

Treatment of systematic uncertainties in b-jet identification and measurement of Higgs boson decays to b-quarks with the ATLAS detector

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Abstract of the Dissertation

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The Higgs boson was discovered in 2012, and since then the ATLAS and CMS collaborations have been analyzing an ever increasing number of collisions from the LHC collider to pin down the properties of this particle as precisely as possible. Among the measurements performed, especially interesting is the measurement of the Higgs boson decays to two b-quarks. However, this decay mode is hard to observe because of the large background from multi-jet production. To measure the Higgs boson decaying to two b-quarks, the best Higgs boson production channel is the associated production with a vector boson (VH) where one vector boson, either the W or Z boson, is produced in association with a Higgs boson. If the vector boson decays leptonically into neutrinos or charged leptons, the leptons will provide a handle to reduce the large multi-jet background. This thesis work involves multiple efforts on increasing the signal significance of the VH, $H \rightarrow b\bar{b}$ analysis including optimizing the event selection, adding a new control region for the top back-

ground and using machine learning methods to purify the W +jets background in a dedicated control region and ultimately to get a better constraint on the normalization factor for this background. Each attempt increases the signal significance of the analysis by several percent. Apart from the $H \rightarrow b\bar{b}$ analysis work, the thesis work also involves inventing two new approaches to treat systematic uncertainties related to b -jet identification, which plays a crucial role in enabling the $H \rightarrow b\bar{b}$ measurement and also in many other ATLAS analyses. The first allows for the correct correlation of b -jet identification systematic uncertainties across multiple analyses. The second new treatment provides an estimate of the systematic uncertainties on identifying b -jets with especially large transverse momentum. This is particularly relevant for events in the “boosted” VH , $H \rightarrow b\bar{b}$ analyses

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Chapter 1

Introduction

Humankind has always been curious about whether there exist fundamental building blocks of the universe, and if so, what they are. Around the 5th Century BC, Democritus first proposed the atomic hypothesis, i.e. everything is composed of 'atoms', where an atom is the smallest building block of the universe and all of them are indivisible. Since then, human's understanding of the 'atom' has been deepened progressively. In the year 1804, John Dalton formulated the modern atomic theory, in which he proposed that elements are composed of atoms, and each element's atoms are identical in mass and properties. After that in late 19-20th Century, JJ.Thomson's discovery of the electron and Ernest Rutherford's discovery of the nucleus marked the human's first understanding of the atom's structure and the discovery of subatomic particles. Then the theory of quantum mechanics is developed and used to explain the behaviour of sub-atomic particles. Then the Standard Model theory unified the electromagnetic, strong and weak forces, explaining the interactions of subatomic particles and providing a comprehensive framework for modern particle physics. The Standard Model has been very successful in explaining the particle interactions and predicting the types of elementary particles, the fundamental building blocks of the universe.

In 2012, the Higgs boson, a particle predicted by the Standard Model, is discovered by the ATLAS and CMS experiments at the Large Hadron Collider (LHC). This completed the discovery of all the particles predicted by the Standard Model, but constituted just a starting point for measuring the properties of the Higgs boson. The Higgs boson is responsible for endowing the other particles with mass through coupling, where the coupling strength is proportional to either the mass (fermions) or the mass squared (vector bosons) of the particle. Therefore the measurement of Higgs boson coupling to massive particles such as bottom quarks plays a determinant role in probing deviations from the Standard Model. Measuring the Higgs boson decays to two b-quarks

($H \rightarrow bb$) is crucial for measuring the coupling strength to b -quarks since there is no easy way to access this coupling through Higgs production. Also, among the various decay modes of the Higgs boson, $H \rightarrow bb$ is expected to be the most copious decay mode and its partial decay width Γ_{bb} is expected to dominate the total Higgs boson decay width. Therefore it is crucial to measure the rate of $H \rightarrow bb$ decays. The best way to measure the $H \rightarrow bb$ mode is to look at Higgs bosons produced in association with a W or Z vector boson, the so called 'VH' production channel. This is because leptons or neutrinos from vector boson decays can provide a handle to reduce the large multi-jet background. The $VH, H \rightarrow bb$ analysis constitute one of the main parts of this thesis. The identification of b-jets is important in $H \rightarrow bb$ analysis since selection of $H \rightarrow bb$ signal requires identifying the final state b-jets decay from Higgs boson. Here the b-jet is a spray of hadrons and other particles originating from the hadronization of b-quarks.

This thesis represents a summary of a 4-years-long research period on the ATLAS experiment, focused on $VH, H \rightarrow bb$ analysis and flavor tagging performance. The studies are documented in the following chapters. A brief introduction is as follows.

The work on the $VH, H \rightarrow bb$ analysis involves several developments for improving the measurement precision and the analysis robustness. This includes the optimization of the selection procedure for identifying the b-jets. Also, a detailed study has been performed to separate and purify the W+jets background from the $t\bar{t}$ background in order to improve the estimate of the W+jets background normalization. Another improvement made is the combined use of the top background control region from both $VH, H \rightarrow bb$ and $VH, H \rightarrow cc$ analysis selections in order to pin down the top background more precisely. Some work has also been carried out to test new techniques based on deep neural networks for estimating the modeling systematic uncertainty of the W+jets background.

On the flavor tagging performance side, this thesis work involve designing two new approaches of treating flavor tagging systematic uncertainties. The first approach enables different physics analyses to correctly correlate b -jet identification (b -tagging) uncertainties when their physics results are combined. In ATLAS b -tagging calibration, the number of original uncertainties is $O(100)$. To reduce the number of original uncertainties, an eigenvector decomposition method was developed to transform the original uncertainties into the so called eigenvector uncertainties which are of the order of $O(10)$. However, eigenvector uncertainties related to different b -tagging setups cannot be correlated directly. In this thesis, the so called eigenvector recomposition method is developed to revert eigenvector uncertainties back to the original un-

certainties. This allows them to be correctly correlated among various physics analyses but without the need of evaluating the original uncertainties one-by-one. The second development is the estimation of b -tagging uncertainties at high jet transverse momentum based on both in-situ b -tagging calibration uncertainties and additional Monte Carlo(MC) based extrapolation uncertainties to reach the high transverse momentum region. This uncertainty estimation is derived for the first time in the so called b -tagging pseudo-continuous scheme, where jets are classified according to the ratio of probabilities assigned to the jet by the b -tagging algorithm for being a b -jet rather than a c - or *light*-jet.

The thesis is structured as follows. Chapter 2 focuses on the theoretical background with an introduction to the Standard Model and to the Higgs properties. Chapter 3 is a general introduction to the LHC and to the subsystems of the ATLAS detector. Chapter 4 is focused on flavor tagging, mainly presenting the two new approaches to treat flavor tagging systematic uncertainties. Chapter 5 describes the final Run-2 $VH, H \rightarrow b\bar{b}$ analyses and several improvements to it introduced in this thesis. Finally, Chapter 6 summarizes the whole thesis work.

Chapter 2

Theoretical background

2.1 Standard model

2.1.1 Standard model particles

The universe consists of particles as building blocks and the law of physics can be explained by the interaction between particles. The Standard Model is for now the best theory explaining the particles and their interaction. In the world of low energy, the fundamental building blocks are atoms, which consists of a nucleus with electrons orbiting around. Both nucleus and electrons are charged particles and they are attracted by electrical force which could be explained by Quantum Electrodynamics (QED). The nucleus consists of protons and neutrons, which are bound by the strong force described by Quantum Chromodynamics (QCD). Nucleus sometimes could decay and produce one electron/positron and electron anti-neutrino/electron neutrino. This process is called nuclear β decay and could be explained with weak force. The picture is completed with gravity, which is very weak compared to three other forces. The proton and neutron are composite particles. Protons consist of two up-quarks and one down-quark. Neutrons consist of two down-quarks and one up-quark. The up-quarks and down-quarks, electrons and electron neutrinos do not have internal structure (to current knowledge) and therefore are elementary particles. These particles are in the "low energy" world. However, in the "high energy" world such as in LHC collisions, there are two more copies of up-quarks and down-quarks, electrons and electron neutrinos. They are for example the muon (μ) as a heavier electron, and the charm quark as a heavier up-quark. These particles are called second generation and third generation particles. The experiments results show that there are only three generations of particles. Also, each charged particle has a counterpart anti-particle which has nearly the same physical properties but is carrying opposite charge. For

Standard Model of Elementary Particles					
three generations of matter (fermions)			interactions / force carriers (bosons)		
	I	II	III		
mass	$\approx 2.2 \text{ MeV}/c^2$	$\approx 1.28 \text{ GeV}/c^2$	$\approx 173.1 \text{ GeV}/c^2$	0	$\approx 124.97 \text{ GeV}/c^2$
charge	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	0	0
spin	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1	0
QUARKS	u up	c charm	t top	g gluon	H higgs
	d down	s strange	b bottom	γ photon	
	e electron	μ muon	τ tau	Z Z boson	
LEPTONS	ν_e electron neutrino	ν_μ muon neutrino	ν_τ tau neutrino	W W boson	
				GAUGE BOSONS VECTOR BOSONS	SCALAR BOSONS

Figure 2.1: A table of all elementary particles predicted by Standard Model. [1]

instance, the anti-particle of the electron is the positron which carries positive charge. Apart from these particles which are spin-half fermions, there are also particles of spin-1 as force carriers. As mentioned above, there are three types of forces in the Standard Model: electromagnetic force, strong force and weak force. The electromagnetic force carrier is a particle called photon. The gluon is the strong force carrier. W and Z bosons are weak force carriers. The elementary particles are completed with one last particle called the Higgs boson. The Higgs boson is different from all particles discussed above since it is a spin-0 scalar particle. The field describing the Higgs boson, unlike other particles whose field has zero vacuum expectation values, has non-zero vacuum expectation value. This provides a mechanism which endows mass to all other particles. The Higgs boson is discovered in 2012 in ATLAS [13] and CMS [14] at the LHC. The mass of the Higgs boson is measured to be $\approx 125 \text{ GeV}$. The research to measure the properties of Higgs boson is one of the main parts of this thesis work. Figure 2.1 lists all elementary particles and their properties.

2.1.2 QED and QCD

The electromagnetic force and weak force are both described by Quantum Electrodynamics (QED) in the Standard Model. The Lagrangian for the fermion

fields is[15]:

$$\begin{aligned}\mathcal{L}_F = \sum_i \bar{\psi}_i (i\not{\partial} - m_i - \frac{m_i H}{v}) \psi_i - \frac{g}{2\sqrt{2}} \sum_i \bar{\psi}_i \gamma^\mu (1 - \gamma^5) (T^+ W_\mu^+ + T^- W_\mu^-) \psi_i \\ - e \sum_i Q_i \bar{\psi}_i \gamma^\mu \psi_i A_\mu - \frac{g}{2 \cos \theta_W} \sum_i \bar{\psi}_i \gamma^\mu (g_V^i - g_A^i \gamma^5) \psi_i Z_\mu\end{aligned}\quad (2.1)$$

where the ψ represent fermion fields $\psi_i = \begin{pmatrix} \nu_i \\ l_i^- \end{pmatrix}$ for leptons and $\begin{pmatrix} u_i \\ d_i' \end{pmatrix}$ for quarks. The d_i' is defined as $d_i' \equiv \sum_j V_{ij} d_j$, where V is CKM matrix. Also in the Lagrangian, the e is the positron electric charge and θ_W is the weak mixing angle. The term A_μ is photon field, $W_\mu^\pm$ is W boson field and Z_μ is Z boson field. The Yukawa coupling of H to fermion field is in the first term and will be explained in detail in section 2.2. The second term in the Lagrangian describes charged current weak interactions.

The strong force is described by Quantum Chromodynamics (QCD). The QCD Lagrangian is[15]:

$$\mathcal{L} = \sum_q \bar{\psi}_{q,a} (i\gamma^\mu \partial_\mu \delta_{ab} - g_s \gamma^\mu t_{ab}^C \mathcal{A}_\mu^C - m_q \delta_{ab}) \psi_{q,b} - \frac{1}{4} F_{\mu\nu}^A F^{A\mu\nu}, \quad (2.2)$$

where the $\psi_{q,a}$ is quark-field spinors for quark whose flavor is q and mass is m_q . Since there are 3 colors, the color-index a runs from 1 to 3. The γ^μ are the Dirac γ -matrices. The g_s is the strong coupling constant. The $\mathcal{A}_\mu^C$ is the gluon field. Since there are 8 types of gluon, the C is running from 1 to 8. t_{ab}^C is generator of SU(3) group.

The term $F_{\mu\nu}^A$ is field tensor:

$$F_{\mu\nu}^A = \partial_\mu \mathcal{A}_\nu^A - \partial_\nu \mathcal{A}_\mu^A - g_s f_{ABC} \mathcal{A}_\mu^B \mathcal{A}_\nu^C \quad (2.3)$$

$$[t^A, t^B] = i f_{ABC} t^C \quad (2.4)$$

where f_{ABC} is SU(3) group's structure constant.

2.2 Higgs mechanism

2.2.1 Standard model Higgs boson

Higgs generate mass for gauge boson [16] [17] [18] [19] . In the Salam-Weinberg model, the field can be expressed as:

$$\phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix} \quad (2.5)$$

The Lagrangian for this field can be expressed as:

$$\mathcal{L} = (\partial_\mu \phi)^\dagger (\partial_\mu \phi) - V(\phi), \quad (2.6)$$

where $V(\phi)$ is the potential term of the Lagrangian, which can be expressed as:

$$V(\phi) = \mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2 \quad (2.7)$$

This form of potential lead to broken symmetry. This is more intuitive if the field is a one-dimensional field. In this case, considering the Lagrangian has a one dimensional potential, $V(\phi) = \frac{1}{2}\mu^2\phi^2 + \frac{1}{4}\lambda\phi^4$. Here the λ is required to be positive since the minimum of potential has to be finite. However, there is no such restriction for μ^2 . Figure 2.2 shows the field potential when μ^2 is positive and negative. In the latter case, the field can be chosen to be either $+v$ or $-v$ leading to spontaneously symmetry breaking.

Similarly to the 1-dimensional field, in the Salam-Weinberg model, if $\mu^2 < 0$, the symmetry is spontaneously broken and there will be infinite many minima given by:

$$\phi^\dagger \phi = \frac{1}{2}(\phi_1^2 + \phi_2^2 + \phi_3^2 + \phi_4^2) = \frac{v^2}{2} \quad (2.8)$$

Like in the 1-dimensional field, the minimum of the field is no longer sitting at 0. Without loss of generality, the minima can be chosen to be:

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix} \quad (2.9)$$

The field can be expanded at this minimum with expression of:

$$\phi(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h \end{pmatrix} \quad (2.10)$$

where h is the field expansion around the minimum and it is also the higgs field. The perturbation term for other field term turns out to be the so called

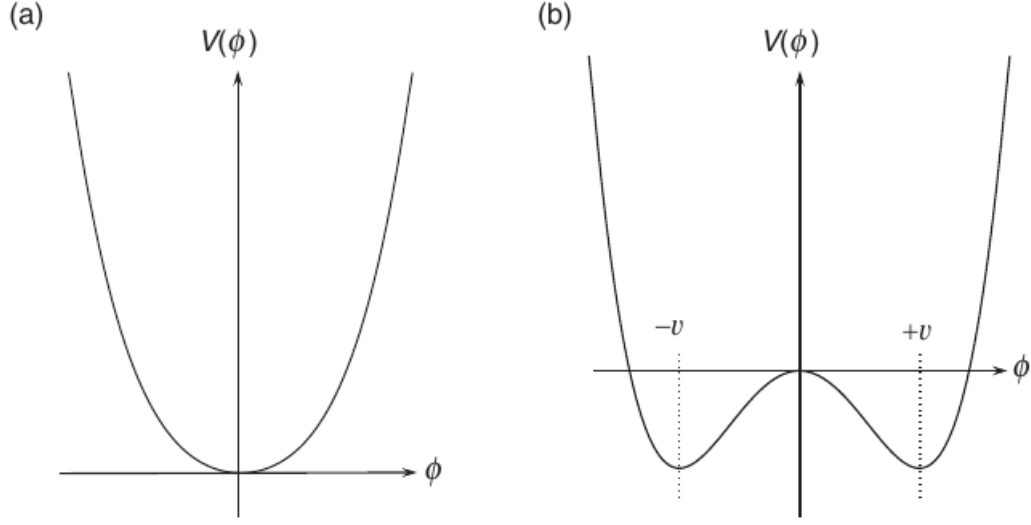


Figure 2.2: Figure (a) shows scalar field potential when $\lambda > 0$. Figure (b) shows scalar field potential when $\lambda < 0$.

Goldstone bosons and they can be absorbed by a re-definition of the covariant derivative D_μ , therefore are not written in the field expansion for simplicity. In the Glashow-Salam-Weinberg (GSW) model, the Lagrangian needs to obey $SU(2) \times U(1)$ local gauge symmetry, therefore one can re-express the derivative into covariant derivative to be:

$$\partial_\mu \rightarrow D_\mu = \frac{1}{2}[2\partial_\mu + (ig_w \boldsymbol{\sigma} \cdot \mathbf{W}_\mu + ig' B_\mu)] \quad (2.11)$$

The first term of the Lagrangian in Equation 2.6 becomes:

$$\begin{aligned} (D_\mu \phi)^\dagger (D_\mu \phi) &= \frac{1}{2}(\partial_\mu h)(\partial^\mu h) + \frac{1}{8}g_w^2(W_\mu^{(1)} + iW_\mu^{(2)})(W^{(1)\mu} - iW^{(2)\mu})(v+h)^2 \\ &\quad + \frac{1}{8}(g_W W_\mu^{(3)} - g' B_\mu)(g_W W^{(3)\mu} - g' B^\mu)(v+h)^2 \end{aligned} \quad (2.12)$$

The coefficient of the quadrature term $W_\mu^{(1)}W^{(1)\mu}$ and $W_\mu^{(2)}W^{(2)\mu}$ reveal the mass of W boson to be:

$$m_W = \frac{1}{2}g_w v \quad (2.13)$$

The last term in the right hand side of the equation can be expressed as:

$$\frac{v^2}{8} \begin{pmatrix} W_\mu^{(3)} & B_\mu \end{pmatrix} \begin{pmatrix} g_w^2 & -g_w g' \\ -g_w g' & g'^2 \end{pmatrix} \begin{pmatrix} W^{(3)\mu} \\ B^\mu \end{pmatrix}, \quad (2.14)$$

where the two-by-two non-diagonal matrix is the mass matrix. The eigenvalues of this matrix give the mass of Z boson and photon, their mass is:

$$m_\gamma = 0, m_Z = \frac{1}{2}v\sqrt{g_w^2 + g'^2}, \quad (2.15)$$

where v represent the vacuum expectation value of Higgs field. It is measured to be 246 GeV. The Higgs mechanism spontaneously breaks the $U(1) \times SU(2)$ gauge group symmetry successfully generating the mass of $W^\pm$ and Z^0 bosons.

2.2.2 Higgs boson coupling to Vector bosons

The W^+ and W^- field is expressed as [19]:

$$W^\pm = \frac{1}{\sqrt{2}}(W^{(1)} \mp iW^{(2)}) \quad (2.16)$$

With this, one can rewrite the second term in the right hand side of Equation 2.12 to become:

$$\frac{1}{4}g_W^2 W_\mu^- W^{+\mu} (v + h)^2 = \frac{1}{4}g_W^2 v^2 W_\mu^- W^{+\mu} + \frac{1}{2}g_W^2 v W_\mu^- W^{+\mu} h + \frac{1}{4}g_W^2 W_\mu^- W^{+\mu} h h \quad (2.17)$$

The first term shows the mass of W^+ and W^- . The second term is $WW h$, showing the triple coupling of the Higgs boson with a pair of $W^\pm$ bosons. The coupling strength is:

$$g_{HWW} = \frac{1}{2}g_W^2 v = g_W m_W = \frac{2m_W^2}{v} \quad (2.18)$$

Therefore the coupling strength is proportional to the mass of the W boson squared. The third term $WW h h$ shows the quartic coupling between the Higgs and the W bosons. Similarly, the coupling strength between the Higgs and the Z boson is $g_{HZZ} = g_Z m_Z$, which is also proportional to the mass of Z boson.

2.2.3 Higgs boson coupling to Fermion particles

The Lagrangian for leptons in the Standard Model needs to be invariant under the $SU(2) \times U(1)$ gauge symmetry [19]. A term of the form $-g_f(\bar{L}\phi R + \bar{R}\phi^+ L)$ satisfies this requirements. Here the ϕ is the same field as in equation 2.5, and ϕ^+ is the hermitian conjugate of ϕ . Therefore, for example, the Lagrangian of

electron and electron neutrino can have the form of:

$$\mathcal{L}_e = -g_e [(\bar{\nu}_e \quad \bar{e}_e)_L \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} e_R + \bar{e}_R (\phi^{+*} \quad \phi^{0*}) \begin{pmatrix} v_e \\ e \end{pmatrix}_L] \quad (2.19)$$

Expanding the field at minimum as expressed in Equation 2.10, the Lagrangian becomes:

$$\mathcal{L}_e = \frac{g_e}{\sqrt{2}} v (-\bar{e}_L e_R - \bar{e}_R e_L) + \frac{g_e}{\sqrt{2}} h (-\bar{e}_L e_R - \bar{e}_R e_L) \quad (2.20)$$

Here the g_e is Yukawa coupling:

$$g_e = \sqrt{2} \frac{m_e}{v} \quad (2.21)$$

However, the above is only for charged lepton and down-quark. For up-quarks, the Lagrangian is given by using the conjugate of field ϕ :

$$\phi_c = -i\sigma_2 \phi^* \quad (2.22)$$

This gives the Lagrangian of the form:

$$\mathcal{L} = g_f [\bar{L} \phi_c R + (\bar{L} \phi_c R)^\dagger], \quad (2.23)$$

where g_f is the Yukawa coupling between fermion and Higgs. The coupling can be expressed as below. It is not predicted by Higgs mechanism but can be chosen to be consistent with fermion mass. [19]:

$$g_f = \sqrt{2} \frac{m_f}{v}, \quad (2.24)$$

and, as mentioned before, v is measured to be 246 GeV and m_f is the mass of the fermion. The fermion coupling to the Higgs boson is also proportional to fermion mass. The Higgs boson can decay to pairs of fermions as long as this is kinematically allowed. Among all of such decays, $H \rightarrow b\bar{b}$ has the largest branching ratio. The decay width of $H \rightarrow b\bar{b}$ is:

$$\Gamma(H \rightarrow b\bar{b}) = \frac{3m_b^2 m_H}{8\pi v^2} \quad (2.25)$$

The branching ratio related to a certain decay mode "i" is defined as:

$$\text{BR}_i = \frac{\Gamma_i}{\sum_k \Gamma_k} \quad (2.26)$$

Decay mode	Branching ratio
$H \rightarrow bb$	57.8%
$H \rightarrow WW^*$	21.6%
$H \rightarrow \tau^+\tau^-$	6.4%
$H \rightarrow gg$	8.6%
$H \rightarrow cc$	2.9%
$H \rightarrow ZZ^*$	2.7%
$H \rightarrow \gamma\gamma$	0.2%

Table 2.1: Branching ratio of Higgs boson predicted by Standard Model [20] [19], assuming an m_H mass corresponding to the measured value.

