}$
Multi-jet	590800 ± 4200	529400 ± 3500	–
Z +jets	16100 ± 2800	12000 ± 2100	–
W +jets	3050 ± 720	2510 ± 500	–
Top	16200 ± 1900	15900 ± 2000	3737 ± 68
$W(\ell\nu)$	–	–	53 ± 16
H	400 ± 1500	300 ± 1300	–
Total	626530 ± 810	560090 ± 770	3790 ± 66
Data	626532	560083	3791

Table I.4: Post-fit yields and associated uncertainties of all considered processes in fiducial SRL, SRS and $\text{CR}_{t\bar{t}}$, as found in the fiducial Higgs boson measurement fit. The single top-quark production and $t\bar{t}$ process are combined as *Top*.

Process	SRL	SRS	$\text{CR}_{t\bar{t}}$
Multi-jet	591000 ± 410	371000 ± 2400	–
Z +jets	16400 ± 2800	9300 ± 1500	–
W +jets	3080 ± 720	1690 ± 340	–
Top	16000 ± 1700	8700 ± 1100	2062 ± 50
$W(\ell\nu)$	–	–	41 ± 12
$H(p_T^H < 450 \text{ GeV})$	98 ± 8.4	41.6 ± 2.7	–
$H(p_T^H > 450 \text{ GeV})$	-30 ± 1300	-10 ± 700	–
Total	626530 ± 810	390660 ± 640	2103 ± 48
Data	626532	390665	2104

Table I.5: Post-fit yields and associated uncertainties of all considered processes in jet- p_T -binned SRL, SRS and $\text{CR}_{t\bar{t}}$, in the differential Higgs boson measurement [5]. The Higgs boson yields are measured in fiducial volumes defined by Higgs boson p_T . $p_T^{H,1/2/3/4} \equiv p_T = 300 - 450, 450 - 650, 650 - 1000, > 1000$ GeV. The single top-quark production and $t\bar{t}$ process are combined as *Top*. Continued on the following page.

SRL			
Jet p_T [GeV]	450 – 650	650 – 1000	> 1000
Multi-jet	509500 ± 3700	72400 ± 1100	5580 ± 360
Z +jets	13100 ± 2200	2600 ± 780	390 ± 270
W +jets	2300 ± 520	630 ± 160	98 ± 30
Top-quark	13200 ± 1200	2360 ± 280	153 ± 47
$H(p_T^{H,\text{out}})$	38.1 ± 7.6	5 ± 1	0.289 ± 0.058
$H(p_T^{H,0})$	-290 ± 880	-15 ± 46	-0.9 ± 2.9
$H(p_T^{H,1})$	-900 ± 1400	-28 ± 46	-0.47 ± 0.78
$H(p_T^{H,2})$	58 ± 71	250 ± 310	2.9 ± 3.5
$H(p_T^{H,3})$	–	14 ± 24	60 ± 100
Total	537040 ± 750	78180 ± 280	6283 ± 79
Data	537038	78177	6283

SRS			
Jet p_T [GeV]	250 – 450	450 – 650	650 – 1000
Multijet	157400 ± 2900	340600 ± 2100	48020 ± 710
Z +jets	3900 ± 2400	8000 ± 1300	1640 ± 530
W +jets	800 ± 160	1370 ± 250	365 ± 83
Top-quark	7800 ± 1000	7320 ± 750	1150 ± 160
$H(p_T^{H,\text{out}})$	41.1 ± 8.2	19.7 ± 3.9	1.96 ± 0.39
$H(p_T^{H,0})$	-400 ± 1300	-110 ± 330	-5 ± 16
$H(p_T^{H,1})$	-130 ± 210	-450 ± 740	-8 ± 13
$H(p_T^{H,2})$	–	90 ± 110	140 ± 170
$H(p_T^{H,3})$	–	–	25 ± 43
Total	169420 ± 420	356910 ± 600	51320 ± 230
Data	169418	356910	51324

Table I.5: (Cont.) Post-fit yields and associated uncertainties of all considered processes in jet- p_T -binned SRL, SRS and $\text{CR}_{t\bar{t}}$, in the differential Higgs boson measurement [5]. The Higgs boson yields are measured in fiducial volumes defined by Higgs boson p_T . $p_T^{H,1/2/3/4} \equiv p_T = 300 - 450, 450 - 650, 650 - 1000, > 1000$ GeV. The single top-quark production and $t\bar{t}$ process are combined as Top .