While the $H \rightarrow bb$ decay mode is the primary tool to determine the Higgs boson coupling to b-quarks, a modification of this coupling would also result in significant modification of other branching ratios, because of the large impact on the total Higgs boson width. The branching ratio Higgs boson of major decay modes are listed in Table 2.1.

2.3 Higgs boson with high transverse momentum

The latest Higgs combination result from ATLAS[21] and CMS[22] shows that the Higgs cross-section measurement at transverse momentum below 400 GeV are so far consistent with Standard Model predictions. However, there is still a chance that the cross-section of Higgs boson decays especially at high transverse momentum deviate from Standard Model prediction. Therefore, the measurement of $H \rightarrow bb$ decay in the high transverse momentum region described in section 5 of this thesis is an important part of the $H \rightarrow bb$ analysis. This is also related to the estimation of b-jet identification uncertainties described in section 4.3. Many beyond Standard Model (BSM) theories have been developed and several have deviation from Standard Model at high-transverse momentum. In order to probe such potential deviations, it is highly beneficial to develop a general theory framework including additional freedom for BSM theories and also including some of our Standard Model theory knowledge at the same time. A framework called standard model effective field theory (SMEFT) is developed [23],[24],[25]. It assumes new physics are at a higher scale than the measurement and it is a consistent theory which represents an

extension to the Standard Model. The Lagrangian of SMEFT is:

$$\mathcal{L} = \mathcal{L}_{SM} + \sum \frac{c_i}{\Lambda^2} O_i^{d=6} + \sum \frac{c_i}{\Lambda^4} O_i^{d=8}, \quad (2.27)$$

where the first term on the right hand side is standard model Lagrangian and the terms that follow are corrections to the SM providing BSM effects. The Λ is energy scale of new physics, O_i^d are d dimension operators. The c_i is Wilson coefficients. The first correction term is suppressed by $\frac{1}{\Lambda^2}$ therefore the BSM effect has an order of $O(\frac{p_T^2}{\Lambda^2})$ and, although suppressed, it will become larger at high transverse momentum, thus making this kinematic region particularly sensitive to BSM physics.

2.4 Higgs boson search at the LHC

2.4.1 Higgs discovery

The Higgs boson was discovered in 2012 by ATLAS [13] and CMS [14] with Run-1 data. The analysis involves multiple decay channels of the Higgs boson such as $H \rightarrow \gamma\gamma$, $H \rightarrow ZZ^*$, $H \rightarrow WW^*$, $H \rightarrow \tau^+\tau^-$ and $H \rightarrow b\bar{b}$. There are large QCD background with multi-jet final states produced by the LHC. Therefore the signal with hadronic final state is more difficult to extract and the most sensitive channels are $H \rightarrow \gamma\gamma$ and $H \rightarrow ZZ^* \rightarrow 4l$. Figure 2.3 shows the result from $H \rightarrow \gamma\gamma$ analysis in ATLAS and $H \rightarrow ZZ \rightarrow 4l$ analysis in CMS. The measured combine significance was 5.9σ in ATLAS [13] and 5.0σ in CMS [14]. The Higgs mass was measured to be $m_H = 126.0 \pm 0.6$ GeV in ATLAS [13] and $m_H = 125.3 \pm 0.6$ GeV in CMS [14]. In 2015, the combined measurement using Run-1 data from ATLAS and CMS was published to be [26]:

$$m_H \simeq 125.09 \pm 0.21(\text{stat}) \pm 0.11(\text{syst})\text{GeV} = 125.09 \pm 0.24(\text{tot})\text{GeV} \quad (2.28)$$

2.4.2 Higgs coupling to bottom quarks

Among various decay modes of the Higgs boson, $H \rightarrow b\bar{b}$ is expected to have the largest branching ratio according to the Standard Model(SM), therefore it is one of the best channels to test for the deviation from SM prediction. However, the large multi-jet background at the LHC make this decay channel hard to be observed. The Higgs production mode VH is the best production channel to observe the $H \rightarrow b\bar{b}$ process since the associated vector boson could

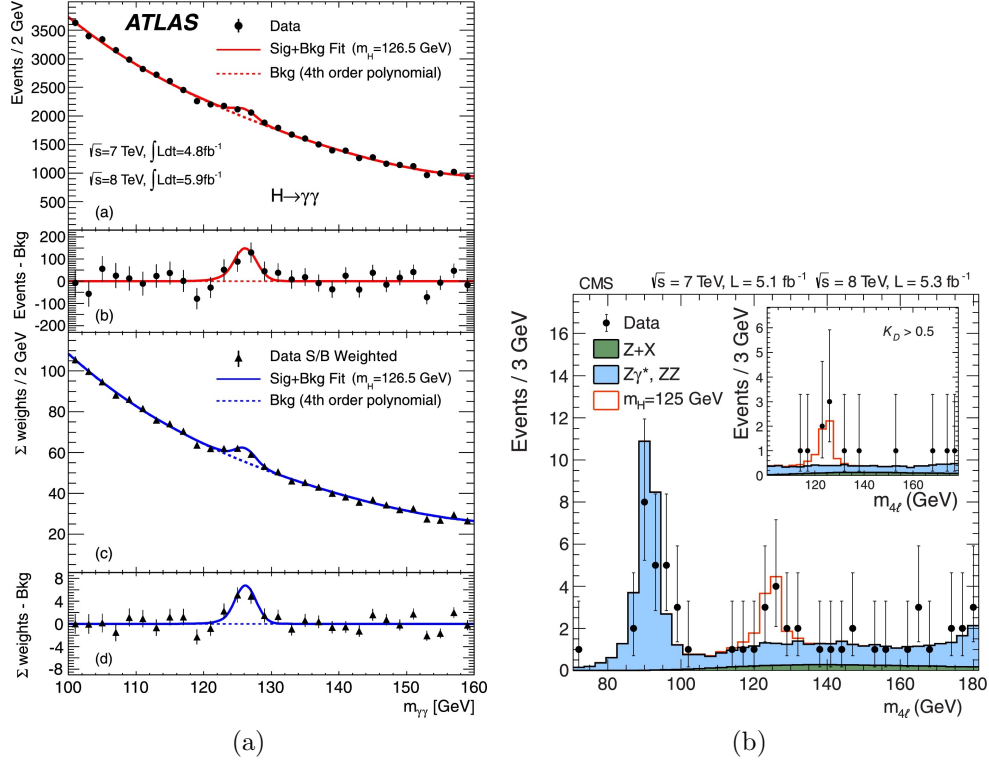


Figure 2.3: Figure (a) shows $m_{\gamma\gamma}$ distribution in ATLAS $H \rightarrow \gamma\gamma$ analysis. The solid line shows the expected distribution of signal and background events. Figure (b) shows m_{4l} distribution in CMS $H \rightarrow ZZ^* \rightarrow 4L$ analysis. The blue shows the expected background of $Z\gamma^*$ and ZZ . The red shows the expected distribution from Higgs boson decay.

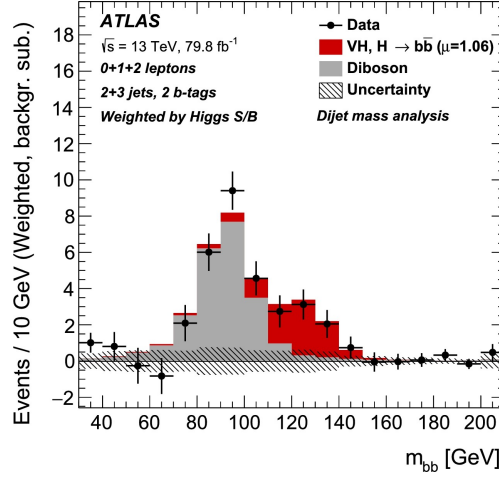


Figure 2.4: Figure shows the m_{bb} distribution after subtracting all background except diboson processes in $VH, H \rightarrow bb$ analysis. All events in all analysis regions are summed up and weighted by S/B, where S is fitted signal events and B is fitted background events.[2]

decay into leptons, which provide a clean signature for triggering and selecting the $VH, H \rightarrow bb$ signal events. The Higgs boson decay mode $H \rightarrow bb$ was observed in the VH production channel in 2018 [2]. The observed significance was 4.9σ [2]. The result of combined Run-I and Run-II analysis yields an significance of 5.4σ [2]. The ratio of measured and expected event yield was $1.01 \pm 0.12(\text{stat.})^{+0.16}_{-0.15}(\text{syst.})$.

The result was further improved in the analysis published in 2021[27]. The new result observed significance of 4.0 and 5.3 for WH and ZH production channel. The thesis work on $H \rightarrow bb$ described in Chapter 5 are about improvements on this latest $VH, H \rightarrow bb$ analysis [27].

Chapter 3

Large Hadron Collider and ATLAS detector

3.1 Large Hadron Collider

The Large Hadron Collider (LHC) is now the largest particle collider ever. It was built by European Organization for Nuclear Research (CERN) on the France-Switzerland border near Geneva. The length of the whole tunnel is 27km. The center of mass energy of particle collision at the LHC is 13.6 TeV, one order of magnitude larger than its predecessor Tevatron. The large center of mass energy and high luminosity at the LHC enable the discovery of Higgs boson. Apart from colliding proton beams, it can also collide heavy nuclei (Pb-Pb collision).

After some initial acceleration stages, the particle beams are accelerated in the Super Proton Synchrotron (SPS). Then they are accelerated in the 27km-long LHC ring until the particles in the beam reach 6.8 TeV energy (after about 28 mins). At that point, the speed of the beams reaches $0.999999990c$, then the two beams of particles collide in the center of the four LHC detectors (ATLAS, CMS, LHCb, ALICE) with center of mass energy of 13.6 TeV. Although it requires more efforts to collide two beams head-on, the collider design provides higher center of mass energy than fixed target apparatus [28].

3.1.1 Luminosity

Discoveries in high energy physics experiments not only rely on the center of mass energy, but they often require a high number of events giving high statistical power to make the result significant enough over the backgrounds in order to claim discovery. The number of expected events depends on the

luminosity of the collider as described below:

$$N_{events} = L \times \sigma, \quad (3.1)$$

where L is the instantaneous luminosity and σ is the cross section of a certain process only depending on the underlying physics. Therefore, higher luminosity gives a higher number of events. High luminosity is essential for rare events such as Higgs boson production. The luminosity can be expressed as:

$$L = \frac{f_r \gamma N_b^2 n}{4\pi \epsilon_n \beta^*} R \quad (3.2)$$

where f_r is the revolution frequency, γ is the relativistic gamma factor, N_b is the number of particles per bunch, n is the number of bunches per beam, ϵ_n is the normalized transverse emittance and β^* is the beta function at the collision point. R is the luminosity geometrical reduction factor from the crossing angle which can be further expressed by:

$$R = 1/\sqrt{1 + \frac{\theta_c \sigma_z}{2\sigma^*}} \quad (3.3)$$

where θ_c is the crossing angle at the interaction point, σ_z is the rms bunch length and σ^* is the rms transverse beam size at crossing point [28].

This thesis work focuses on analysing data collected from 2015 to 2018 (ATLAS Run 2). The cumulative luminosity versus time is shown in Figure 3.1. The overall luminosity in Run 2 is 139 fb^{-1} .

3.1.2 Detectors at the LHC

The LHC has four experimental detectors each located at one interaction point where two particle beams traveling in opposite directions collide. Two of the four detectors are general purpose detector: ATLAS (A Toroidal LHC Apparatus) and CMS (Compact Muon Solenoid). The other two are ALICE (A Large Ion Collider Experiment) and LHCb (Large Hadron Collider beauty). The location of the four detectors are illustrated in figure 3.2.

- ATLAS is one of the two general purpose detectors at the LHC. When LHC is operating, beam traveling from opposite directions collide at the center of the ATLAS detector. The final state particles go through detector of multiple layers covering almost the full solid angle. The particles' energy and path can be measured and the magnet system in the ATLAS detector produces strong magnetic fields which make it also

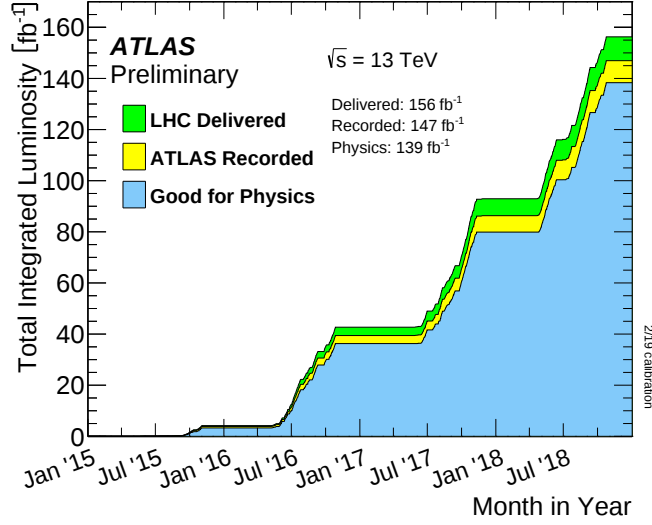


Figure 3.1: Cumulative luminosity versus time delivered to ATLAS (green), recorded by ATLAS (yellow, and certified to be good quality data (blue) during stable beams for pp collisions at 13 TeV center-of-mass energy in 2015-2018 (ATLAS Run 2). [3]

possible to measure the momentum of charged particles. With these measuring abilities, ATLAS can be used to detect the remnants of rare particles such as Higgs boson and to search for extra dimensions and explore undiscovered particles which could be dark matter. The size of the ATLAS detector is 46 m long, 25 m high and 25 m wide and overall weight of 7,000 tonne which makes it the largest volume particle detector built around the world.

- CMS is also one of the two general purpose detectors located at the one of the interaction points in the LHC ring. Similarly to ATLAS, it can also detect rare particles such as Higgs bosons, search for extra dimensions and search for dark matter candidate particles, but it has a different technical design compared to the ATLAS detector, built with a single huge solenoid magnet around it which can produce a strong magnetic field for measuring the final state charged particles' momentum. The CMS detector is 21 m long, 15 m wide and 15 m high, with an overall weight of 14,000 tonne. It is the heaviest one among the four detectors at the LHC.
- ALICE is a detector for research on the quark-gluon plasma which has high energy densities. Differently from ATLAS and CMS, which are

mostly designed to analyse pp collisions, ALICE is designed to analyse collisions of lead ions that produce strongly interacting quark-gluon plasma. This quark-gluon plasma in the extreme condition is similar to what happened right after the big bang and is a good source for understanding the color confinement of quarks and gluons. Here the color confinement means no isolated quarks and gluon can exist in our universe. With the ALICE detector, scientists can study how quarks and gluons becomes colorless particles through cooling down. The ALICE detector is 26m long, 16 m high and 16 m wide and has an overall weight of 10,000 tonne.

- LHCb is a particle detector mainly for research on b -quarks. Unlike fully enclosed detectors such as ATLAS and CMS, the LHCb detector is mostly focusing on detecting forward particles which travel in the direction close to the beam line, where the b -quark production cross section is highest. The detectors extend layer by layer in the beam line direction for 20 meters. In the collisions, other flavors of quarks are also produced, therefore it is important to distinguish them from b -quarks. A movable tracking detector provides more information for identifying b -quarks from the others. The size of LHCb is 21 m long, 10 m high and 13 m wide, with an overall weight of 5,600 tonne.

3.2 ATLAS detector

3.2.1 Detector overview

The same coordinate system is used in all physics analyses in ATLAS [6]. Therefore it is useful to introduce it from the beginning. The z axis is defined to be in the beam line of counter-clockwise direction. The x - y plane is transverse to the z axis: the y axis is pointing upward and the x axis is pointing to the center of the LHC ring. The azimuthal angle ϕ is around the z axis. The polar angle θ is measured from the z axis. The rapidity is defined by $y = 1/2 \ln[(E + p_z)/(E - p_z)]$. If particle is massless, pseudo-rapidity is equivalent to rapidity as defined by $\eta = -\ln \tan(\theta/2)$. The transverse momentum p_T , transverse energy E_T and missing transverse energy E_T^{miss} are all defined in the direction in the x - y plane. The angle ΔR is defined by $\Delta R = \sqrt{\Delta\eta^2 + \Delta\phi^2}$.

The overall view of the ATLAS detector and all major components are pointed out and shown in Figure 3.4. In general, the ATLAS detector is symmetric in the beam line direction. The innermost part of the detector is the inner tracking detector (ID) surrounded by a Solenoid magnet. Three

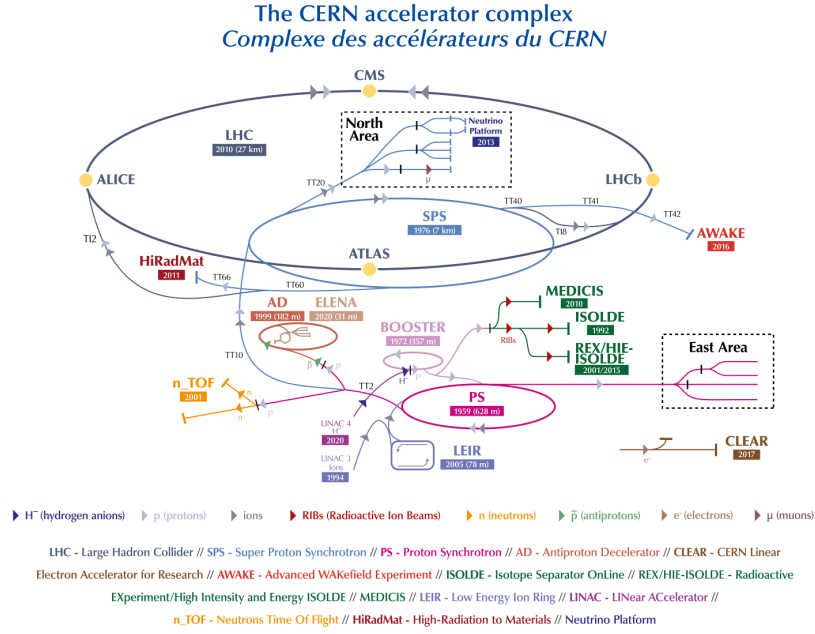


Figure 3.2: The locations of detectors in the LHC ring. [4]

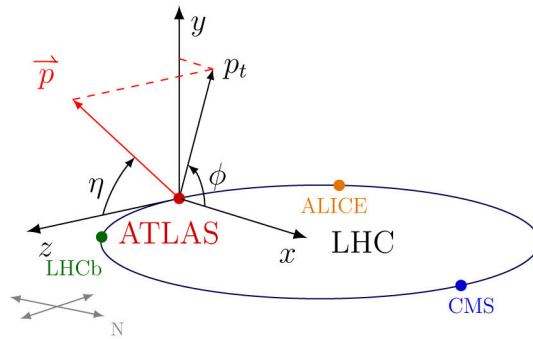


Figure 3.3: The coordinate system used in ATLAS detector.[5]

systems of Toroid magnets, one barrel and two end-caps, are built surrounding the calorimeter.

The magnetic field in the inner detector is 2T provided by a superconducting solenoid. The inner detector mainly consist of an inner part and an outer part. The inner part is a high resolution pixel and strip silicon detector. It allows for high precision momentum measurements, particle identification and vertex detection in high particle fluxes environment. The outer part is a straw detector which also helps refining the particle trajectory measurements and can also detect transition radiation, which contributes to electron identification.

The calorimeter consists of liquid-argon(LAr) electromagnetic calorimeter in the inner part and scintillator-tile hadronic calorimeter in the outer part. The electromagnetic calorimeter has high granularity and covers an angle of $|\eta| < 3.2$. The hadronic calorimeter, including the central barrel and two extended barrels, has a coverage of $|\eta| < 1.7$.

The muon spectrometer surrounds the calorimeter. Toroid magnets are inside this system, and provide a high magnetic field. Together with the three layers of muon tracking chambers, they allow to precisely measure muon tracks.

The LHC bunch crossing rate is around 40MHz. However, not all the events are interesting physics-wise and it is anyway impossible to record all data onto the disc/tape with this high frequency. Therefore a trigger system is in place to filter out uninteresting events on the fly. There are two levels of trigger, Level-1 (L1) and Level-2 (L2). Before ATLAS Run-2, L1 trigger was upgraded so that it could reduce the event rate from 40MHz to 100kHz. L2 further reduces the event rate down to a few hundred Hz. [29]

3.2.2 Inner Detector(ID) Tracking system

The Inner Detector (ID) is used to record track information of charged particles coming from particle collisions. The particle track density is exceptionally high in ATLAS, making it crucial to have fine detector granularity in order to accurately measure track momentum and vertex. The Pixel detector with the newly installed insertable B-layer (IBL), Semiconductor Tracker (SCT) and Transition Radiation Tracker (TRT) can make this high precision measurement possible. The layout of ID including the four components are shown in Figure 3.5. The track momentum measurement precision from ID is complemented by the measurement precision from electromagnetic calorimeter.

Pixel Detector

The Inner Detector consists of multiple elements, with the Pixel Detector [8] positioned as its innermost subsystem. The longitudinal angle covered by the

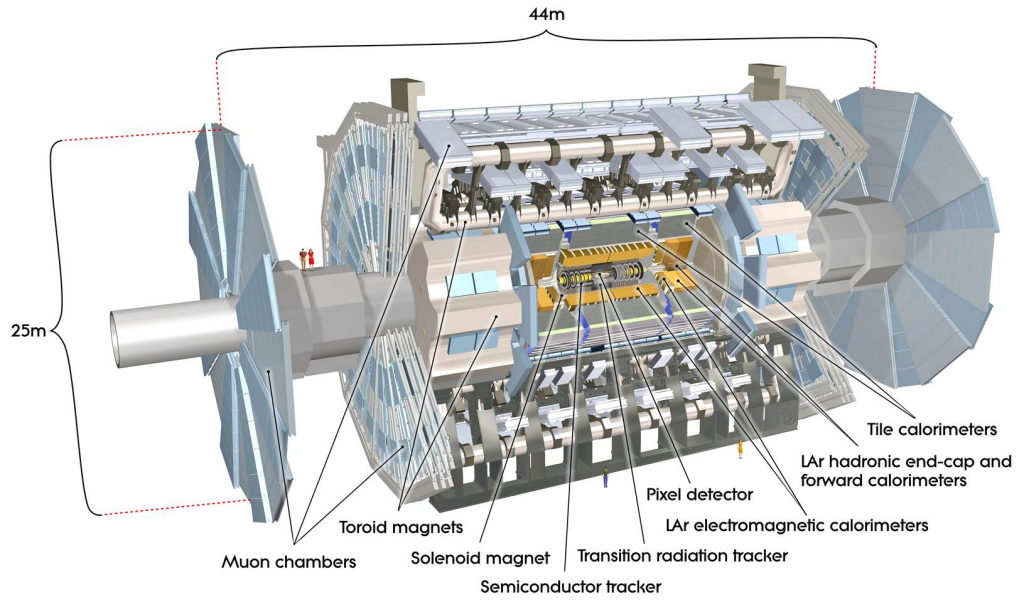


Figure 3.4: Overall layout of the ATLAS detector.[6]

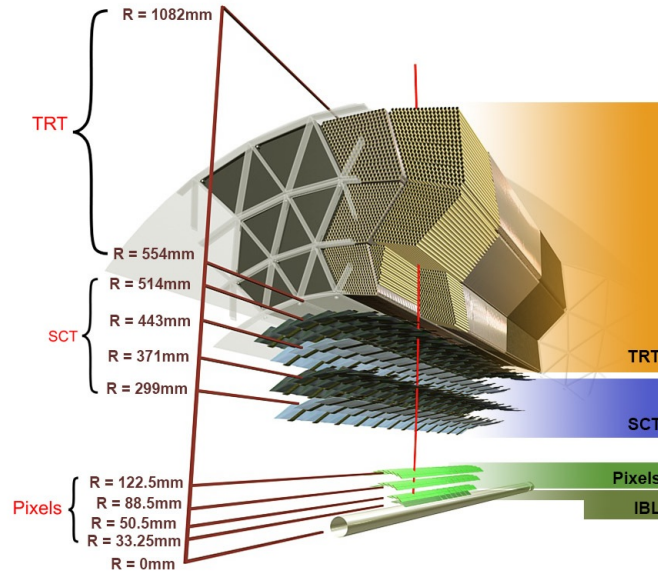


Figure 3.5: Inner detector of.[7]

Pixel detector is $|\eta| < 2.5$. The most inner layer of pixel detector is the Insertable B-layer [30]. It is a new layer of pixel detector that was installed after Run-I between the beam pipe and the B-Layer, the previous closest detector layer to the beam line. The installation was done during the LS1 shutdown just before Run-2. The motivation of the IBL is to provide additional accuracy and robustness to the tracking system given that the readout bandwidth of the B-layer is limited in high luminosity environment and also the front end electronics of the tracking system are damaged by high exposure to radiation. The expected operation time of IBL is until the end of Phase-I, before the HL-LHC (high luminosity LHC) upgrade.

The IBL consists of 14 carbon staves installed 33.25mm from the beam line and is built around the new beam pipe of radius 23.5mm. The longitudinal coverage of IBL is $|\eta| < 3$. Each carbon stave has 20 pixel sensor modules and each of them is connected to a read-out channel. Each pixel in the IBL has a size of $250\mu m$ in the longitudinal direction and $50\mu m$ in the ϕ direction, resulting in IBL's high granularity. All modules are glued onto the stave with a separation of just $200\mu m$ to minimize the dead region.

On the outside of the IBL, there are three barrel layers. Three endcap disc layers are installed on each side of the barrel. The configuration is shown in Figure 3.6. The pixel detector consists of modules of silicon sensors. The size of the smallest detecting unit is one pixel and the nominal pixel size is $50\mu m$ in ϕ direction and $400\mu m$ in the longitudinal direction. Each module consists of 46,080 pixels. There are in total around 67 million pixel electronics channels for the three layers of barrel and around 13 million channels in the 6 endcap disc. All of the modules are mounted on the stave, which is used to support and cool the modules. Each stave consists of 13 modules. The total length of active region of one stave is about 801 mm. The stave are mounted to half shell. Each barrel layer consists of two half shells.

The tracking system is used for reconstructing charged particles' trajectories therefore it is crucial in flavor tagging, which is an important part of this thesis work and is introduced in section 4.1. Since IBL can provide an additional high precision hit information of the particle closer to the beam line, with this information, the track can be extrapolated more accurately to the interaction point during track reconstruction, allowing for a more precise vertex location. This is especially helpful for low- p_T particles, since they are subject to more multiple scattering and an additional detector layer closer to the interaction point can significantly mitigate this effect. The high granularity of IBL is helpful for improving the resolution in the longitudinal (z_0) and transverse (d_0) projection of the impact parameter. As a consequence, additional information from the IBL improves the primary and secondary vertex

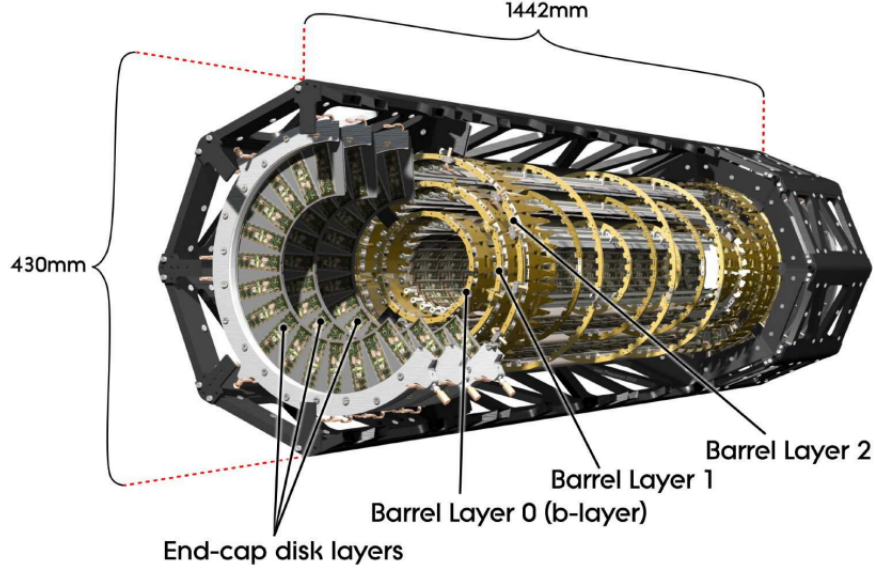


Figure 3.6: Pixel Detector [8]

reconstruction and resolution. The secondary vertex resolution is a crucial factor impacting flavor tagging performance. The light-jet (c-jet) rejection was improved by up to 4 (1.8) and the b-jet efficiency was improved by up to 85% after the addition of the IBL. [30]

SemiConductor Tracker(SCT)

The SemiConductor Tracker [9] is installed in between the Pixel Detector and the Transition Radiation Tracker (TRT). The SCT consists of 4088 modules of silicon-strip sensors. Also, it consists of four barrels and two endcaps. Each endcap has 9 disks as shown in Figure 3.7. The average hit efficiency of SCT modules is $99.74 \pm 0.04\%$. Each disk or barrel gives two strip measurements, which can then be combined to give a single space point measurement. The design of the layout of barrels and endcaps is such that each particle originating in the beam-interaction region has at least eight strip measurements (equivalent to four space-points) from the SCT. Each module of the SCT consists of four silicon-strip sensors. Identical sets of sensors are glued back to back with an angle of 40 mrad in order to provide a transpassing particle's space point. Each endcap has three rings of modules. The strip sensors are placed in the radial direction in the endcap rings. All sensors are $285 \mu\text{m}$ thick.

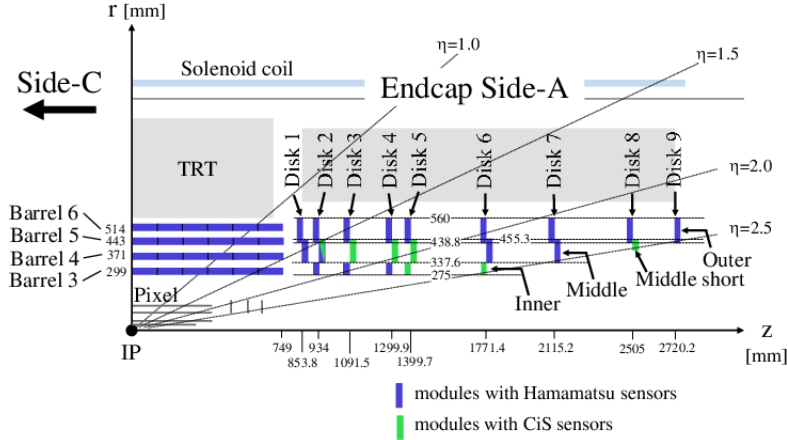


Figure 3.7: Inner Detector SemiConductor Tracker [9].

Transition Radiation Tracker(TRT)

The Transition Radiation Tracker(TRT)[31] is a straw tube detector. It consists of 4 mm diameter straw tubes. Inside each tube, there is a $31 \mu\text{m}$ gold-plated tungsten wire. During operation, the wall of the tube is on voltage of 1.5kV, while the wire inside is grounded. The tube is filled with a gas mixture of 70% Xe, 27% CO₂ and 3% O₂. When a particle transpasses a tube, it ionizes the gas mixture inside the tube and the resulting electrons will move towards the tungsten wire due to the electric field between the high voltage wall and the wire. Once they hit the wire, they produce an electric signal, which is read by both ends of the tube as a signal of the particle passing by. The maximum readout rate of the TRT is 100kHz.

There are in total 52,544 straws in the barrel region covering the area of radius 0.5 to 1.1m and the longitudinal angle $|\eta| < 1$. The straws are aligned parallel to the beam axis. There are 122,880 straws in the endcap regions covering $0.8\text{m} < |Z| < 2.7\text{m}$ and $1 < |\eta| < 2$, each one with a length of 0.4 m. The straws are aligned perpendicular to the beam line axis.

The space between straws is filled with polymer fibers in the barrel region and foils in the endcap region. When highly relativistic particles travel across a material boundary, they will create transition radiation and this effect depends on the relativistic factor $\gamma = E/m$. Therefore transition radiation is helpful to identify light particles such electrons.

The design of the TRT makes it complementary to the Pixel and SCT detector. Although the single point resolution of the TRT is $120 \mu\text{m}$, larger than silicon trackers, the TRT usually has much more hits than the silicon tracker, typically 30 hits per track. partially compensating for the lower resolution.

The TRT reaches large radii providing a longer lever arm that is particularly important for measuring the track momentum.

3.2.3 Calorimeter

The ATLAS calorimetry system utilizes various techniques in different parts. The ATLAS calorimeter consists of two main parts, an electromagnetic calorimeter which is used to measure the energy of photons and electrons and a hadronic calorimeter which is used to measure the energy of hadrons. The schematic of the ATLAS calorimeter is shown in Figure 3.8. The system in total covers a large range of $|\eta| < 4.9$. The coverage is larger than the inner detector which has $|\eta| < 2.5$ coverage. The granularity is fine enough for precise measurements of electrons and photons calorimeter regions where the $|\eta|$ matches the inner detector. In the other region of the calorimeter, the granularity is coarser but it is sufficient for jet reconstruction and measuring E_T^{miss} . The calorimeter needs to be thick enough to yield a precise measurement on the particle energy and to limit particles (except muons) from leaking into muon spectrometer. The electromagnetic calorimeter thickness is >22 radiation lengths in the barrel and >24 radiation lengths in the endcap. The radiation length is defined as the amount of matter traversed by high energy particles where they will lose energy by bremsstrahlung and e^+e^- pair production [15] by roughly a factor $1/e$. Together with the large coverage of the calorimetry system of η , the calorimetry system provide precise measurement on η , which is crucial for some physics analyses such as searches for supersymmetric particles.

Electromagnetic calorimeter

The electromagnetic calorimeter is a lead-Liquid Argon(LAr) scintillating detector. The detector is interleaved with lead plates and liquid argon. To make argon liquid, the temperature is cooled down to $-174^\circ C$. The lead is used as absorber and LAr is used as ionization medium. Absorbers and scintillators are installed interleaved. The thickness of lead is optimized to give the best energy resolution in η . When the calorimeter is operational, the absorber lets the high-energy particle traveling through shower into low energy particles. Then these particles travel further into the LAr section and ionise the LAr. Electrons and photons are produced during this process, and because of the high voltage electrons/ions drift towards the electrodes producing electric signals and that can be measured to get the energy lost by the particle traveling through. The calorimeter consists of two parts, a barrel part covering the region $|\eta| < 1.475$, and an endcap part covering the region $1.375 < |\eta| < 3.2$. The barrel consists of two half barrels, which are connected at position $z=0$,

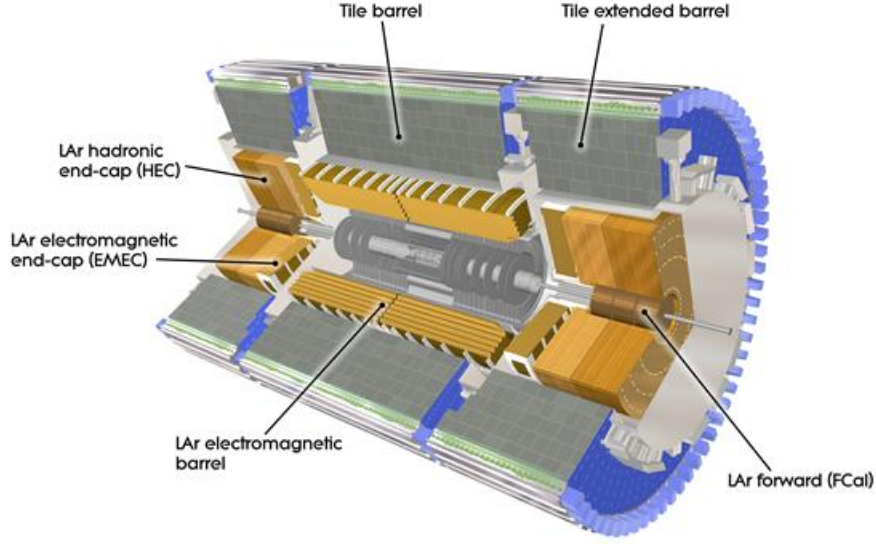


Figure 3.8: ATLAS calorimeter system [6].

except for a separation of 4mm. The endcap consists of two coaxial wheels. The inner wheel covers the region $1.375 < |\eta| < 2.5$, the outer wheel covers the region $2.5 < |\eta| < 3.2$. Both the barrel and endcap are divided into three longitudinal layers in $|\eta| < 2.5$ as shown in Figure 3.9. The cell size of the first layer is 0.003125 in $|\eta|$. The second layer absorb most of the energy of particles so it has fine granularity in η and ϕ . The cell size is $\Delta\eta \times \Delta\phi = 0.025 \times 0.025$. The third layer mostly collects the tails of the electromagnetic shower and therefore is coarsely segmented in η .

The resolution of the calorimeter can be expressed as:

$$\frac{\sigma_E}{E} = \frac{a}{\sqrt{E}} \oplus \frac{b}{E} \oplus c, \quad (3.4)$$

where for the ATLAS electromagnetic calorimeter, a is a stochastic term of $10\%\sqrt{GeV}$, b is a noise term around 200 MeV and c is a constant term around 0.2%.

The uniformity is measured to be 0.5% in barrel region and 0.6% in endcap.

Hadronic calorimeter

The Tile Calorimeter [6] is installed outside the electromagnetic calorimeter in the barrel region. The barrel of the Tile Calorimeter covers the region $|\eta| < 1.0$. The extended barrel covers the region $0.8 < |\eta| < 1.7$. The Tile Calorimeter

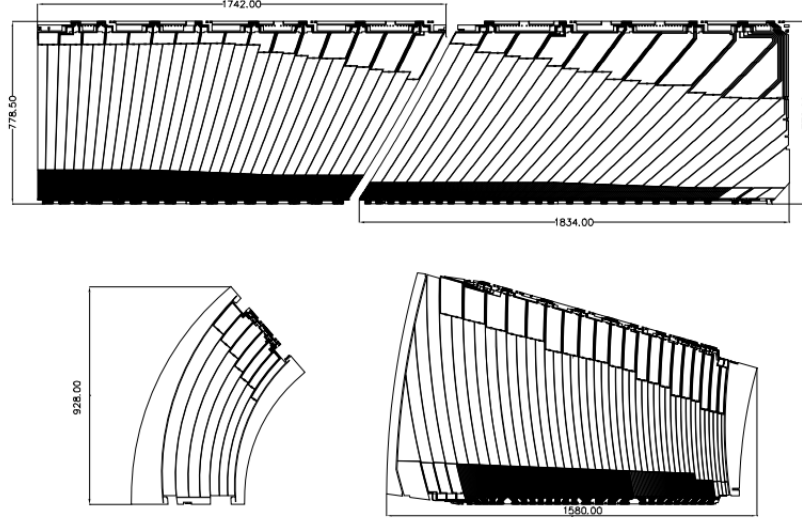


Figure 3.9: Electromagnetic calorimeter layout of three layers in barrel (top), endcap inner (bottom left) and outer (bottom right) wheels. [6]

is built with steel as absorber and scintillating tiles as active material. The inner radius of the Tile Calorimeter is 2.28m while the outer radius is 4.25m. The detector consists of three layers, each of them has thickness of 1.5, 4.1 and 1.8 hadronic interaction lengths(λ) in barrel and 1.5, 2.6 and 3.3 λ in the extended barrel. Here the interaction length is defined as the mean distance the hadron can travel before having an inelastic nuclear interaction with the calorimeter material. The total thickness of the Tile Calorimeter is 9.6 λ at $\eta = 0$. The Tile Calorimeter is the heaviest part of the ATLAS experiment weighing about 2900 tonne. For ATLAS Run-2 data, the jet energy resolution is measured to be smaller than 10% for jets with energy above 100 GeV [32].

The LAr hadronic end-cap Calorimeter (HEC) [6] is installed right behind the electromagnetic calorimeter endcap. There are two wheels for each endcap. The HEC is designed to cover the range of $1.5 < |\eta| < 3.2$ so that it overlaps with the Tile Calorimeter at smaller $|\eta|$ and with the Forward Calorimeter at higher $|\eta|$, in order to prevent material density drop in the connection region. The calorimeter uses copper plate as absorber, installed interleaved with a 8.5mm gap filled with LAr which is used as active material.

The LAr Forward Calorimeter (FCal)[6] is located in the center of the wheels of electromagnetic calorimeter and HEC endcap. However, the inner face of FCal doesn't line up with the inner face of the electromagnetic calorimeter endcap and is more to the outside direction to prevent neutron albedo in the inner detector. Therefore the FCal density must be high in order to stop

forward hadrons in shorter depth corresponding to about 10λ .

3.2.4 Muon System

The layout of the ATLAS Muon System [6, 33] is shown in Figure 3.10. The magnetic field from the large superconducting air core toroid magnet provides bending power for particles' tracks. The toroid consists of three parts, two endcap toroids covering the region $1.6 < |\eta| < 2.7$ and one barrel toroid covering the region $|\eta| < 1.4$. The endcap toroids line up with the barrel toroid on both sides of the ATLAS detector. Each toroid set consists of eight large superconducting coils uniformly distributed in the cylindrical layer around the beam axis. The magnetic field provided by the endcap toroids ($1.6 < |\eta| < 2.7$) and barrel toroid ($|\eta| < 1.4$) are between 2 to 5 Tm, and varies depending on azimuth angle. The magnetic field is weaker in the transition region $1.4 < |\eta| < 1.6$. The muon momentum is measured based on the muon track curvature. The muon track is measured by three stations installed in the toroid.

The three stations each occupy one cylindrical layer around the beam axis and are equipped by Monitored Drift Tubes (MDT). Each station can measure the muon position with a precision of $50 \mu m$. The Monitored Drift Tubes are aligned and form multiple layers, then put into chambers. The MDTs are filled with 93% Ar, 7% CO₂ at 3 bar pressure. The high pressure provides better spatial resolution for high p_T particles. Similar to the TRT in the inner detector, the Monitored Drift Tubes also contain a high voltage wire (3.1kV) inside each tube, so when a muon goes accross the gas in the tube, gas is ionized and charged particles are attracted to the wire creating an electric signal. The signal is then processed for measuring the position of the muon.

The outer two stations both have Resistive Plate Chambers (RPC) equipped, used for trigger. The outer layer has one RPC for high p_T ($p_T > 20$ GeV) trigger and the middle layer has two RPC for low p_T ($p_T > 6$ GeV) trigger. The RPC is constructed with two resistive plate with separation of 2mm. High volatege is applied through Graphite electrodes on the plate. A gas mixture of 94.7% C₂H₂F₄, 5% C₄H₁₀ and 0.3% SF₆ is filled in between the two plates. When muons fly through the RPC ionizing the gas, charged particles will be traveling under 5 kV/mm electric field to the plates generating electric signals for triggering. The typical space-time resolution is $1cm \times 1ns$.

In the endcap region, MDTs are also employed across three stations installed at each side of the endcap. Each station is mounted to a big disk installed perpendicular to the beam axis. Endcap use Thin Gap Chambers (TGC) as different technical design for trigger. The TGC is a multiwire proportional chamber filled with a gas mixture of 55% CO₂, 45% n-pentane. The

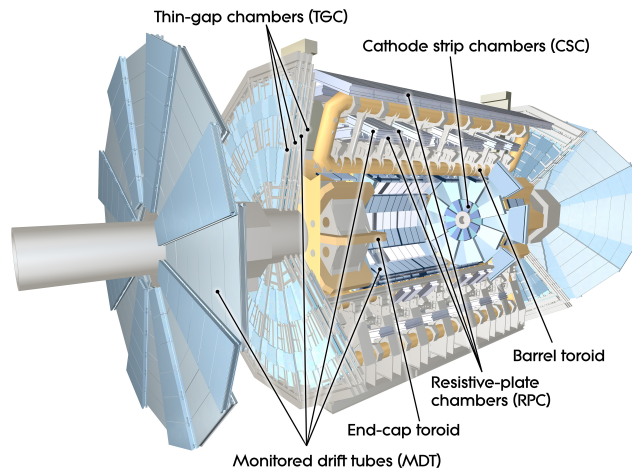


Figure 3.10: Schematic of the ATLAS Muons subsystem. [6]

efficiency of the chambers is tested to be 99.9% when operating offline using muon beams.