$\text{CR}_{t\bar{t}}$				
Jet p_T [GeV]	250 – 450	450 – 650	650 – 1000	> 1000
Top-quark	1676 ± 43	1606 ± 41	426 ± 21	27.7 ± 6
$W(\ell\nu)$	12.3 ± 3.5	22.9 ± 6.5	14 ± 4	5.9 ± 1.7
Total	1688 ± 43	1628 ± 41	440 ± 21	33.6 ± 5.8
Data	1687	1628	442	34

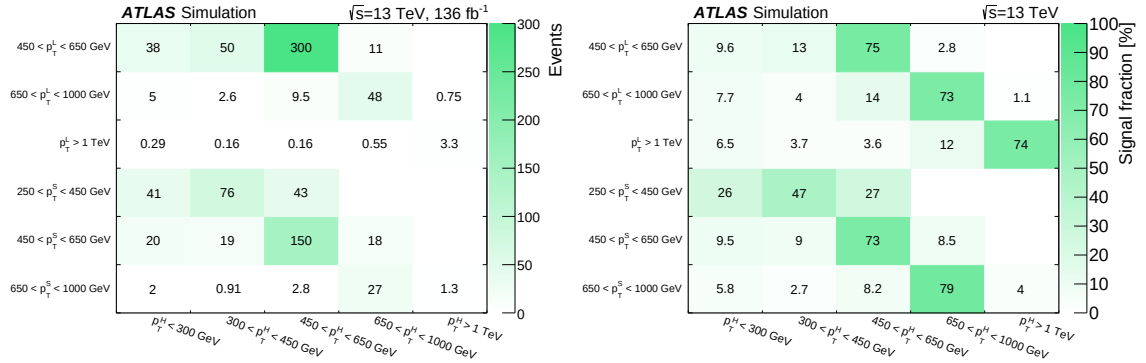


Figure I.1: The expected (a) yields and (b) percent contributions of each truth- p_T -binned Higgs boson component (x -axis) within each jet- p_T -binned signal region (y -axis) [5]. p_T^L denotes SRL p_T^{jet} bins, and p_T^S denotes SRS bins.

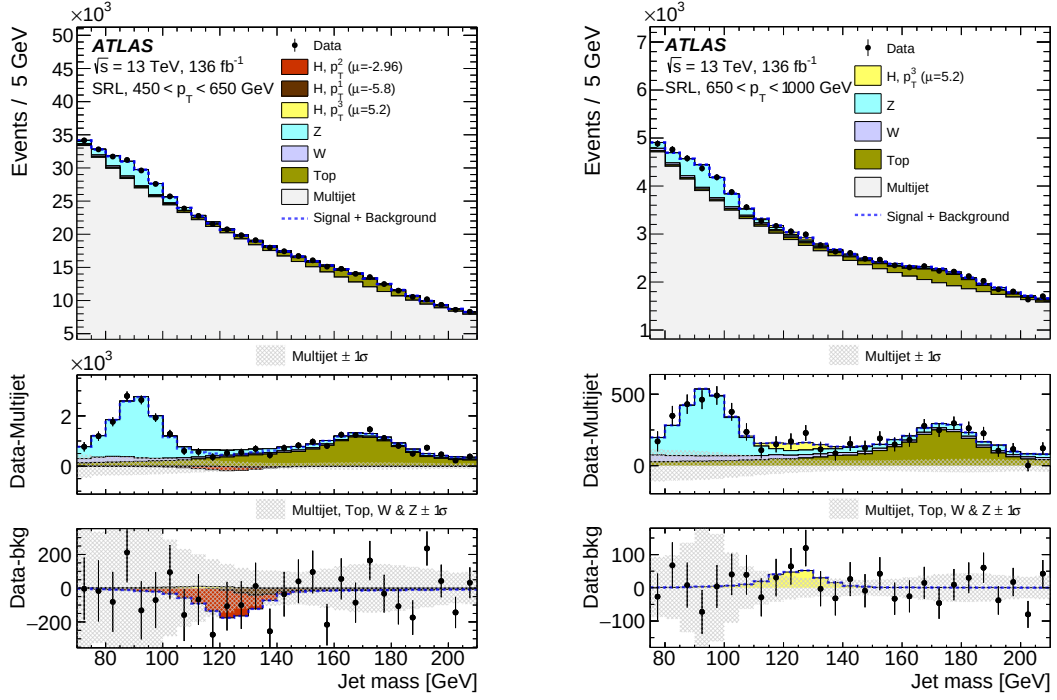
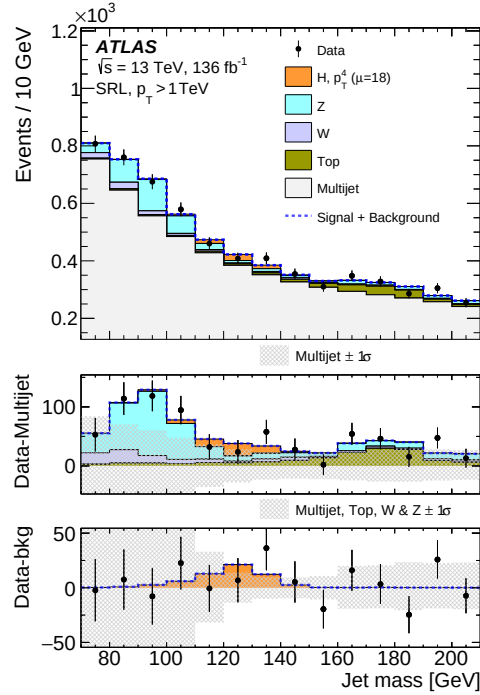
(a) SRL1, $p_T^{\text{jet}} \in [450, 650]$ GeV(b) SRL2, $p_T^{\text{jet}} \in [650, 1000]$ GeV(c) SRL3, $p_T^{\text{jet}} > 1$ TeV