Chapter 4

Flavor tagging

4.1 Flavor tagging basics

The identification of jets containing b -hadrons against c - and *light*-flavored jets is a core element of many physics analyses in ATLAS, such as the study of Higgs boson decays into a pair of b -quarks produced in association with a vector boson (also referred to as $VH, H \rightarrow b\bar{b}$ in this thesis in Chapter 5) [34]. The sequence of algorithms used to identify these jets is known as b -tagging. The procedure is based on multivariate algorithms relying on specific kinematic properties of the b -hadron decays (i.e. long lifetime, high mass, high decay multiplicity); more details can be found in Ref. [35]. The b -tagging algorithms are applied independently on each jet in the event. In particular, the performance of a b -tagging algorithm is quantified by its probability to tag a real b -jet, also referred to as b -tagging efficiency ϵ_b , against the probability to wrongly tag (mis-identify) c - and *light*-flavored jets as b -jets, defined as ϵ_c and ϵ_{light} respectively.

The flavor-tagging-efficiency ϵ_f for a given jet flavor f is defined as the probability for such jets to be b -tagged. It is estimated using

$$\epsilon_f = \frac{N_f^{b\text{-tag}}}{N_f}, \quad (4.1)$$

where $N_f^{b\text{-tag}}$ is the number of b -tagged jets of flavor f , and N_f is the total number of jets of flavor f . The rejection is defined as $1/\epsilon_f$ [10]. The efficiency is usually parameterized as a function of the transverse momentum p_T of the tagged jet. For simplicity, this is the only kinematic variable used in this thesis but the method can be easily extended to multiple kinematic dependencies (e.g. η). In case of multiple kinematic dependencies, the N-

dimensions can be mapped into a 1-dimensional index identifying a specific bin in the N -dimensional space. The efficiencies are measured in data in well defined control samples ($\epsilon_{\text{data}}(p_T)$), and compared to the corresponding efficiencies predicted by the Monte Carlo (MC) simulation ($\epsilon_{\text{MC}}(p_T)$)¹. The MC efficiency is calibrated to match the efficiency in data using dedicated calibration analyses described for example in Ref. [10]. Scale factors (SF) are derived as ratios of efficiencies in data and simulation. In particular, the scale factors are measured separately for each flavor and in bins of jet transverse momentum (and jet pseudorapidity for *light*-jets) for each combination of algorithm and working point. The working point is defined as a particular threshold of the b -tagging output discriminant above which the jet is considered as b -tagged. It can be tuned to yield a tighter or looser selection based on the b -jet tagging efficiency. Currently working points are defined corresponding to b -jet tagging efficiencies of roughly 85%, 77%, 70% and 60%, as determined inclusively on a Monte Carlo sample of $t\bar{t}$ events before any data-based calibration is applied. Different methods are used to calibrate the tagging efficiencies of b -, c - and *light*-flavored jets [36] [37]. The resulting scale factors are applied, jet-by-jet, as multiplicative event weights to any simulated physics sample where b -tagging is applied during event reconstruction and selection. The scale factors are defined as:

$$\text{SF}(p_T) = \frac{\epsilon_{\text{data}}}{\epsilon_{\text{MC}}}(p_T) \quad (4.2)$$

In case of discrete p_T bins, the SF becomes:

$$\text{SF}_i = \frac{\epsilon_{\text{data},i}}{\epsilon_{\text{MC},i}} \quad (4.3)$$

where i is the index of the p_T bins, $i \in \{1, \dots, N\}$, and N is the total number of p_T bins. For every b -tagged jet passing the b -tagging requirement, the SF is applied directly as an event weight. In order to conserve the overall normalization – so $p(\text{tagged jet}) + p(\text{non-tagged jet}) = 1$ – for every b -tagged jet which does not pass b -tagging requirement (non-tagged jet), an inefficiency SF is applied:

$$\text{SF}_{\text{ineff}} = \frac{1 - \text{SF}(p_T) \cdot \epsilon_{\text{MC}}(p_T)}{1 - \epsilon_{\text{MC}}(p_T)}. \quad (4.4)$$

In many physics analyses, the distribution of the b -tagging output discriminant is different for the signal and the different backgrounds and can therefore be used to enhance the analysis sensitivity. In order to correctly use this binned distribution, rather than just the tagged/non-tagged binary in-

¹The MC efficiency estimates for each of the flavors is provided by the full simulation of the ATLAS detector based on Geant4.

formation, the distribution needs to be calibrated in each bin. The so-called "pseudo-continuous" calibration simultaneously calibrates a binned version of the continuous output values of the b -tagging discriminant, expressed in intervals of the b -tagging efficiency². It thus considers the dependence of the scale factors both on p_T and on the b -tagging score. This calibration gives more freedom to the analyses when developing their b -jet selection. For example, jets in the same event can be selected with b -tagging requirements corresponding to different efficiency working points to increase the signal over background ratio of the analysis. This is, however, a more complex procedure from the calibration point of view, as the scale factors are derived as a function of both jet kinematics and simultaneously for all b -tagging bins. In the pseudo-continuous case no inefficiency SFs are applied as the SFs are already extracted as a function of the binned b -tagging score, while simultaneously applying a constraint that the total number of jets of a given flavor in each jet p_T bin and across all b -tagging score bins must be preserved.

The total uncertainty on the scale factors is calculated considering both statistical and systematic uncertainties on the measured and simulated efficiencies entering in the calibration analyses. For example, about ~ 100 separate uncertainty sources are considered for the b -jet SFs. In this thesis, these uncertainties will be referred to as original b -tagging uncertainty sources.

4.2 Eigenvector Recomposition

4.2.1 Introduction to eigenvector recomposition

As described in section 4.2.2, an eigenvector decomposition method is used to reduce the number of flavor-tagging uncertainty components in the analyses while correctly preserving correlations across jet kinematic bins, and – for the pseudo-continuous WP calibration – also across b -tagging score bins. In brief, the set of original b -tagging uncertainty sources (~ 100 for b -jets) is decomposed and replaced by a smaller set of eigenvector uncertainties [10], which are then used in physics analyses. The eigenvectors are strictly related to the diagonalization of a specific covariance matrix, so when combining different analyses, the eigenvectors computed starting from different flavor-tagging setups (i.e. b -tagging algorithm, working point, jet collection) can not be directly correlated, since they correspond to different combinations of the same

²Concisely, each bin of the b -tagging output score distribution will be referred to as *b -tagging score bin* in the text.

sources of uncertainties. A similar procedure is also used in ATLAS to reduce the number of jet calibration uncertainties, as described in Ref. [38].

This section introduces a new method to correlate the b -tagging calibration uncertainties across analyses using different flavor-tagging setups. The method is encoded into a tool that takes the likelihood function of a given analysis as input, and replaces all the flavor-tagging related nuisance parameters corresponding to the eigenvector uncertainty components with new nuisance parameters corresponding to the complete set of *original* b -tagging uncertainty sources. In this way, the likelihood functions of multiple analyses can be easily re-expressed in terms of the same original b -tagging uncertainty sources, making their correlation possible. This is very useful for example in combination analyses, such as the combination of all Higgs boson measurements. An additional feature naturally emerging from this approach is the possibility to correlate the recomposed original uncertainty sources with the analogous uncertainties affecting the physics analyses. For example, the recomposed jet energy calibration uncertainty components from the flavor-tagging calibration could be correlated across different calibration setups but also with the same jet calibration components of the physics analyses being combined. This additional feature will not be further discussed in the text as it strongly depends on the meaning of the systematic uncertainties in the input analyses being combined. As an additional simplification, only b -jet uncertainties will be considered in the following sections of this thesis, but the method is applicable to other flavors as well.

In a similar context, a different technique has been developed in ATLAS in the jet energy scale (JES) calibration domain to allow for the correlation of the leading JES uncertainties across different experiments, jet types and data taking years [39], and a concrete application of this technique can be found in the context of the $H \rightarrow b\bar{b}$ analysis, as reported in Ref. [40].

Correlation of uncertainties between different b -tagging setups

In order to better understand the impact of the recomposition tool when combining multiple physics analyses, one important step consists in quantifying the level of correlation between the uncertainties coming from different b -tagging setups. The larger the correlations, the more the uncertainties need to be carefully treated in combination to avoid biases in the final result. As an example, this section focuses on quantifying the correlation of the total b -jet uncertainties between two analyses using the same tagger and working point, but different jet collections. This particular example uses Variable Radius (VR) track jets [41] and Particle Flow (PF) jets [42]. The correlation between uncertainties coming from different setups can be assessed through

the correlation matrix:

$$\rho_{ij} = \frac{\sum_{k=1}^M u_{ik}^{\text{PF}} \cdot u_{jk}^{\text{VR}}}{\sqrt{V_i^{\text{PF}} \cdot V_j^{\text{VR}}}} \quad (4.5)$$

where the indices i, j are the kinematic bin indices of the two flavor-tagging setups, k is the index running over the original b -tagging uncertainty sources and u_{ik}^{PF} is the effect of the uncertainty on the SF in the kinematic bin i for the PF setup. The total number of original uncertainty sources common to both flavor-tagging setups is denoted by M , while V_i^{PF} in the denominator is the total SF variance in the kinematic bin i :

$$V_i^{\text{PF}} = \sum_{k=1}^M (u_{ik}^{\text{PF}})^2 \quad (4.6)$$

The analogous terms for the VR setup are u_{ik}^{VR} and V_i^{VR} . Figure 4.1 shows the correlation of the total b -tagging SF uncertainties between two different jet collections: Variable Radius Track Jets and Particle Flow Jets, using the DL1r tagger at the 70% working point. The correlations can be as high as 50%, so a proper correlation of the b -tagging uncertainties between analyses using these two different jet collections is important. The recomposition method introduced in this thesis enables physics analyses to account for such correlations, e.g. in the context of modeling or tracking uncertainty sources.

Brief introduction to the $VH, H \rightarrow b\bar{b}$ analysis

Most of the cross-checks presented in this chapter have been performed on the $VH, H \rightarrow b\bar{b}$ analysis discussed more in details in Chapter 5. This section will thus introduce the analysis and summarise the key points needed to understand the following sections. A more extended discussion of this analysis can be found in Chapter 5.

The analysis aims at studying the Standard Model Higgs boson decay to a pair of bottom quarks, also referred to as $H \rightarrow b\bar{b}$, which is expected to happen with a branching ratio of about 58%. The search is carried out selecting the Higgs boson produced in association with a leptonically decaying vector boson (VH) to ensure high background rejection thanks to the additional leptonic signatures in the final state. The analysis version used in this chapter of the thesis refers to the first version of the full Run-2 analysis, carried out on 13 TeV data collected with the ATLAS detector between 2015 and 2018 [34], while Chapter 5 describes improvement towards the second version of the full Run-2 analysis.

The $VH, H \rightarrow b\bar{b}$ signatures are categorized by the decays of the vector

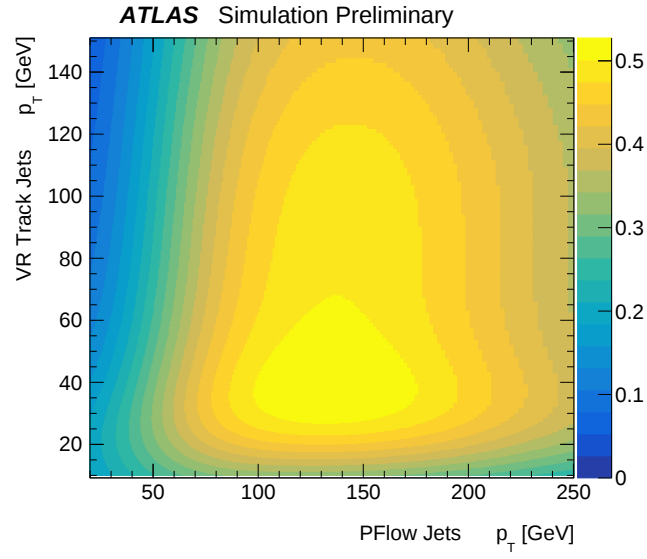


Figure 4.1: Correlation between the total b -tagging SF uncertainty for VR Track Jets and PFlow Jets, both tagged using the DL1r algorithm at the 70% Working Point, as a function of the respective jet p_T

bosons (Z or W) into: $ZH \rightarrow \nu\nu bb$, $WH \rightarrow \ell\nu bb$ and $ZH \rightarrow \ell\ell bb$. Depending on the number of charged leptons in the final state, the events are thus referred to as 0-, 1- and 2-lepton channels. The main backgrounds are $t\bar{t}$, Z +jets, W +jets (also referred to as V +jets in the text) and single top-quark production. The Higgs boson candidate is reconstructed from exactly two b -tagged small-radius calorimeter jets, using the MV2c10 b -tagging algorithm at the 70% working point.

A multivariate analysis (MVA) making use of Boosted Decision Trees (BDTs) is implemented to separate the Higgs boson signal from the backgrounds. Different multivariate discriminants are reconstructed, trained and evaluated in each lepton channel and signal region separately. The input variables used for the BDTs are chosen to maximise the separation power. One of the leading discriminating variables is the invariant mass of the di-jet system, also abbreviated to m_{bb} . This variable will appear later in thesis Chapter 5, as it has been used to validate the recomposition tool³.

The events are categorised in Signal Regions (SRs) and Control Regions (CRs). The CRs are designed to control the normalisation of the main backgrounds (top and V +jets) in the fit. The results are obtained from a simultaneous likelihood fit that combines together all channels and analysis regions. The BDT classifier score is used as fitting variable. All the cross-checks shown in section 4.2.4 and 4.2.5 have been performed taking the BDT distribution of the 1-Lepton SR as an example.

4.2.2 The eigenvector recomposition method

This section will first show a brief overview of the eigenvector (EV) *decomposition* method, currently used to reduce the number of flavor-tagging related uncertainty components in physics analyses. Then, the second part will describe the eigenvector *recomposition* method.

Brief overview of the eigenvector *decomposition* method

As summarised in the introduction, the scale factors measurement is affected by M sources of statistical and systematic uncertainty sources, typically around $\mathcal{O}(100)$ for each jet-flavor calibration analysis. Each source of uncertainty $k \in \{1, \dots, M\}$ is assumed to have a correlated effect on all p_T bins and, generalising to the pseudo-continuous case, on different b -tagging score bins. Partially correlated or uncorrelated uncertainty sources such as the statistical uncertainties

³An m_{bb} -based analysis is used to validate the nominal MVA analysis, since m_{bb} provides a more straightforward physical interpretation of the result.

in the calibration analysis ⁴ are treated by decomposing them into multiple correlated uncertainty components. For the b -jet and c -jet calibrations, the main sources of systematic uncertainty are related to the MC modeling, the jet energy scales and the statistical uncertainties (the latter for both data and simulation). From here the covariance matrix V_{ij} of the scale factors between two different p_T bins ($i, j \in \{1, \dots, N\}$) is given by:

$$V_{ij} = \sum_{k=1}^M u_{ik} u_{jk}, \quad (4.7)$$

where i and j are p_T -bin indices, k denotes the uncertainty component and u the bin-dependent SF uncertainty amplitude. The mathematical description of how to derive this covariance matrix can be found in Appendix .1.

Note that, as shown in Eq. 4.6, the diagonal element V_{ii} of the covariance matrix is equal to the total uncertainty squared. The covariance matrix is in general not diagonal, which means that the scale factor uncertainty sources are correlated across different kinematic bins [38]. Being symmetric and positive-definite, the total covariance matrix can be diagonalized, so as to provide orthogonal uncorrelated uncertainty components through its eigenvectors. After the diagonalization, the covariance matrix contains the eigenvalues λ_i^2 :

$$V \xrightarrow{\text{Diagonalize}} \begin{pmatrix} \lambda_1^2 & & & \\ & \lambda_2^2 & & \\ & & \ddots & \\ & & & \lambda_N^2 \end{pmatrix} \quad (4.8)$$

There are in total N eigenvectors which could be used to construct a matrix with element v_{ik} , one for each dimension of the covariance matrix. The eigenvector uncertainty can be calculated by multiplying the eigenvector with the corresponding eigenvalue. To be specific, the i^{th} p_T bin of k^{th} eigenvector uncertainty is:

$$\tilde{u}_{ik} = \lambda_k v_{ik}. \quad (4.9)$$

The variance V_i in the i^{th} kinematic bin should be exactly the same in the

⁴Most calibration analyses do a simultaneous fit of the scale factors across kinematic bins, and events do typically contain more than one jet, thus statistical uncertainties from such calibration analyses turn out to be partially correlated and partially uncorrelated across bins.

two bases, and can thus be written as:

$$V_i = \sum_{k=1}^N (\tilde{u}_{ik})^2 = \sum_{k=1}^M (u_{ik})^2 \quad (4.10)$$

After discarding the negligible eigenvector uncertainties (smaller than 10^{-20} for all kinematic bins) arising from the smoothing procedure described in Ref. [36], one ends up with a set of L eigenvectors, with $L \leq N$. Since normally $L \ll M$ this leads to a great reduction in the number of uncertainty components. These L eigenvectors, derived separately for each tagging setup (combination of algorithm and working point), are used as uncorrelated systematic uncertainty components in the physics analyses. When applying the eigenvector decomposition method to the pseudo-continuous calibration, no change is required in the formalism, apart from the index i which is generalized to all combinations of jet kinematic bins and b -tagging score bins considered in the calibration.

Mathematical description of the eigenvector *recomposition*

Using the results of the EV decomposition, described in the previous section 4.2.2, the original b -tagging calibration uncertainty sources λ_i are expressed in the basis defined by the eigenvectors. The total SF variation in each p_T bin i , referred to as T_i , can be expressed as:

$$T_i = \sum_{k=1}^L \theta_k \lambda_k v_{ik} = \sum_{k=1}^L \theta_k \tilde{u}_{ik} \quad (4.11)$$

where $k \in \{1, \dots, L\}$, is the eigenvector index and θ_k are the nuisance parameters used in the analysis.

At the same time, T_i can also be expressed as a function of the *original* sources of systematic uncertainties:

$$T_i = \sum_{j=1}^M \eta_j u_{ij} \quad (4.12)$$

where η_j is one of the M nuisance parameters representing the original sources of systematic uncertainties.

Combining (4.11) and (4.12) and rewriting it in matrix form:

$$(\eta_1 \quad \dots \quad \eta_M) \begin{pmatrix} u_{1,1} & \dots & u_{N,1} \\ \vdots & \ddots & \vdots \\ u_{1,M} & \dots & u_{N,M} \end{pmatrix} = (\theta_1 \quad \dots \quad \theta_L) \begin{pmatrix} \lambda_1 v_{1,1} & \dots & \lambda_1 v_{N,1} \\ \vdots & \ddots & \vdots \\ \lambda_L v_{1,L} & \dots & \lambda_L v_{N,L} \end{pmatrix} \quad (4.13)$$

Note that the left hand side is not exactly equal to the right hand side since some negligible eigenvector uncertainty components might be discarded. However the discarded uncertainties are too small ($< 10^{-20}$ in all kinematic bins) to be visible in any of the tests performed in this thesis, the two sides of equation above can be treated as equal. The previous equality can be written shortly as:

$$\boldsymbol{\eta} \cdot U = \boldsymbol{\theta} \cdot \tilde{U} \quad (4.14)$$

One can see that the non-square matrix $\tilde{U}$ in Eq. 4.13 has dimension $L \times N$. Each row of matrix $\tilde{U}$ is an eigenvector times eigenvalue. Therefore, $\tilde{U}$ is a matrix with rank L . In this case, it is known that the right inverse $\tilde{U}_{\text{right}}^{-1} = \tilde{U}^T(\tilde{U}\tilde{U}^T)^{-1}$ is a pseudo-inverse (Moore–Penrose inverse) of $\tilde{U}$ and therefore must be unique, thus multiplying the expression above by $\tilde{U}_{\text{right}}^{-1}$ leads to an expression for $\boldsymbol{\theta}$ in terms of $\boldsymbol{\eta}$:

$$\boldsymbol{\theta} = \boldsymbol{\eta} \cdot U \cdot \tilde{U}_{\text{right}}^{-1} \quad (4.15)$$

One can hence define a dimension $M \times L$ matrix:

$$\text{Re} \equiv U \tilde{U}_{\text{right}}^{-1} \quad (4.16)$$

that translates the uncertainties between the original set and the eigenvector decomposed uncertainty set.

Most physics analyses using b -tagging in ATLAS rely on a maximum-likelihood fit to extract their parameters of interest, with the diagonalized b -tagging uncertainties encoded in the nuisance parameters θ . The corresponding likelihood function is:

$$\mathcal{L} = L(\boldsymbol{\mu}, \theta_1, \theta_2, \dots, \theta_L) P(\theta_1) P(\theta_2) \dots P(\theta_L), \quad (4.17)$$

where $\boldsymbol{\mu}$ is the vector of the parameters of interest, for example the Higgs boson production signal strengths, and the $P(\theta_k)$ represent the Gaussian priors centered at zero and with variance set to unity which constrain the values of the corresponding components of the flavor-tagging systematic uncertainty encoded as eigenvectors. This likelihood function has the same form as the likelihood written explicitly in Equation 5.19.

The aim of the eigenvector recomposition approach is to transform the likelihood function in Eq. 4.17, back into the corresponding likelihood function where the b -tagging uncertainty components are encoded into the nuisance parameters η of the original sources of systematic uncertainties:

$$\mathcal{L} = L(\boldsymbol{\mu}, \eta_1, \eta_2, \dots, \eta_M) P(\eta_1) P(\eta_2) \dots P(\eta_M), \quad (4.18)$$

where the $P(\eta_k)$ again represent Gaussian priors.

The nuisance parameters θ (after diagonalization) and the nuisance parameters η (before diagonalization) represent the exact same uncertainties in the space of the b -tagging scale factors, i.e. the same central values and same covariance matrix. The results of the two maximum-likelihood fits for Eq. 4.17 and Eq. 4.18 will thus be identical (within numerical accuracy) in terms of parameters of interest (POIs) and any nuisance parameters (NPs) unrelated to b -tagging. However, since the space of the θ parameters is lower-dimensional than the space of the η parameters, a transformation from the θ to the η space of parameters requires a replacement of the (lower-dimensional) prior constraints in θ with the complete set of prior constraints in the η . The latter will include not only the directions in the η space already spanned by variations of the θ parameters, but also additional directions that keep the b -tagging scale factors invariant and to which the analysis likelihood is thus insensitive. The identity between the two likelihood functions and the procedure to transform one into the other is demonstrated and justified in more detail in Appendix .2.

In order to modify Eq. 4.17 to make it identical to Eq. 4.18 the eigenvector recomposition tool proceeds through the following steps:

1. The priors $P(\theta_1)P(\theta_2)\dots P(\theta_L)$ are removed;
2. The variables $\boldsymbol{\theta}$ are expressed as a function of $\boldsymbol{\eta}$, by using Eq. 4.15, thus effectively replacing the $\boldsymbol{\theta}$ with the $\boldsymbol{\eta}$;
3. The original priors $P(\eta_1)P(\eta_2)\dots P(\eta_M)$ are added back.

With these substitutions, the analysis likelihood function becomes equivalent to Eq. 4.18, in the sense that they will both converge towards the same postfit SFs and the same postfit impact of the b -tagging systematic uncertainties. Its b -tagging nuisance parameters will now be encoded again in the $\boldsymbol{\eta}$, representing the original systematic variations. It should be noted that Eq. 4.18 is the likelihood function one would have obtained without applying the eigenvector decomposition (diagonalization) method in first place. One notable feature of this procedure is that it is agnostic with respect to the observable used in the analysis and the detailed structure of the likelihood

function, which means the method can be applied without specific and detailed knowledge of a particular analysis.

Treatment of the statistical uncertainties in the scale factors The recomposition tool is designed to recombine both the systematic and the statistical components of the total calibration uncertainty. However after they have both been recomposed, at the moment, only the systematic components can be correctly correlated across different calibrations. The correlation between the statistical NPs across different setups is not straightforward to evaluate, since it requires taking the event overlap between the different calibrations into account, e.g. through direct evaluation or through bootstrap techniques, see Ref. [43] and references therein for more details. Thus, missing a dedicated study, it is only possible to correlate the *original* uncertainty sources that have a systematic origin. One exception to this is the case of the b -jet calibrations differing from each other only by their working points, with the events used for the tighter WP calibration being a subset of the looser one. Since these are currently all derived from the more generic pseudo-continuous calibration, common nuisance parameters among different working points are already used, thus describing in a coherent way the impact of statistical uncertainties on common/orthogonal events in the calibration analysis. In a similar way, the treatment of the statistical uncertainties could be improved in the future also for setups with different b -tagging algorithms or jet collections.

The impact of this approximation is expected to be small as in the current calibrations the systematic component is largely dominant over the statistical component, especially for the region of jet kinematics relevant for most physics analyses in ATLAS. In Figure 4.2 the systematic component is compared to the total uncertainty for the particle flow b -jet efficiency calibration at the 70% working point. The statistical component starts to be significant only for jet p_T above 200 GeV, while in the bulk of the kinematic range the systematic component accounts for more than 90% of the total uncertainty, with a peak of 98% around 80-90 GeV.

4.2.3 Validation of the eigenvector recomposition

The method derived above and its implementation in the ATLAS software have been verified through multiple crosschecks and validation tests. This section summarizes the most relevant ones, performed based on the $VH, H \rightarrow b\bar{b}$ analysis.

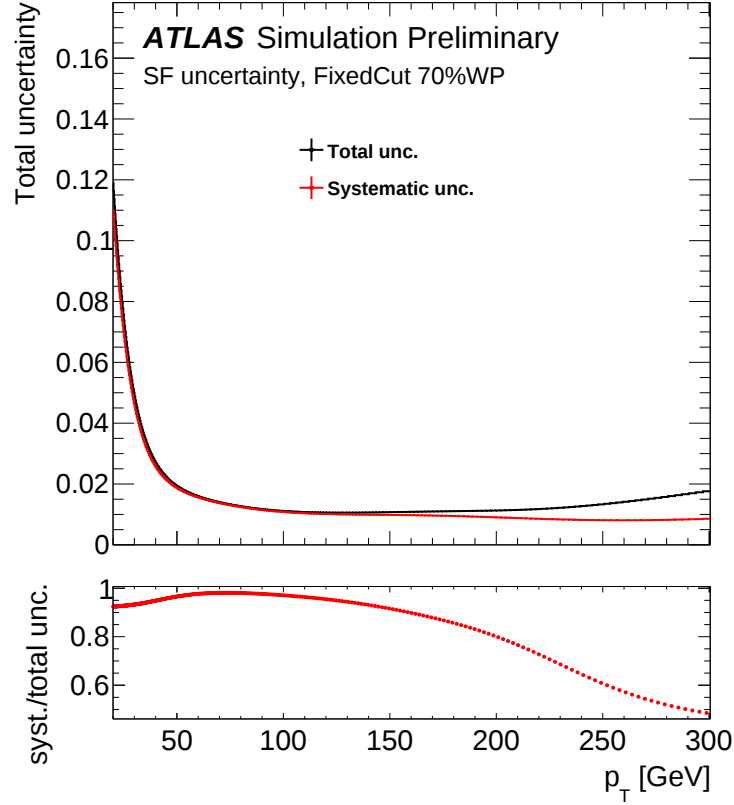


Figure 4.2: The upper panel shows the total uncertainty compared to its systematic component as a function of p_T , for the particle flow b -jet calibration at the 70% working point. The bottom panel shows the ratio between the systematic component and the total uncertainty.

Recomposed uncertainties

The procedure to modify the likelihood function introduced in section 4.2.2, and based on the relation between nuisance parameters expressed in Eq. 4.15, is in principle all what is needed to apply the recomposition method to the analysis likelihood function. However, in addition, one can also derive an equation that relates systematic variations for a generic analysis *observable* in the space of eigenvector variations, to the same variations expressed in the space of the original sources of uncertainties. Here and throughout this chapter the impact of b -tagging uncertainties on the expected event yield (in each of the bins of a physical observable such as m_{bb}) is assumed to be linear, following the likelihood formalism used across most ATLAS analyses. To yield the best possible approximation of the full non-linear dependence, the variations of the yields (binned in such observables) are linearized with respect to variations of the underlying nuisance parameters around their $\pm 1\sigma$ variations (see Section 4.1 in Ref [44]). As a consequence, the recomposition method can be applied to any analysis observable in the same way as to the underlying b -tagging scale factor variations.

Considering that a given kinematic observable has R different bins, the flavor-tagging-related variations of the event yield in each bin r can be expressed both in the eigenvector space (i.e. the SFs *diagonal* space), or in the space of the original sources of SF uncertainties (i.e. the *original* space):

$$b_r = \sum_{j=1}^M \eta_j \Delta y_{rj} = \sum_{k=1}^L \theta_k \Delta d_{rk} \quad (4.19)$$

where r is the index of the kinematic bin considered, with $r \in \{1, \dots, R\}$, b_r is the total systematic variation for the given observable in bin i , Δy_{rj} is the 1-sigma systematic variation corresponding to the j^{th} source of original uncertainty for the bin r which affects the yields in that bin, and Δd_{rk} represents the impact of the k^{th} eigenvector uncertainty component on bin r .

Rewriting (4.19) in matrix form, one obtains:

$$\boldsymbol{\eta} \cdot \mathbf{Y} = \boldsymbol{\theta} \cdot \mathbf{D} \quad (4.20)$$

or more explicitly:

$$(\eta_1 \quad \dots \quad \eta_M) \begin{pmatrix} \Delta y_{1,1} & \dots & \Delta y_{R,1} \\ \vdots & \ddots & \vdots \\ \Delta y_{1,M} & \dots & \Delta y_{R,M} \end{pmatrix} = (\theta_1 \quad \dots \quad \theta_L) \begin{pmatrix} \Delta d_{1,1} & \dots & \Delta d_{R,1} \\ \vdots & \ddots & \vdots \\ \Delta d_{1,L} & \dots & \Delta d_{R,L} \end{pmatrix} \quad (4.21)$$

The goal here is to determine the matrix Y . To obtain the matrix Y , Eq. (4.15) can be plugged into Eq. (4.21) to get:

$$\boldsymbol{\eta} \cdot Y = \boldsymbol{\eta} \cdot U \cdot \tilde{U}_{\text{right}}^{-1} \cdot D \quad (4.22)$$

This identity remains valid for any arbitrarily chosen set of values for the components of the $\boldsymbol{\eta}$ vector. Therefore $\boldsymbol{\eta}$ can be removed from both sides to get the recomposed original sources of uncertainty⁵:

$$Y = U \cdot \tilde{U}_{\text{right}}^{-1} \cdot D \quad (4.23)$$

Comparison between *single* recomposed uncertainties and original sources

This section aims at verifying if a *single* uncertainty source recomposed using the recombination method matches the *original* uncertainty source before the decomposition and recombination steps. As a concrete example, the impact of each original uncertainty source has been quantified on the $VH, H \rightarrow b\bar{b}$ dijet-mass (m_{bb}) observable. In order to establish the reference for this check, the analysis has been re-run disabling the decomposition step. In this way the b -tagging systematic variations remain equal to the original sources, rather than being decomposed into flavor-tagging eigenvectors.

At the same time, each original uncertainty source can also be derived from the flavor-tagging eigenvectors using the recombination method, by applying the Y matrix as in Eq. (4.23). A comparison of the derived uncertainty source and the original one (also referred to as "reference" in the figures) for the leading original uncertainty source of the b -jet calibration analysis – namely the Parton Shower (PS) modeling uncertainty⁶ – is shown in Figure 4.3 along

⁵On the right hand side of Eq. 4.23, matrix U and $\tilde{U}_{\text{right}}^{-1}$ are derived from the standard ATLAS b -tagging calibration analyses. Matrix D refers to the b -tagging eigenvector variations relative to the analysis observable.

⁶This source of uncertainty refers to the $t\bar{t}$ Parton Shower modeling. It has been calculated comparing the nominal generator produced using PowhegBox v2 interfaced to Pythia 8.230 with an alternative sample generated using PowhegBox v2 interfaced to Herwig 7. More details are discussed in Ref. [36].

with their ratio. The recomposed uncertainty source matches with the original reference uncertainty within 0.5% in all the considered bins⁷. These small non-closures have to be attributed not to the recombination method, but to the assumption of linearity, i.e. they are due to the small differences observed between linearizing the relation between the b -tagging scale factor variations and the expected analysis yields (in bins of the m_{bb} observable) around the $\pm 1\sigma$ variations of the eigenvector uncertainties, versus applying the same linearization around the $\pm 1\sigma$ variations of the original uncertainty sources. It should be noted that a non-closure of this size on single uncertainties will have no appreciable impact on the physics analysis results.

Comparison of *total* eigenvector and recomposed uncertainties

Since the expressions of the uncertainties in the original space and in the SF diagonal space are equivalent, as related by Eq. (4.23), the total flavor tagging uncertainty should be preserved when computing the sum in quadrature of the set of uncertainties in the eigenvector space and in the space of the recomposed uncertainties. In a given bin r of the m_{bb} distribution, the sum in quadrature of the original uncertainty amplitudes (Δy_{rj}) and the sum in quadrature of the eigenvectors (Δd_{rl}) , defined in the $VH, H \rightarrow b\bar{b}$ analysis phase space, can be defined as follows:

$$\sqrt{\sum_{j=1}^M (\Delta y_{rj})^2} = \sqrt{\sum_{l=1}^L (\Delta d_{rl})^2} \quad (4.24)$$

Eq. (4.24) has been experimentally verified using the m_{bb} distribution, to see if the sum in quadrature of the recomposed uncertainty sources is equal to the sum in quadrature of the uncertainty components in the SF diagonal space.

The result of this validation check is shown in Figure 4.4, where for simplicity the two terms in Eq. (4.24) have been rewritten as:

$$\sqrt{\sum \Delta Y^2} = \sqrt{\sum \Delta D^2} \quad (4.25)$$

The two total uncertainties are exactly the same within the numerical

⁷Detailed studies discussed in section 4.2.5, show that this matching works only if no significant *pruning* is applied to the eigenvector uncertainty components at analysis level. Pruning the uncertainty components is a widely spread practice in physics analyses and it consists in removing uncertainties, in this case the single eigenvectors, that have sub-leading effects, region by region. More details about the pruning procedure used in $VH, H \rightarrow b\bar{b}$ can be found in Ref. [45]

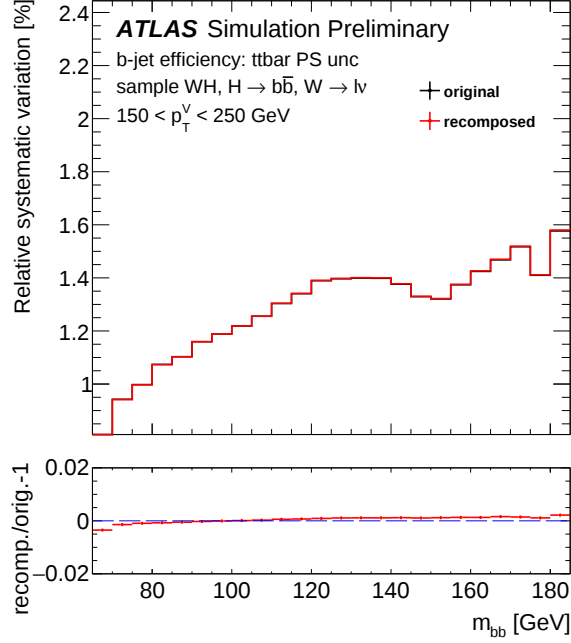


Figure 4.3: Comparison between reference (black) and recomposed (red) systematic variation of the m_{bb} observable corresponding to the leading single source of uncertainty of the b -jet efficiency calibration, i.e. the parton shower uncertainty on the top anti-top process. The lower panel shows the ratio of the derived uncertainty source over original (reference) uncertainty. Both recomposed uncertainty source and original uncertainty source are computed on $VH, H \rightarrow b\bar{b}$ signal events in the one lepton channel (targeting the WH production mode). The pseudo-continuous calibration is used. The residual difference is typically less than 10^{-2} .

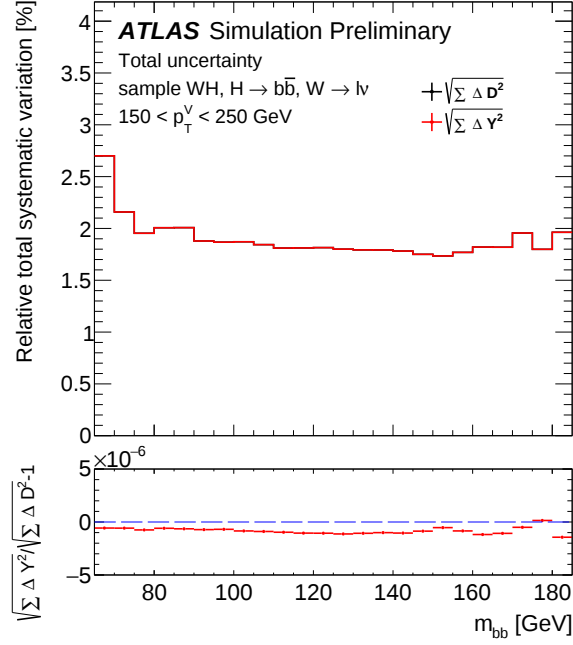


Figure 4.4: Comparison between the total systematic variations $\sqrt{\sum \Delta Y^2}$ and $\sqrt{\sum \Delta D^2}$ relatively to the nominal yields for the m_{bb} distribution. The bottom panel shows their ratio, which is within the available numerical precision (10^{-6}).

precision available (10^{-6}). In this case the linearization always happens at the $\pm 1\sigma$ points of the eigenvector uncertainty components, and no re-linearization is applied when moving to the space of recomposed uncertainty sources. So, since both are coming from the same run of the $VH, H \rightarrow b\bar{b}$ analysis, almost perfect closure is observed. This differs from the previous section, where the linearization was applied first in the space of the original uncertainty sources and then in the space of the eigenvector uncertainty components.

4.2.4 Implementation in statistical analyses

This section will focus on the application of the recomposition tool to real physics analyses. The tool is designed to be applied at the latest stages of the analyses, directly on the analysis workspaces (WS). This ensures flexibility and applicability even a-posteriori on already published ATLAS analyses.

The workspace mentioned in this section is based on the RooWorkspace class [46], built with HistFactory [47]. The tool has been tested only on workspaces built with HistFactory, however its applicability is expected to be

independent from the chosen statistical analysis framework. As described in section 4.2.1, all the fits shown in this section are based on first version of the full Run 2 $VH, H \rightarrow b\bar{b}$ one-lepton workspace, which uses an MVA-based classifier, named BDT(VH) hereafter, as fitting variable in the Signal Regions (SR).

Workspace modification: technical details

All the tests described in this section are performed modifying the $VH, H \rightarrow b\bar{b}$ analysis workspace. The WS is modified using the relation derived in Eq. (4.15):

$$\boldsymbol{\theta} = \boldsymbol{\eta} \cdot \boldsymbol{U} \cdot \tilde{\boldsymbol{U}}_{\text{right}}^{-1} \quad (4.26)$$

After this modification, the eigenvector nuisance parameters (NPs) in the likelihood are replaced by a linear combination of nuisance parameters representing the *original* calibration uncertainty sources. The matrices $\boldsymbol{U}$ and $\tilde{\boldsymbol{U}}_{\text{right}}^{-1}$ have been computed from the original set of uncertainty sources for the given analysis b -tag setup, and can be applied to any other analysis using the same setup. The newly introduced NPs encoding the original uncertainty sources are constrained using Gaussian priors with mean equal to zero, and standard deviation equal to one. Only the b -jet related uncertainties have been modified, but the method can be applied identically to all jet flavors. In this particular workspace the total number of original uncertainty sources is $M = 127$, while the number of eigenvector uncertainty components is $L = N = 45$, as no smoothing is applied to the b -tagging SFs. After pruning L is reduced to 4 eigenvectors (see section 4.2.5 for more details).

Inspection of the uncertainties

Section 4.2.3 shows the validation of the method at histogram level (prior to the workspace creation) within $\sim 1\%$ accuracy. This study aims at cross-checking that the recomposed uncertainty in the modified workspace is equal to the original source uncertainty histogram given by the analysis before creating the WS⁸. The results are shown in Figure 4.5. The $\sim 0.2\%$ residual non-closure has been discussed in section 4.2.3.

⁸Note that during the generation of the $VH, H \rightarrow b\bar{b}$ workspace, the BDT(VH) histogram is rebinned by a specific algorithm explained in Ref. [34]. Therefore, before making the comparison, the standard histogram has been rebinned by the same algorithm.

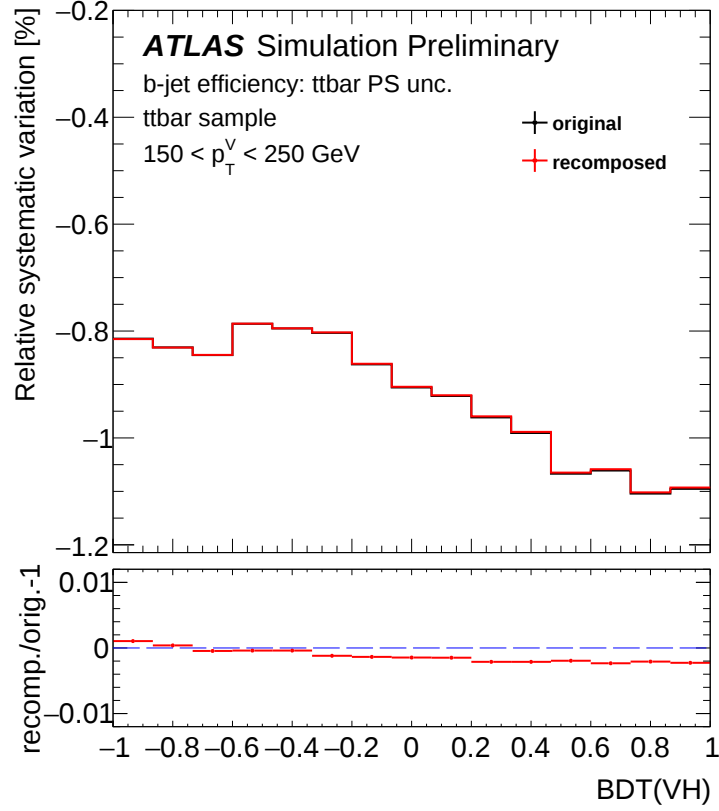


Figure 4.5: Comparison between the *original* uncertainty source and the *recomposed* uncertainty source. The upper panel shows the systematic variation, while the lower panel shows $\frac{\text{recomposed}}{\text{standard}} - 1$. The test is performed on the $t\bar{t}$ MC-modeling related uncertainty source "b-jet efficiency: $t\bar{t}$ PS uncertainty" on the MVA classifier output used in the $VH, H \rightarrow b\bar{b}$ analysis.

Effects on the recomposed uncertainties

From the equivalence of the expression of the uncertainties in the original and in the recomposed spaces, it is expected that the post-fit b -tagging SFs nuisance parameter value of the modified workspace match the fitted parameter values of the eigenvectors in the standard workspace. To check this expectation, since the original NPs and eigenvector NPs are related by Eq. 4.15, the pull values of the b -tagging NPs fitted from the modified workspace are used to calculate the pull values of the corresponding eigenvector NPs by Eq. 4.27:

$$\boldsymbol{\theta}_{\text{calculated}} = \boldsymbol{\eta} \cdot U \cdot \tilde{U}_{\text{right}}^{-1} \quad (4.27)$$

Then $\boldsymbol{\theta}_{\text{calculated}}$ can be compared with the eigenvector NPs pulls $\boldsymbol{\theta}_{\text{standard}}$ of the standard workspace. This calculation was performed for the 4 leading b -tagging eigenvector NPs, where the agreement was found to be better than 10^{-4} .

4.2.5 Pruning effects

The pseudo-continuous b -tagging calibration leads to 45 eigenvectors after the decomposition. In order to ease the convergence of the fit and reduce the computation time, a pruning procedure is usually applied at physics analysis level, excluding the smallest eigenvector uncertainty components from the fit (sometimes small uncertainty components are combined according to the method presented in Ref. [48]). The pruning criteria have a negligible impact on the final result. However, a pruned sub-set of the flavor-tagging eigenvectors by construction loses a certain amount of information on the total uncertainty. This might lead to accuracy losses when applying the recombination. This section aims at studying these effects on the accuracy of the recomposed uncertainty sources.

Eigenvector pruning effects and the accuracy of the recomposed uncertainties

In order to quantify how pruning affects the accuracy of the recomposed uncertainty sources, the flavor-tagging uncertainty components of the $VH, H \rightarrow b\bar{b}$ workspace have been recomposed into the original uncertainties, using three different sub-sets of eigenvectors, corresponding to three different pruning thresholds:

- The first case corresponds to the full set of 45 eigenvectors with no pruning applied.