Figure I.2: The post-fit distributions of data and model processes in (a) SRL1, (b) SRL2, and (c) SRL3 regions from the differential Higgs boson measurement [5], where $p_T^{H,1/2/3/4} \equiv p_T^H = 300 - 450, 450 - 650, 650 - 1000, > 1000$ GeV. The single top-quark production and $t\bar{t}$ process are combined as *Top*.

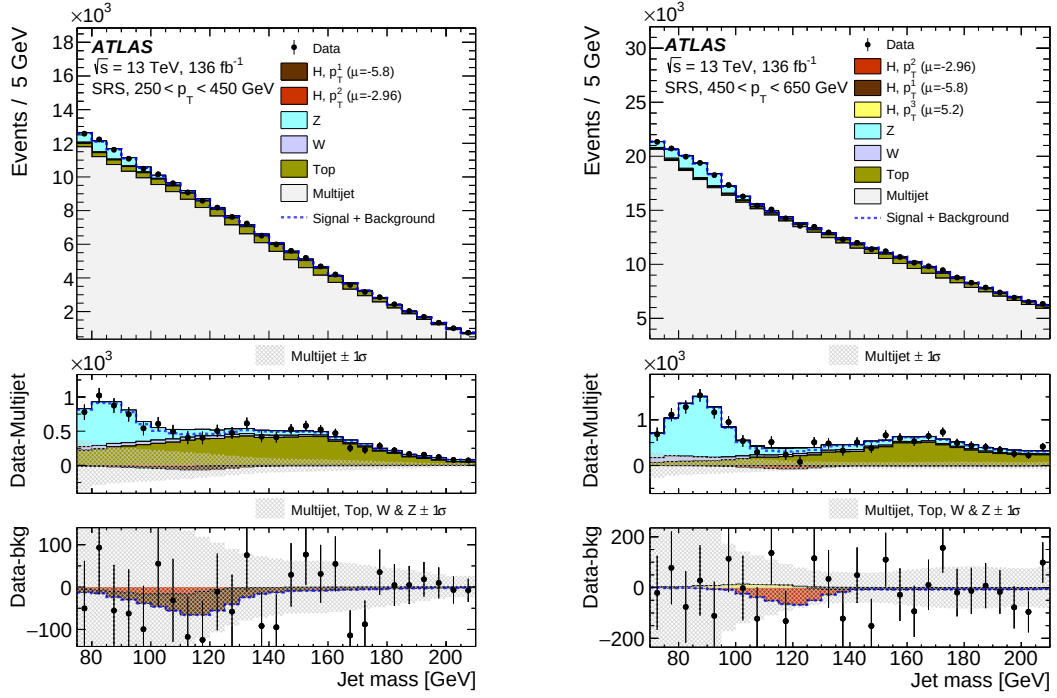
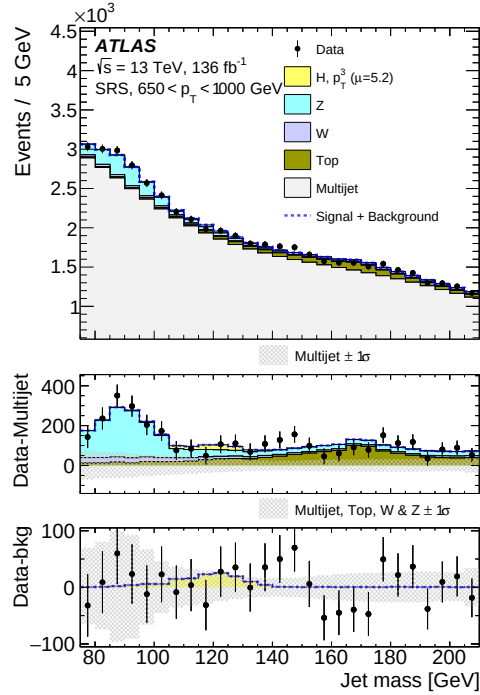
(a) SRS0, $p_T^{\text{jet}} \in [250, 450]$ GeV(b) SRS1, $p_T^{\text{jet}} \in [450, 650]$ GeV(c) SRS2, $p_T^{\text{jet}} \in [650, 1000]$ GeV