- The second case corresponds to 29 EV, which is the number of uncertainty components after the dedicated pruning step of the $VH, H \rightarrow b\bar{b}$ analysis. The analysis keeps all the eigenvectors for which the variation is above 1% in at least one p_T bin in at least one of the three considered b -tagging score bins 100-70%, 70-60% and 60-0%.
- The third case corresponds to 4 EV, which is the number of b -tag uncertainty components after applying the pruning criteria of the $VH, H \rightarrow b\bar{b}$ 2019 fit. These are applied on top of the pruning criteria described before. An uncertainty is pruned if its normalisation or shape effect is smaller than 0.5%. In addition, the uncertainties on the very small background processes (their yield is less than 2% of the signal) are pruned. In non-sensitive regions (where the signal is less than 2% of the background in each bin) the uncertainty components are pruned if the impact is smaller than 0.5% of the total background.

These numbers correspond to the number of uncertainty components in the specific region tested here ($150 < p_T^V < 250$ GeV, SR, 2 jets, 1 lepton).

The comparison of one of the leading uncertainty sources: " b -jet efficiency: $t\bar{t}$ bar PS" recomposed starting from 45, 29 and 4 eigenvectors is shown in Figure 4.6. In all the three cases the "standard" uncertainty source (in black) represents the original reference histogram before the creation of the workspace. The corresponding accuracy loss is respectively 0.1%, 1% and 20% for 45, 29 and 4 eigenvectors.

For completeness, the test has been enlarged also to the top 10 recomposed uncertainty sources impacting the BDT(VH) histogram. The sources of uncertainty have been ordered by their impact on the $t\bar{t}$ background yields.

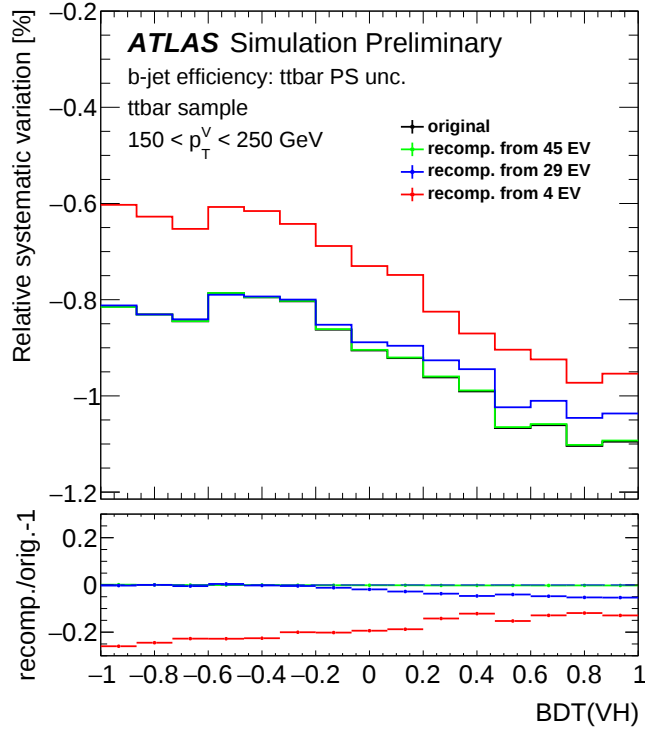


Figure 4.6: Comparison between the b -jet efficiency $t\bar{t}$ bar PS uncertainty recomposed starting from 45 (full set, "recomp. from 45 EV" label in green), 29 ("recomp. from 29 EV" label in blue) and 4 ("recomp. from 4 EV" in red) eigenvector uncertainty components. The original uncertainty source (black) is labeled as "original".

Uncertainty Name	Impact on $t\bar{t}$ yield (%)	Rel. deviation from original unc. (%)		
		45 Eigen	29 Eigens	4 Eigens
ttbar PS	0.84	0.09	1	22
PDF4LHC NP. 1	0.63	0.09	6	48
diboson modeling	0.56	0.07	15	43
pile-up reweighting	0.51	0.14	24	23
single top DR vs DS	0.49	0.06	5	57
PDF stat. NP. 1	0.45	0.18	1	8
Jet Energy Resolution	0.41	0.48	14	25
MC stat.	0.39	0.17	39	136
fake correction	0.39	0.20	5	56
Z+jets modeling	0.31	0.03	4	25

Table 4.1: Top 10 original uncertainty sources impacting the $t\bar{t}$ yield in the 1L 2jet $150 < p_T^V < 250$ SR. The second column shows their impact on the $t\bar{t}$ yield. The three last columns show the relative loss of accuracy when the recomposition is performed starting from 45, 29 and 4 eigenvector (EV) uncertainty components respectively. This relative deviation is calculated by using the sum of the absolute difference in each bin between the recomposed histogram and the original histogram.

The relative deviation between each recomposed and original uncertainty source is calculated as the sum of the absolute yield difference between the two histograms in each bin and it is shown in the last three columns of Table 4.1. The accuracy loss on the recomposed uncertainty sources spans between 1% to ~40% with 29 eigenvectors. With 4 eigenvectors the accuracy loss increases, with losses between 10% and up to ~130%. In order to get accurate recomposed uncertainties and correctly correlate the b -tagging uncertainty components for example in downstream combinations, the various input analyses must have similar pruning settings. The most conservative suggestion would be to remove the pruning on the eigenvector uncertainty components before applying the recombination tool.

A complementary test consists in checking whether the pruning affects the closure between the total uncertainty calculated before and after the recombination step. Figure 4.7 shows the total relative variation calculated using 4, 29 and 45 eigenvectors and the corresponding original uncertainty sources recomposed from those eigenvector sets. The difference remains within 2×10^{-3} , which implies that the total uncertainty is conserved after recombination, independently from the chosen pruning threshold.

4.3 High-pT extrapolation uncertainties in pseudo-continuous scheme

4.3.1 Introduction to high-pt-extrapolation

The basic of b -tagging analysis including pseudo-continuous b -tagging(PCBT) is introduced in section 4.1. To be more specific, in PCBT, the overall normalization is obtained imposing the following constraint:

$$\sum_{i=1}^5 \epsilon_{p_T}^i S F_{p_T}^i = 1 \quad (4.28)$$

$$\sum_{i=1}^5 \epsilon_{p_T}^i = 1 \quad (4.29)$$

where i runs from 1 to 5, representing the 5 tag weight bins, $\epsilon_{p_T}^i$ is the tagging efficiency in the given bin and $S F_{p_T}^i$ is the efficiency scale factor associated to that tag weight bin. The product of efficiency and scale factor gives the calibrated efficiency. This constraint means that the sum of calibrated b -tagging efficiency is equal to 1. The constraint is still valid when considering a variation on the scale factor due to a specific SF calibration uncertainty.

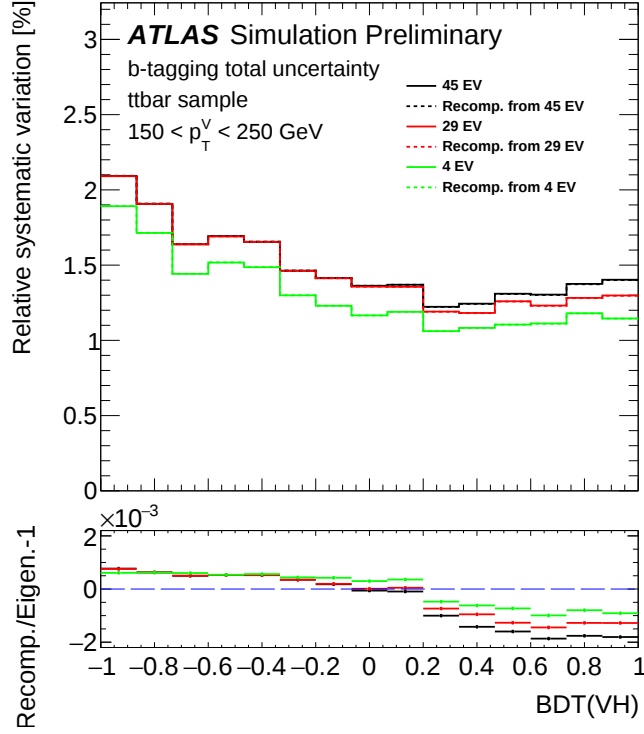


Figure 4.7: Sum in quadrature of the relative uncertainties calculated from 4, 29 and 45 eigenvectors (solid lines) and sum in quadrature of all recomposed uncertainties based on 4, 29, 45 eigenvectors (dashed lines). The bottom panel shows the ratio between the sum in quadrature of the total recomposed uncertainty sources and the corresponding sum in quadrature of the eigenvector uncertainties.

As described in Ref. [11], in the fixed cut working point case, the b-tagging uncertainties in the high p_T region were evaluated by summing all sources of systematic uncertainties in quadrature to get a single monotonic uncertainty. However, the quadrature summed uncertainty cannot guarantee Eq. 4.28 to still be valid. Therefore, a new method is needed to evaluate the uncertainties of b-tagging in the high p_T region with the PCBT scheme.

4.3.2 Derivation of the extrapolation uncertainties

The p_T value that determines the division between high p_T region and the standard in-situ calibration region is called the p_T *reference point*. The SFs in the extrapolation region are related to the SFs at the highest p_T reference point of the in-situ calibration region by:

$$SF_{p_T} = SF_{p_T,ref} \cdot R(p_T) \quad (4.30)$$

where R is a factor depending on p_T . The value of R is assumed to be equal to one since the SFs do not have a strong dependence on p_T , as reported in Ref [49]. However, R has associated uncertainties that need to be evaluated and propagated as additional extrapolation uncertainties to cover possible deviations from unity. The relative uncertainty of the SF in the high- p_T extrapolation region can be expressed as $\Delta_{rel}(SF_{p_T})$. It depends on the relative SF uncertainty at the reference point $\Delta_{rel}(SF_{p_T,ref})$ determined by the in-situ calibrations and on the relative uncertainty of R , defined as $\Delta_{rel}(R)$, as follows:

$$\Delta_{rel}(SF_{p_T}) = \frac{\Delta(SF_{p_T})}{SF_{p_T}} = \frac{\Delta(SF_{p_T} \cdot R)}{SF_{p_T} \cdot R} \quad (4.31)$$

$$\cong \frac{\Delta(SF_{p_T,ref}) \cdot R + SF_{p_T,ref} \cdot \Delta(R)}{SF_{p_T} \cdot R} \quad (4.32)$$

$$\cong \Delta_{rel}(SF_{p_T,ref}) + \Delta_{rel}(R) \quad (4.33)$$

The relative variation of R is evaluated from Monte-Carlo samples as described below. Please note that the statistical uncertainties in the high- p_T region are inherited from the statistical uncertainties of the highest p_T bin in the standard calibration region. Therefore in the current procedure, only the systematic variations are evaluated in the high p_T region.

In the in-situ calibration analyses, the variation of the MC efficiency systematic uncertainty induces a variation of the b -tagging efficiency measured in data. In addition, the variation on MC will change the expected flavour fraction in data, therefore also changes the efficiency measured in data. In

contrast, in deciding a MC-based uncertainty, the impact on the predicted b -tagging efficiency due to a certain systematic uncertainty is checked in MC, and applied to the data-based measurement of the efficiency.

$$\Delta_{syst}(\epsilon_{data}^{meas}) = (\epsilon_{data}^{meas})_{syst} - (\epsilon_{data}^{meas})_{nom} \quad (4.34)$$

$$= (\epsilon_{data}^{meas})_{nom} \frac{(\epsilon_{MC})_{syst} - (\epsilon_{MC})_{nom}}{(\epsilon_{MC})_{nom}} \quad (4.35)$$

$$= SF_{nom} \cdot \Delta_{syst}(\epsilon_{MC}) \quad (4.36)$$

$$= \frac{\epsilon_{data}^{meas,nom}}{\epsilon_{MC}^{nom}} \Delta_{syst}(\epsilon_{MC}) \quad (4.37)$$

Therefore, a known variation of the MC b -tagging efficiency corresponds to a scale factor variation:

$$SF' = \frac{\epsilon_{data} + \Delta(\epsilon_{data})}{\epsilon_{MC}} = \frac{\epsilon_{data}(1 + \Delta_{rel}(\epsilon_{MC}))}{\epsilon_{MC}} = SF(1 + \Delta_{rel}(\epsilon_{MC})) \quad (4.38)$$

Based on the result above, the variation on R becomes:

$$R' = \frac{SF'_{p_T}}{SF'_{p_T,ref}} = \frac{SF_{p_T}(1 + \Delta_{rel}(\epsilon_{MC,p_T}))}{SF_{p_T,ref}(1 + \Delta_{rel}(\epsilon_{MC,p_T,ref}))} \quad (4.39)$$

$$\approx R \cdot (1 + \Delta_{rel}(\epsilon_{MC,p_T}))(1 - \Delta_{rel}(\epsilon_{MC,p_T,ref})) \quad (4.40)$$

$$\approx R \cdot (1 + \Delta_{rel}(\epsilon_{MC,p_T}) - \Delta_{rel}(\epsilon_{MC,p_T,ref})) \quad (4.41)$$

Therefore the relative uncertainty of R due to a certain systematic source is:

$$\Delta_{rel}(R) \approx \Delta_{rel}(\epsilon_{MC,p_T}) - \Delta_{rel}(\epsilon_{MC,p_T,ref}) \quad (4.42)$$

where from Eq. 4.41 to 4.42 the assumption $R = 1$ is used. Now that $\Delta_{rel}(R)$ is achieved, combining Eq. 4.42 with Eq. 4.33, the combined SF variation is:

$$\Delta_{rel}(SF_{p_T}) = \Delta_{rel}(SF_{p_T,ref}) + \Delta_{rel}(\epsilon_{MC,p_T}) - \Delta_{rel}(\epsilon_{MC,p_T,ref}) \quad (4.43)$$

The above equation shows the SF variation in extrapolation region. In the previous study of [11], $\Delta_{rel}(R)$ is derived to be:

$$\Delta_{rel}^2(R) = \sum_{s \in S} \max_{\leq p_T} [\Delta \epsilon_s^{MC}(p_T) - \Delta \epsilon_s^{MC}(p_{T,ref})]^2 \quad (4.44)$$

Where the set S contains all sources of uncertainty. The symbol " $\max_{\leq p_T}$ " means the largest value until the current p_T value. Therefore it enforces the uncertainty to be monotonically increasing. In the fixed cut approach this monotonic trend results in an increase in the uncertainty, which is compensated by the inefficiency scale factors, that are specifically computed imposing the overall normalisation to be constant. However, when imposing the monotonic increase in the pseudo-continuous regime, the constraint defined in Eq. 4.28 does not hold anymore for the corrected efficiencies. In fact, Eq. 4.44 does not preserve the signs of the uncertainties, which will thus always result in positive corrections added to the initial values in each bin. This will therefore lead to the following relation:

$$\sum_{i=1}^5 \epsilon_{p_T}^i SF_{p_T}'^i > 1 \quad (4.45)$$

In the newly derived approach for the pseudo-continuous case shown in Eq. 4.43, the uncertainty is not forced to be monotonically increasing with jet p_T . This preserves the sign of the uncertainty and therefore ensures better closure. To be specific, expanding the left hand side of Eq. 4.28:

$$\sum_{i=1}^5 \epsilon_{p_T}^i SF_{p_T}'^i = \sum_{i=1}^5 \epsilon_{p_T}^i SF_{p_T}^i + \sum_{i=1}^5 \epsilon_{p_T}^i \Delta SF_{p_T}^i = 1 + \sum_{i=1}^5 \epsilon_{p_T}^i \Delta SF_{p_T}^i \quad (4.46)$$

and combining Eq. 4.43 with Eq. 4.46 above:

$$\sum_{i=1}^5 (\epsilon_{p_T}^i \Delta SF_{p_T,ref}^i + \epsilon_{p_T}^i \Delta_{rel}(\epsilon_{p_T}) SF_{p_T,ref}^i - \epsilon_{p_T}^i SF_{p_T,ref}^i \Delta_{rel}^i(\epsilon_{p_T,ref})) \quad (4.47)$$

The unitarity condition imposed in Equation 4.28 is still not completely fulfilled, since the first term in Equation 4.47 is zero only if the efficiencies for extrapolated and reference p_T are the same, while the last two are zero only if the already mentioned efficiencies are the same and the SF measured in data for p_T^{ref} is equal to one, since the SF in the high- p_T region is assumed to be equal to the SF in the in-situ calibration region. However, the closure should already be much better than the result obtained from Eq. 4.44. The

non-closure is cross-checked explicitly in section 4.3.5.

4.3.3 Simulated event samples and object definitions

The in-situ b -jet and c -jet b -tagging calibration analyses are computed on a b, c -jet enriched $t\bar{t}$ data sample, while the *light*-jets b -tagging calibration is performed on data events enriched in Z +jets. Both the $t\bar{t}$ and Z +jets process have a steeply falling spectrum at high p_T , thus there are not enough events at very high jet p_T to perform a data based calibration. Above a certain jet p_T threshold, which depends on flavor and jet reconstruction algorithm, an extrapolation procedure is used, while relies on simulation based systematic uncertainties, such high p_T extrapolations have been computed using a $Z' \rightarrow q\bar{q}$ MC sample. The $Z' \rightarrow q\bar{q}$ sample consists for 30% of $Z' \rightarrow b\bar{b}$, for 30% of $Z' \rightarrow c\bar{c}$ and of 30% $Z' \rightarrow l\bar{l}$ where l represents u, d, s light quarks. The jets in the sample are reconstructed as Variable-Radius Track Jets, for which the jet identification is performed using a variable radius cone depending on the jet p_T [50]. The variable radius parameter used for the VR track jets is $0.02 < R < 0.4$. A variety of tracking and modeling uncertainties are evaluated using the corresponding alternative samples for DL1r [51] b -tagging algorithm listed in Table 4.2. The same table with exact sample name is listed in appendix .8. The Z' samples are generated with a wide Z' mass spectrum, to provide a nearly flat distribution of jet p_T up to 3 TeV. In order to derive systematic variations, nominal samples are generated for each of these samples. A comparison among the nominal samples using different generator setups shows that the largest differences on the b -tagging efficiency for real b -jet is at most 2% across all p_T bins. For most of the p_T bins, the difference is less than 0.2%. Therefore the nominal samples are consistent. This said, the uncertainty evaluation has been performed on pairs of samples with the same generator setup, but with and without a specific systematic variation applied.

The extrapolation uncertainties are evaluated separately for b -, c - and *light*-flavour jets restricting the selection to the two p_T -leading jets in the event and applying an upper cut on b -hadron $p_T < 1000$ GeV. The cut is applied since the b -jets beyond 1000GeV are contaminated a non-negligible fraction of fake tracks, which make the estimate of the track p_T , and thus of the track-jet p_T , unreliable.

4.3.4 Uncertainty evaluation

The extrapolation uncertainties are composed by a modeling and a tracking component. In particular:

Generator	Shower	PDF	Process	Uncertainty Type
Pythia8	Pythia8	NNPDF23LO	$Z' \rightarrow bb/cc/ll$	Tracking
Pythia8	Pythia8	NNPDF23LO	$Z' \rightarrow bb/cc/ll$	Final state radiation
Madgraph	Herwig7	NN23LO1	$Z' \rightarrow bb/cc/ll$	Parton shower
Madgraph	Phythia8	NN23LO1	$Z' \rightarrow bb/cc/ll$	Parton shower

Table 4.2: A list of Z' samples used for evaluating systematic uncertainties of Monte Carlo events.

- **Tracking uncertainties:** fake track rate, tracking efficiency, d_0, z_0 resolution and alignment uncertainties.
- **Modeling uncertainties:** final state radiation modeling, parton shower modeling and quasi-stable uncertainty (the latter only for b -jets).

The quasi-stable uncertainty accounts for the fact that the current default ATLAS simulations does not model the hits from charged hadrons flying in the detector before decaying. High p_T b -hadrons might however decay after traveling through the first few layers (30 to 100mm from collision point for b hadron p_T around 400 to 1200 GeV) of the inner tracker, and having such additional hits has a small but non-negligible impact on the tagging efficiency. The quasi-stable uncertainty affects only b -jets, due to the b -hadron's longer decay time compared to the c and *light*-hadrons. Figures 4.8-4.11 show scale factor variation related to modeling, and tracking, and their combined uncertainty for the 0-60% b -tagging efficiency bin of the pseudo-continuous working point.

Fig. 4.8 shows the variations induced by the modeling uncertainties on the 0 – 60% bin of the pseudo-continuous distributions. The largest modeling uncertainty in this category is due to the parton shower modeling, evaluated comparing nominal sample showered by Pythia8 with alternative sample showered by Herwig7, both generated by Madgraph. The reference p_T is 250 GeV, and the extrapolation region is 250-1000 GeV.

The individual variations in the figure represent the sum of the last two terms of Eq. 4.43, i.e. the scale factor variation with respect to the reference p_T . The first term in Eq. 4.43 is not shown since it purely depends on the standard calibration result. The total uncertainty is the quadrature sum of the individual variations. The aim of showing the total uncertainty in the figure is mainly to compare its magnitude and trend with respect to the different components. A extrapolation uncertainties will actually be delivered to physics analyses as set of eigenvectors that preserve the sign of the uncertainties, as explained in the next section, not just as a single total uncertainty. It is

worth mentioning that, although the individual uncertainties are sometimes not monotonically increasing versus jet p_T – as can be seen for example in the final state radiation systematic variation in Fig. 4.8 – the total uncertainty is in most of the cases still approximately monotonically increasing, especially for b and *light* jets, even if such monotonic increase is not forced externally as with the previous methodology. This behaviour ensures higher uncertainties at higher p_T , which reflects the fact that when moving further away from the p_T reference point, there is less confidence on the assumption that $R = 1$. Fig. 4.9 shows the total **b**-jets uncertainty in the 0 – 60% bin of the pseudo-continuous weight distribution, where the modeling uncertainty dominates and one can see very clearly that the total uncertainty is monotonically increasing with jet p_T .

Fig 4.10 shows the *light*-jets tracking variations in the same bin of the pseudo-continuous tag weight distributions. The reference p_T is 300 GeV and the extrapolation region is 300-1200 GeV. Due to the high *light*-jet rejection of the b -tagging algorithm, the number of light jet in MC passing b -tagging is limited so only three p_T bins are shown in the plot. The uncertainty is dominated by the fake track rate uncertainty and the total tracking uncertainty is monotonically increasing. Fig. 4.11 shows the total *light*-jet uncertainty in the same tag weight bin. Also in this case the total uncertainty is monotonically increasing as a function of p_T . Additional plots are shown in Appendix .5.

4.3.5 Results

As described in section 4.3.2, the sum of the varied efficiencies in the pseudo-continuous bins is not strictly equal to one. In particular, to evaluate the closure one can focus on the closure of the last two terms in Eq. 4.43, which are those that defined on the chosen extrapolation method:

$$\sum_{i=1}^5 \epsilon_{p_T} S F_{p_T, ref} (1 + \Delta_{rel}(\epsilon_{MC, p_T}) - \Delta_{rel}(\epsilon_{MC, p_T, ref})) \quad (4.48)$$

which should be ideally equal to one. The results of the sum as a function of b -jet p_T is shown in Figure 4.12. This test has been performed using only the quasi-stable uncertainty, since it has been proven to be the largest contribution to the extrapolation uncertainty for b -jet. The figure shows the non-closure from two sources—first, the non-closure from the nominal scale factor value. If the scale factor at the p_T reference point is used to calibrate the efficiency in the extrapolation region, then the closure is within 7% as shown by the black line in the plot. The second non-closure sources are from systematic

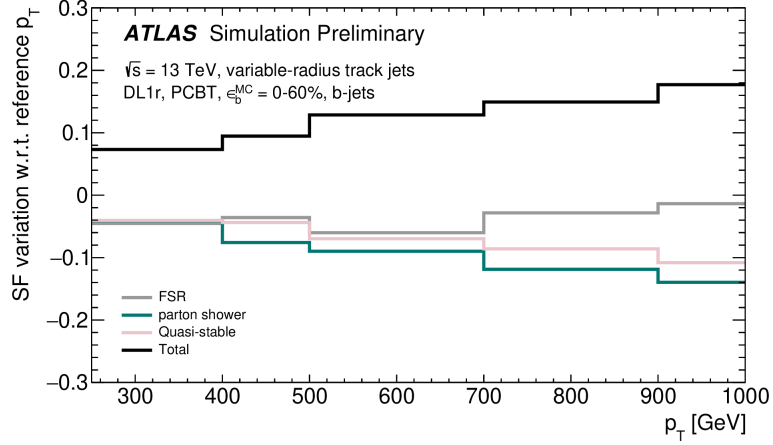


Figure 4.8: Modeling related scale factor variations used to extract the Monte Carlo based extrapolation uncertainties for the DL1r tagger applied to Variable Radius track jets as a function of the reconstructed b -jet p_T . The figure refers to the 0-60% Working Point interval of the pseudo-continuous b -tagging calibration, which is a simultaneous calibration of a binned version of the continuous b -tagging score distribution, expressed in intervals of the b -tagging efficiency [10]. The uncertainties are evaluated on $Z' \rightarrow q\bar{q}$ samples, largely following the method described in Ref. [11]. The monotonic requirement described in Ref. [11] is now dropped and the extrapolation uncertainties are applied to reconstructed $p_T \geq 250$ GeV jets. The events are required to have b -hadron $p_T \leq 1000$ GeV. The contribution from final state radiation is shown in grey, variations pertaining to the parton shower modeling are shown in blue, while the pink curve accounts for the effect of simulating the hits in the detector before the charged b -hadron decay, which is usually not included in the current ATLAS detector simulations. The total variation (black curve) is obtained as the sum in quadrature of the single contributions.

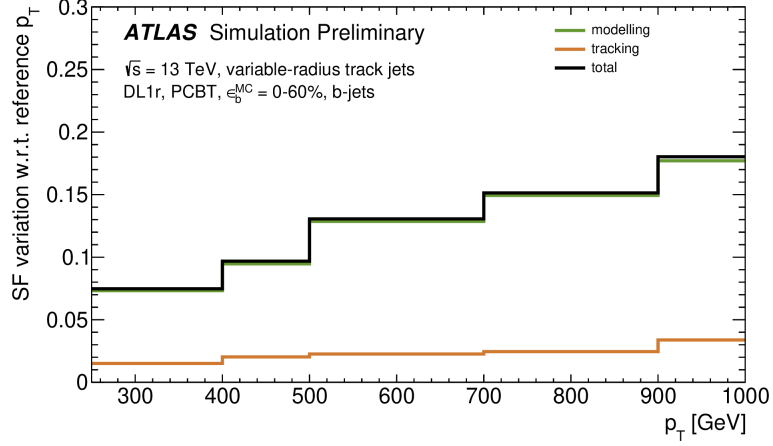


Figure 4.9: Monte Carlo based extrapolation uncertainties for the DL1r tagger applied to Variable Radius track jets as a function of the reconstructed b -jet p_T (black curve). The contribution from experimental uncertainties affecting the reconstruction of tracks is shown in orange. Theoretical uncertainties on the modeling of the jet fragmentation are drawn in green. The total variation is obtained summing in quadrature the single contributions. The figure refers to the 0-60% Working Point interval of the pseudo-continuous b -tagging calibration, which is a simultaneous calibration of a binned version of the continuous b -tagging score distribution, expressed in intervals of the b -tagging efficiency [10]. The uncertainties are evaluated on $Z' \rightarrow q\bar{q}$ samples, largely following the method described in Ref. [11]. The events are required to have b -hadron $p_T \leq 1000$ GeV. The monotonic requirement described in Ref. [11] is now dropped and the extrapolation uncertainties are applied to $p_T \geq 250$ GeV jets.

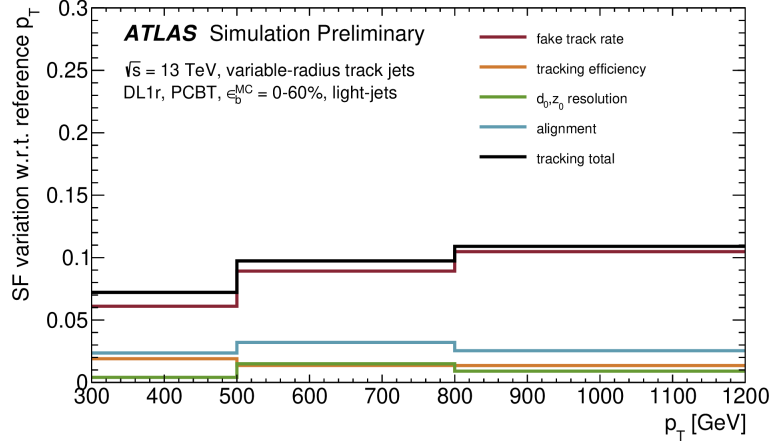


Figure 4.10: Tracking related scale factor variations used to extract the Monte Carlo based extrapolation uncertainties for the DL1r tagger applied to Variable Radius track jets as a function of the reconstructed light-jet p_T . The figure refers to the 0-60% Working Point interval of the pseudo-continuous b-tagging calibration, which is a simultaneous calibration of a binned version of the continuous b-tagging score distribution, expressed in intervals of the b-tagging efficiency [10]. The uncertainties are evaluated on $Z' \rightarrow q\bar{q}$ samples, largely following the method described in Ref. [11]. The monotonic requirement described in Ref. [11] is now dropped and the extrapolation uncertainties are applied to reconstructed $p_T \geq 300$ GeV jets. The uncertainties are categorized into 5 main contributions. The contribution from the fake track rate uncertainties is shown in red, while the one from the tracking efficiency is shown in orange. The d_0 and z_0 resolution uncertainties are shown in green while the alignment uncertainty is shown in blue. The total variation (black curve) is obtained as the sum in quadrature of all the tracking related contributions.

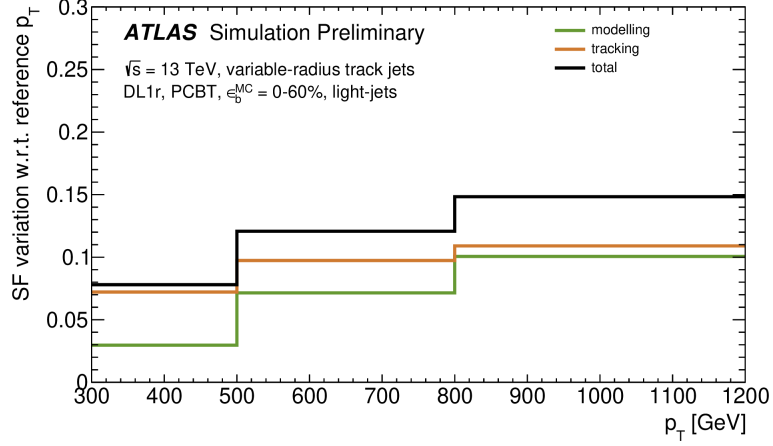


Figure 4.11: Monte Carlo based extrapolation uncertainties for the DL1r tagger applied to Variable Radius track jets as a function of the reconstructed *light*-jet p_T (black curve). The contribution from experimental uncertainties affecting the reconstruction of tracks is shown in orange. Theoretical uncertainties on the modeling of the jet fragmentation are drawn in green. The total variation is obtained summing in quadrature the single contributions. The figure refers to the 0-60% Working Point interval of the pseudo-continuous b -tagging calibration, which is a simultaneous calibration of a binned version of the continuous b -tagging score distribution, expressed in intervals of the b -tagging efficiency [10]. The uncertainties are evaluated on $Z' \rightarrow q\bar{q}$ samples, largely following the method described in Ref. [11]. The monotonic requirement described in Ref. [11] is now dropped and the extrapolation uncertainties are applied to $p_T \geq 300$ GeV jets.

uncertainties. If the quasi-stable systematic uncertainty corrects the scale factor in the extrapolation region and also the reference point scale factor is used in the extrapolation, the closure is within 8% as shown by the green line. Thus the leading contribution to the non-closure comes mainly from the assumption that the scale factor in the extrapolation region is equal to the scale factor at the p_T reference point.

The reason of the non-closure has been further investigated in Figure 4.13. In particular, the non-closure in the lower p_T region just above p_T^{ref} is due to the loosest three tag weight bins, which have SFs at the reference point all larger than 1. This also makes the total efficiency larger than 1. In the higher p_T region, the 85-100% WP has the highest fractional efficiency and a SF of 1.13, which similarly leads to a total efficiency larger than 1 as reported in Figure 4.12.

It is also useful to check the closure of the total uncertainty including all three terms in Eq. 4.43: Result is shown in Figure 4.14.

$$\sum_{i=1}^5 \epsilon_{p_T} SF_{p_T,ref} (1 + \Delta_{rel}(SF_{p_T,ref}) + \Delta_{rel}(\epsilon_{MC,p_T}) - \Delta_{rel}(\epsilon_{MC,p_T,ref})) \quad (4.49)$$

In this case, the uncertainty from the p_T reference point extracted from the in-situ calibration is also included. The result of the total uncertainty in each bin as a function of b -jet p_T is shown in Figure 4.14. An eigenvector decomposition is then performed including the extrapolation uncertainties and the uncertainties from the in-situ calibration at the reference p_T point. More details on the eigenvector decomposition can be found in section 4.3.6 and in Ref. [52]. In the plot, the blue line represents the sum of the efficiency corrected by the largest eigenvector uncertainty. The overall non-closure including all terms reoesentend in 4.49 is within 13%. This is the largest eigenvector uncertainty in the full p_T region considered. Therefore it could provides an estimate of the maximum level of expected non-closure. Furthermore, it should be noted that only the first term of Eq. 4.49 provides a permanent non-closure (up to 8%), while the rest is covered within the extrapolation uncertainty . Such permanent non-closure is typically significantly smaller than the total extrapolation uncertainty.

4.3.6 Implementation in physics analyses

In general, the number of uncertainties from the in-situ b -tagging calibration is in the order of $O(100)$. In order to make them usable in physics analyses this number is reduced to $O(10)$ using a an eigenvector decomposition method [52].

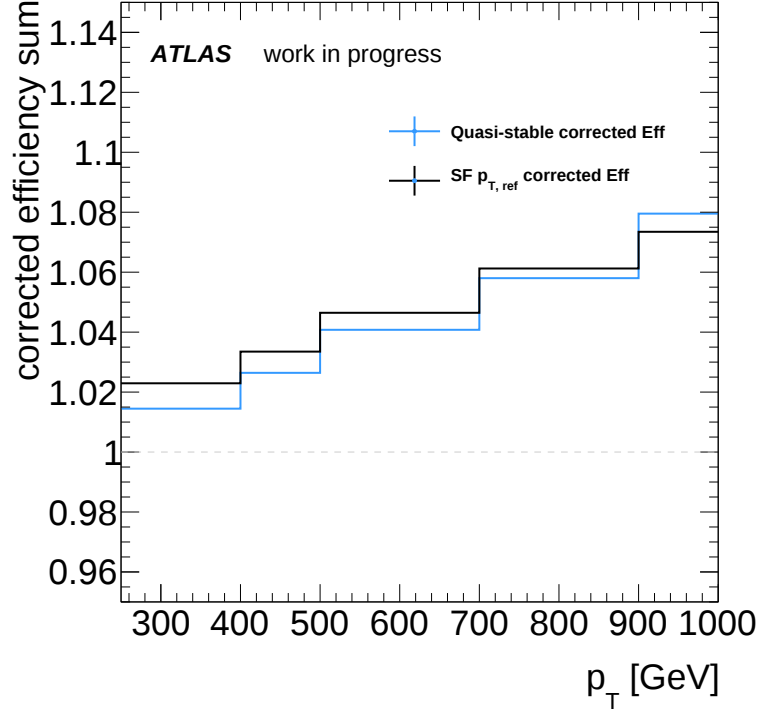


Figure 4.12: Sum of the corrected efficiencies in all b -tagging bins as a function of the b -jet p_T . The sum of the corrected efficiencies as shown in Eq. 4.48 using only the quasi-stable uncertainty, which is the dominant uncertainty for b -jets, is shown in blue. The plot refers to b -jets selected from Z' events. The maximum non-closure remains within 8%. The black line shows the non-closure of the sum of the efficiencies corrected only by the scale factor at the p_T reference point. The non-closure in this case remains within 7.5%.

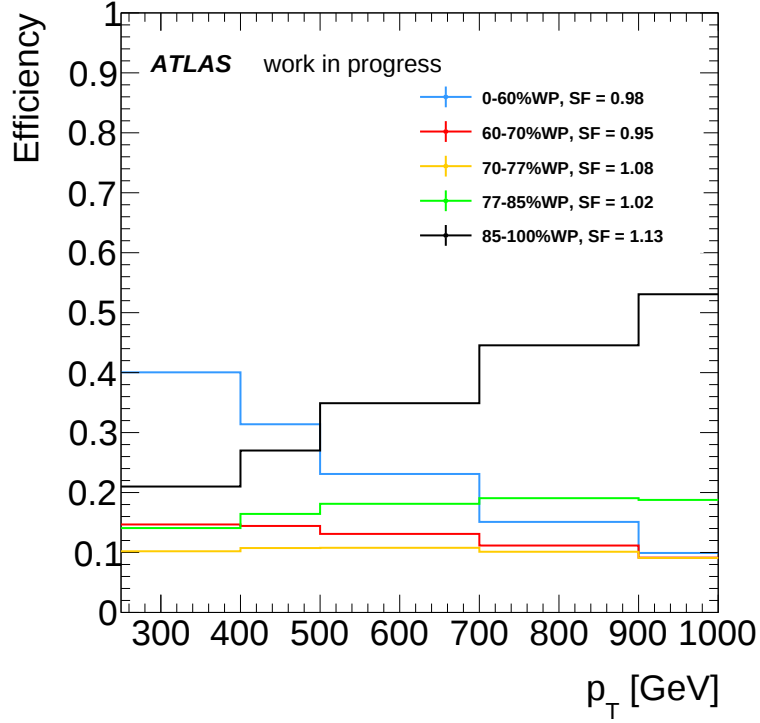


Figure 4.13: The b -tagging efficiency as a function of b -jet p_T for each bin of the pseudo-continuous working point, computed using Z' events. The scale factors at the p_T reference point for each tag weight bins are: 0.98 for the 0-60%, 0.95 for the 60-70% , 1.08 for the 70-77% , 1.02 for the 77-85%, 1.13 for the 85-100% bin.

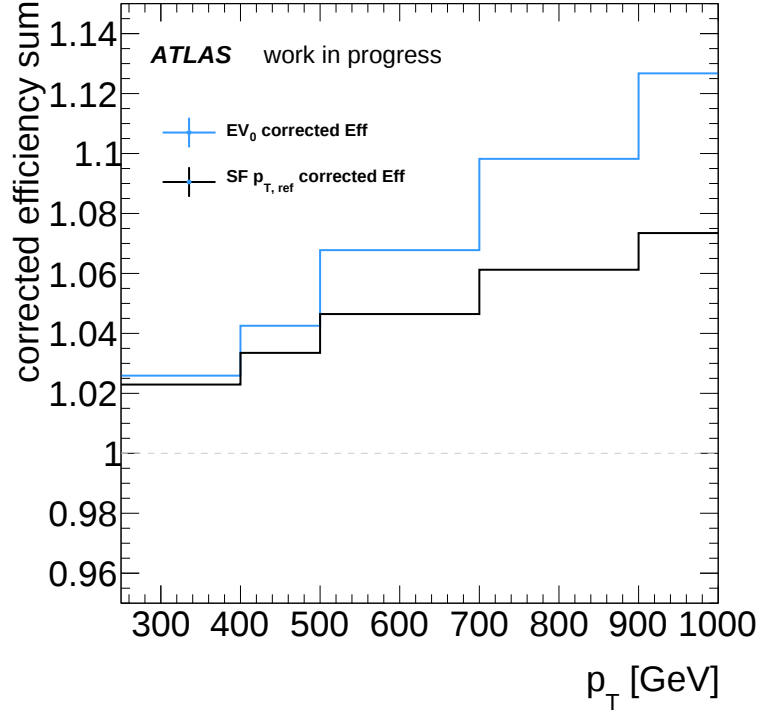


Figure 4.14: Sum of the corrected efficiencies in all b -tagging bins as a function of the b -jet p_T . The largest eigenvector uncertainty for b -jets computed using Z' events is shown in blue. The maximum non-closure remains within 13%. The black line shows the non-closure on the efficiencies corrected only by the scale factor at the p_T reference point. The non-closure in this case remains within 7.5%.

It is also introduced in section 4.2.2 of this thesis.

Eigenvector decomposition in the high- p_T extrapolation region

The eigenvector decomposition in the high p_T region has to include both the uncertainties from the in-situ calibration at the reference point and the additional uncertainties from the extrapolation. There are thus two possible options:

- The first option is to implement the eigenvector decomposition separately for the in-situ calibration region and the high p_T extrapolation region. The advantage is that this allows to fully decorrelate the uncertainties in the in-situ calibration region from the ones in the high p_T region. In physics analyses this separates the contributions from the high- p_T uncertainties and the in-situ calibration uncertainties, such that no nuisance parameter considered in the analysis can mix these two different contributions, simplifying the interpretation of b -tagging systematics
- The second option is to treat high p_T extrapolation uncertainties and the in-situ calibration uncertainties at the same time and then performing an eigenvector decomposition on the whole set of the uncertainties. The advantage of this option is that the implementation is technically easier as the analyses would deal with a single set of eigenvectors. The downside of this method is that it would increase the number of eigenvector uncertainties in the analyses. This is because the number of eigenvectors after decomposition is equal to the dimension of the covariance matrix, which is equal to $N_{p_Tbins} \times N_{TagWeightBins}$. Therefore, after including the high- p_T bins, the number of p_T bins (N_{p_Tbins}) increases which makes the number of flavor tagging eigenvectors increases. Although this can be mitigated by pruning the eigenvector uncertainties, the pruning will make the in-situ calibration no longer 100% accurate as sub-leading components will be lost during the pruning stage.

Considering that certain analyses might be interested in combining with other analyses not particularly sensitive to the high- p_T extrapolation region, the final ATLAS-wide decision was to favour option 1 and actually compute two sets of eigenvectors: one for the in-situ calibration in the low- p_T regime and a second for the high- p_T region. Note that for both options the in-situ calibration uncertainties need to be extended to the high p_T region because the high- p_T extrapolation uncertainties include a term related to the reference p_T (first term in the right-hand side of equation 4.43).

Eigenvector pruning

Based on the discussion above, the eigenvector decomposition has been chosen to be done separately for high- p_T extrapolation uncertainties and in-situ calibration uncertainties. After the eigenvector decomposition of the 17 high- p_T extrapolation uncertainties, the number of eigenvectors (EV) left is:

$$N_{EVs} = N_{TagWeightBins} \times N_{p_Tbins} \quad (4.50)$$

In reality, since the normalization over the full tag weight distribution is always preserved in the in-situ calibration, the number of eigenvectors corresponding to non-zero eigenvalues is as expected to be $N_{EVs} = (N_{TagWeightBins} - 1) \times N_{p_Tbins}$. For b -jets in the current setup $N_{EVs} = 24$. This number is even larger than the number of original uncertainties before eigenvector decomposition. Even considering that some of this eigenvector will have zero eigenvalue, the number of eigenvectors is still very large and needs to be reduced. To do this, the following pruning strategy has been put in place with the aim of maximally preserving the correlations of the uncertainties across jet p_T and tag weight bin:

1. Calculate total uncertainty by summing in quadrature all the eigenvector variations in each in-situ calibration p_T and tag weight bins.
2. Pick one eigenvector uncertainty and take the ratio of the absolute value of each bin over the the total uncertainty in that bin. Sum up the ratio value obtain in each bin.
3. Find the eigenvector uncertainty that gives the highest value and mark it as the first eigenvector in the ranking.
4. Iteratively pick the other eigenvector uncertainties and repeat the two steps above. Keep ranking the uncertainties as in previous steps until a certain threshold is met.

This threshold represents the amount of total uncertainty that is retained by the eigenvectors in the list. For this work the threshold has been set to 99.5% for b -jets, 99% for c -jets and *light*-jets, meaning that the selected eigenvectors were able to retain 99.5% (99%) of the total uncertainty. After this iterative process, 4 EVs for b -jets, 2 EVs for c -jets and 3 EVs for *light*-jets have been retained as final eigenvectors to define the high- p_T extrapolation uncertainties in physics analyses. The first eigenvector uncertainty for b -jets in the 0 – 60% tag weight distribution is shown in Figure 4.15. The plot shows that the first eigenvector uncertainty represent a large fraction of the

total uncertainty. Also, note that the high- p_T uncertainties are set to 0 in the in-situ calibration region with jet p_T below 250GeV. After the pruning, some correlations between different tag weight & p_T bins have been lost, but the procedure adopted limit such lost to less than 12% as shown in Figure 4.16. The uncertainties are also summed in quadrature and plotted in different tag weight & p_T bins in Figure 4.17. The bottom panel in the same figure shows the ratio between the sum in quadrature of four eigenvectors and the sum of all uncertainties: this ratio vs. larger than 90% everywhere. Note that the sum over the ratio value of each bin of the bottom panel histogram is the optimization target in the pruning procedure.