Figure I.3: The post-fit distributions of data and model processes in (a) SRS0, (b) SRS1, and (c) SRS2 regions from the differential Higgs boson measurement [5], where $p_T^{H,1/2/3/4} \equiv p_T^H = 300 - 450, 450 - 650, 650 - 1000, > 1000$ GeV. The single top-quark production and $t\bar{t}$ process are combined as Top .

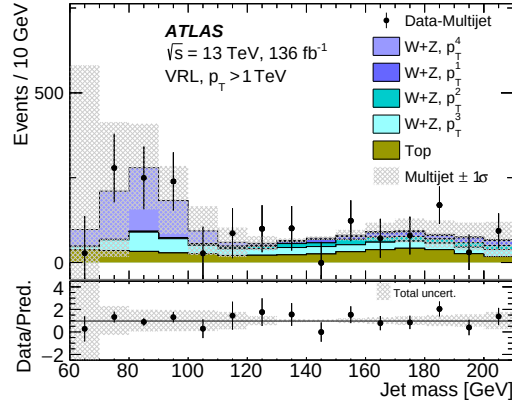
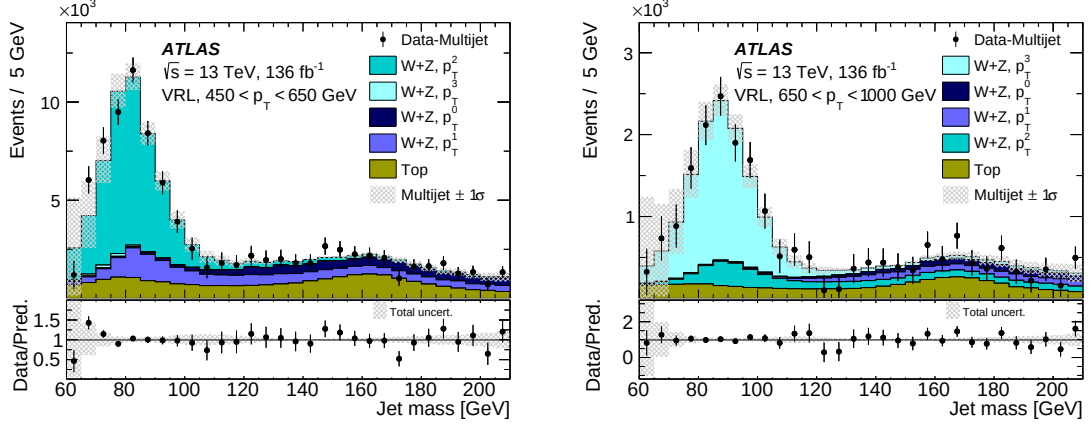


Figure I.4: The post-fit distributions of data and model processes in (a) VRL1, (b) VRL2, and (c) VRL3 regions from the differential V +jets measurement fit in VRL regions [5], where $p_T^{1/2/3/4} \equiv p_T = 300 - 450, 450 - 650, 650 - 1000, > 1000$ GeV. The single top-quark production and $t\bar{t}$ process are combined as Top .