4.3.7 Validation

The extrapolation uncertainties, along with all in-situ calibration results have been stored in the official ATLAS b -tagging calibration file and are then used in all physics analyses that require b -tagging of high p_T jet. The validation has been performed on Variable-Radius Track jets using the pseudo-continuous calibration for b -, c - and *light*-jets. Since option 1 described in section 4.3.6 has been chosen, the uncertainties within the in-situ calibration region should be identical between before and after adding the high- p_T extrapolation uncertainties. Figure 4.18 shows that the in-situ calibration uncertainties are not affected by adding the high- p_T extrapolation uncertainties as desired. This is also tested for all calibration uncertainties below the jet p_T reference point. For the original in-situ calibration uncertainties in the new implementation, the SF variations are extended to high- p_T because the value of the in-situ calibration variations at the reference point provides the first term required to calculate the extrapolation uncertainty at high- p_T , as shown in equation 4.43. In practice the original in-situ uncertainties are extended to high- p_T values by just copying the value of the SF variations for the reference p_T bin to all newly-added high jet p_T bins. A striking consequence of such p_T extension, even before adding any extrapolation uncertainty, is a change induced in the eigenvector variations obtained from eigenvector decomposition. The difference in the first eigenvector variation for b -jets before and after the high p_T extension is shown in figure 4.19. The differences are coming from the fact that the SF variation of the reference p_T bin is magnified, therefore weighting up the importance of the last p_T bin in the eigenvector decomposition/principle component analysis. This leads to a change in the resulting eigenvectors. However, the new eigenvector uncertainties do still correctly represent the in-situ calibration uncertainties.

It worth mentioning that the original in-situ eigenvector uncertainties before high p_T extension can be recovered from those after the high p_T extension

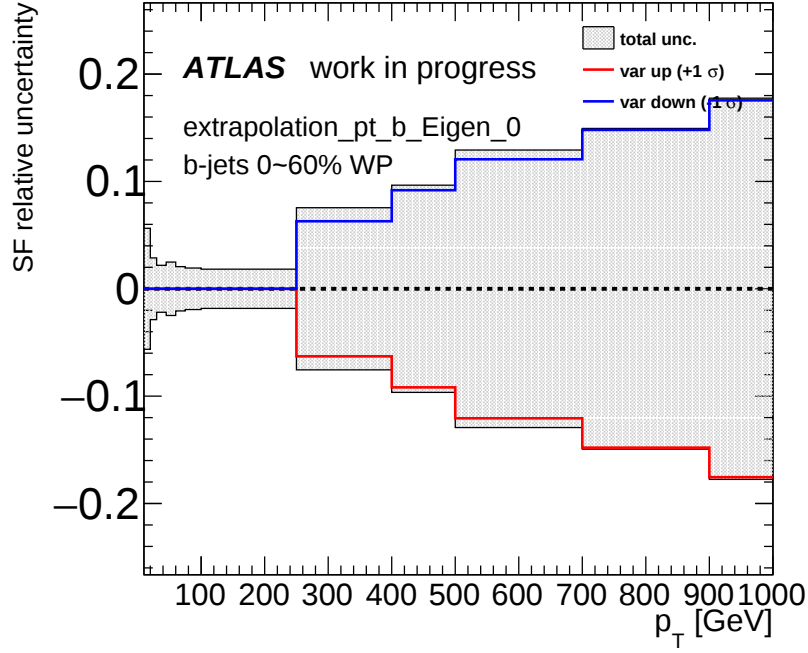


Figure 4.15: The plot shows the relative variation of the scale factor of the $[0,60\%)$ b -tagging efficiency interval for the leading eigenvector variation of the high p_T extrapolation, one for the upward variation (blue) and one for the downward variation (red). The shaded gray area shows the quadrature sum of all uncertainties (in-situ + high- p_T extrapolation) for comparison.

ATLAS preliminary

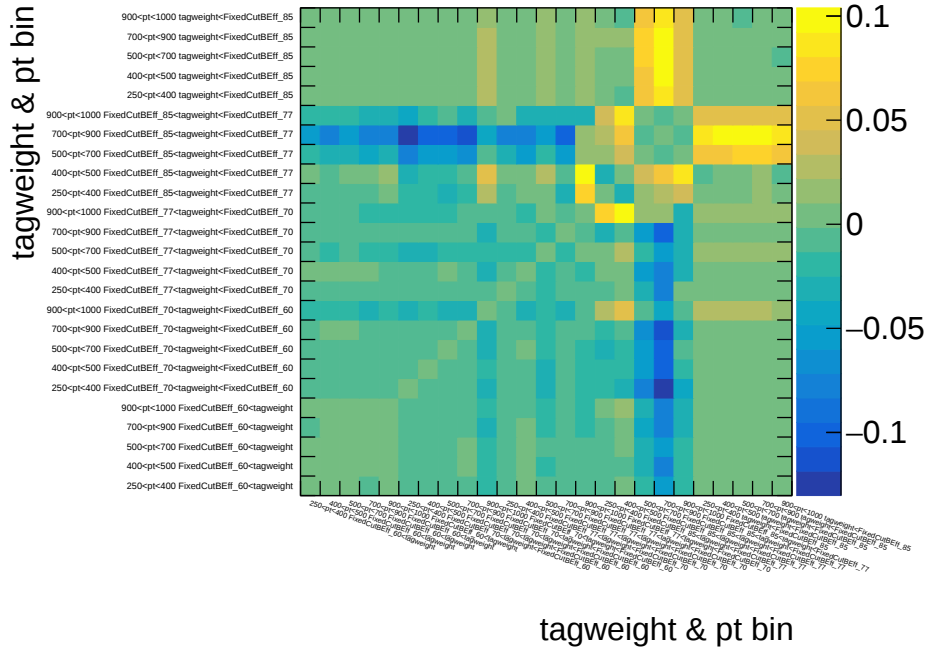


Figure 4.16: The 2d histogram shows the differences between the complete correlation matrix across all tag weight and jet p_T bins in the high p_T extrapolation region, and the approximate correlation matrix based on the four eigenvector variations that survive the pruning procedure.

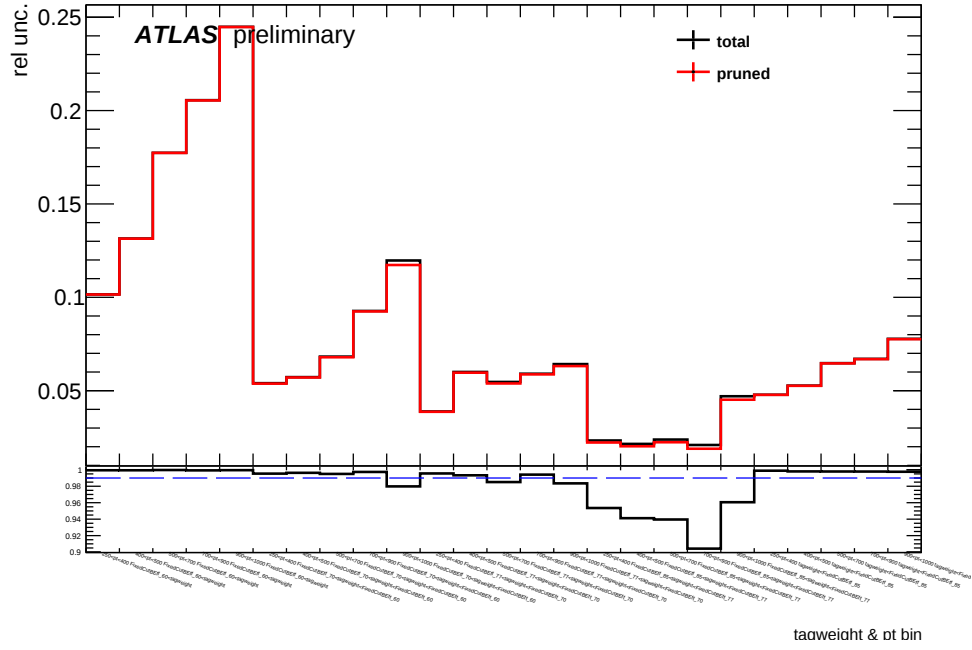


Figure 4.17: The top panel shows the quadrature sum of all extrapolation uncertainties labeled as "total" and the quadrature sum of four remained eigenvector uncertainties of b-jets after pruning labeled as "pruned". The bottom panel shows the ratio between "pruned" and "total".

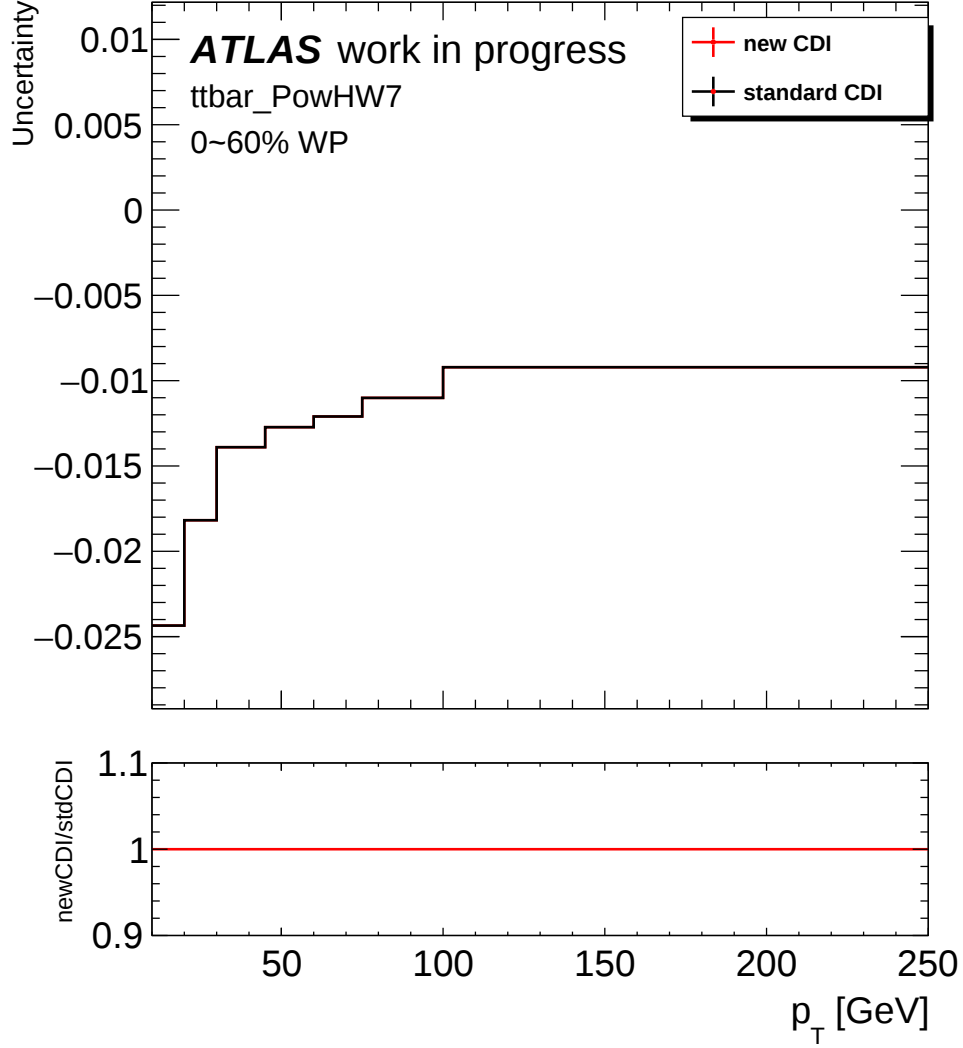


Figure 4.18: Comparison of the size of the leading systematic uncertainty between the in-situ calibration uncertainties before and after adding the extrapolation uncertainties. In this plot, the uncertainty applies to the scale factor of the 0-60% b -tagging efficiency interval, and is shown as a function of jet p_T . In the bottom panel the ratio is between the new CDI(Calibration Data Interface) containing the new extrapolation uncertainty, and the old one without.

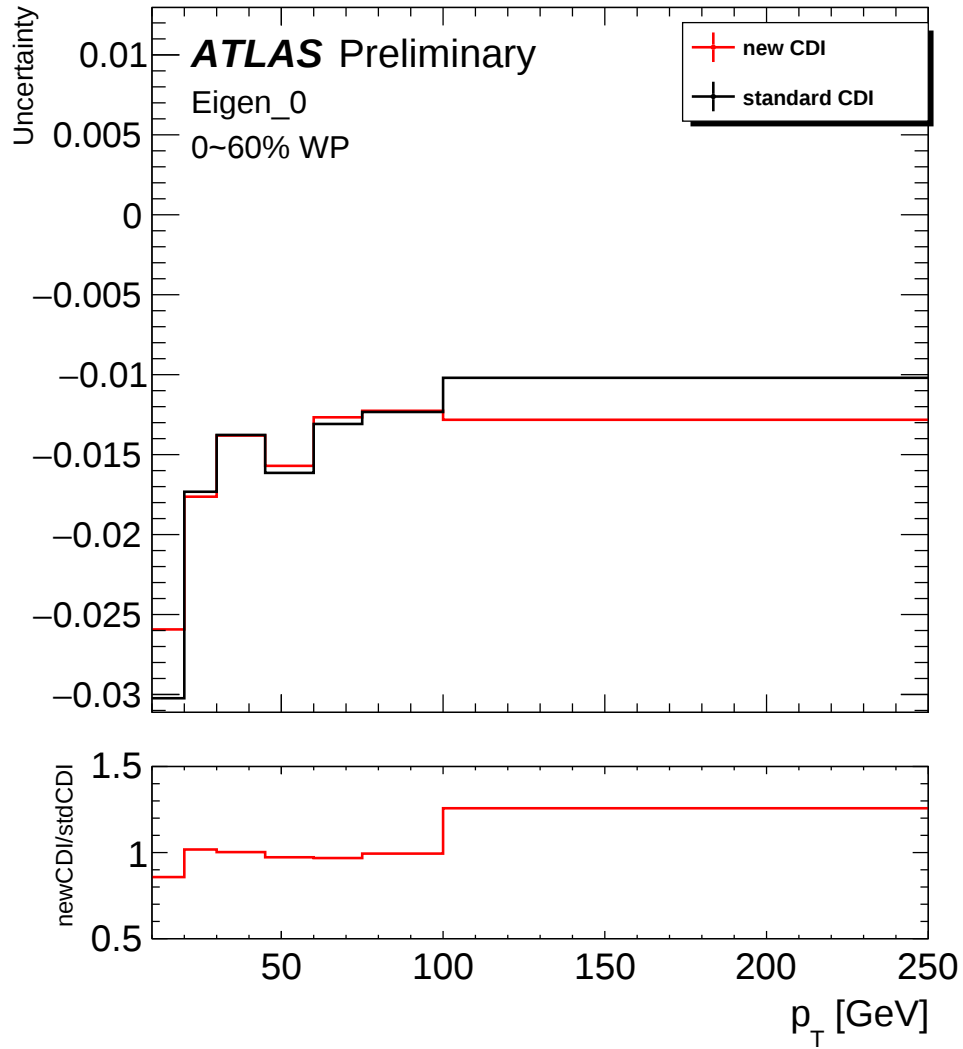


Figure 4.19: The top panel shows the eigenvector variation of the scale factor for the 0-60% tagging efficiency interval before and after the high p_T extension. The bottom panel shows the ratio between the same eigenvector variations after and before the p_T extension.

with some operations based on the following steps:

1. Rescale the last bins(reference jet p_T) of original uncertainties by $\frac{1}{\sqrt{k+1}}$, where k is the number of added p_T bins in the high- p_T region.
2. Perform the eigenvector decomposition on the original uncertainties obtained in step 1. The resulting eigenvalues are exactly the same as the eigenvalues from the original in-situ calibration. Detailed proof is written in appendix .6.
3. Multiplying the last bins of the eigenvectors produced from the previous step by $\frac{1}{\sqrt{k+1}}$. The resulting eigenvector uncertainties are exactly the same as the in-situ eigenvector uncertainties below the p_T reference point. Detailed proof is written in appendix .7.

Although the procedures given above allows to recover the exact same eigenvalues and eigenvectors as those before the high p_T extension, this method has not been finally officially adopted since it is not straight-forward to implement in a way that may prevent cause confusion in the future. This implies that, despite no change in this combined impact, the eigenvector variations of the in-situ calibrations do vary when applying the high p_T extrapolations, and such changes also depend on the number of p_T bins in the extrapolation region.

Another thing worth mentioning is the treatment of in-situ statistical uncertainties in the extrapolation procedure. The statistical uncertainty of b - and c -jet are decomposed into eigenvector uncertainties in the in-situ calibration analysis and therefore can be treated as the form of systematic uncertainties when constructing the covariance matrix. This means that extrapolation procedure is the same for statistical uncertainties of b - and c -jet during the extrapolation, i.e. The uncertainty value of in the reference p_T bin is copied to the extended all bin in high- p_T region. However, there is no eigenvector decomposition performed for light-jet statistical uncertainties therefore the uncertainties in all p_T bin and pseduo-continuous tag weight bins are uncorrelated. During the eigenvector decomposition, such uncertainties values is squared and only added onto the diagonal element of the covariance matrix. To extrapolate such uncertainty, one systematic formed uncertainty is created for each working point interval as the extrapolated statistical uncertainties. The value of in-situ calibration statistical uncertainty of the p_T^{ref} bin is copied to all p_T bins of the newly created uncertainty starting from p_T^{ref} bin. All p_T bins before the p_T^{ref} bin is set to zero. And the uncorrelated statistical uncertainties of the original form remains the same before and not including

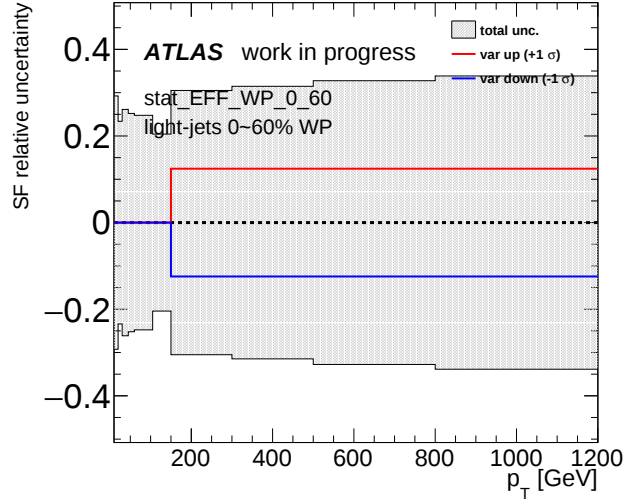


Figure 4.20: The quadrature sum of all systematic form uncertainties are shown in gray. Extended statistical uncertainties of light jet is shown in Red and Blue. The p_T reference bin ranges from 150 to 300 GeV. Therefore uncertainties are set to zero below 150 GeV and constant at above 150 GeV.

p_T reference bin. Therefore in this way, the statistical uncertainties are uncorrelated across all p_T bins and working point tag weight bins in the in-situ calibration p_T region. At the same time, the statistical uncertainties are fully correlated in the high- p_T region with the p_T reference bin. One example of light-jet extended statistical uncertainty is shown in Figure 4.20.

Chapter 5

Measurement of Higgs decay to two b quarks

The Higgs particle was discovered in 2012 [13] [14]. There are various Higgs production channel. The one that has largest cross-section is the gluon-gluon fusion. As for the Higgs boson decay, the largest branching ratio is to two b quarks, which is expected to be about 58%. However, this decay mode is hard to be observed via gluon-gluon fusion Higgs boson production because of large background from multi-jet production. To measure Higgs boson decaying to two b -quarks, the best Higgs boson production channel is the associated production with a vector boson(VH) where one vector boson, either the W or Z boson, is produced in association with a Higgs boson. If the vector boson decays leptonically into neutrinos or charged leptons, the leptons will provide a handle to reducing the large multi-jet background. This chapter is about the measurement of the Higgs boson decay to two b -quarks. It has been discovered and measured in [13] [14] [53]. The following of this chapter will be discussing how this measurement can be improved.

5.1 Event reconstruction and selection

In this analysis leptons are counted to be according to the number of charged leptons, i.e. electrons, muons or taus. There are three possible leptonic decay modes for a vector boson in VH production. If the vector boson is a Z boson, it could decay into two charged leptons or two neutrinos. If the vector boson is W boson, it could decay into one lepton and one neutrino. Therefore the analysis can be divided into three channels: zero lepton, one lepton and two leptons. This thesis will be mainly focusing on the one lepton channel.

After the Higgs boson decays to two b -quarks, due to color confinement,

the b-quarks will shower additional quarks and gluons, then hadronize and become visible in the detector as a jet. However, when the Higgs boson carries large transverse momentum due to the lorentz boost, the two b-jets originating from b-quarks may be merged together into one jet. Therefore the strategy to identify two b-jets in relatively low and high transverse momentum is different. This leads to two different analyses: a *resolved* analysis for when the transverse momentum of the two b-jets system is below 400 GeV and a *boosted* analysis for when two b-jets are above 400 GeV.

The resolved $VH, H \rightarrow$ *analysis* is required to have exactly two *b*-tagged jets, where "b-tagged jets" is explained in section 4.1. The analysis region is splitted into signal region (SR) and control region (CR) which is separated based on the angle separation ($\Delta R(b, b)$) between two candidate b-jets. The SR contains events of which $\Delta R(b, b)$ value is in the middle range. One of the CR, Low- ΔR -CR (CRLow), is defined where $\Delta R(b, b)$ is in the low range. The other one of CR, High- ΔR -CR (CRHigh), is defined where $\Delta R(b, b)$ is in the upper range. Also, the events are splitted into three regions based on transverse momentum of the reconstructed vector boson (p_T^V): $75 \text{ GeV} < p_T^V < 150 \text{ GeV}$, $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$. Furthermore, the events are also splitted into 2,3-jets region, where in the 3-jet region, two of the jets are required to be *b*-tagged and the additional jet is required to be non-*b*-tagged jet.

The boosted $VH, H \rightarrow$ *analysis* is required to have one large-R jet. Large-R jet is calorimeter based jets reconstructed with anti- k_t [54] algorithm with radius parameter $R = 1.0$. The large-R jet is also required to contain at least two track-jet, where track-jet is reconstructed from tracks and has variable parameter ($0.02 < R < 0.4$). The track-jet and large-R jet matching is done by ghost association [55]. The two p_T leading track-jets both required to be *b*-tagged. This *b*-tagging requirement will be further investigated and improved in section 5.1.1. The events are splitted depending on if additional jet of radius parameter $R=0.4$ exist. In 0 and 1-lepton channel, the high purity signal region (HP SR) is defined as event in which no additional jet is present. Otherwise if there are at least one additional jet, the event falls in to low purity signal region (LP SR). Both HP and LP SR requires that the jets outside the large-R jet to be non-*b*-tagged, otherwise, the events will falls into $t\bar{t}$ enriched control region (CR). Also, similar to resolved analysis, boosted analysis is also categorized in different p_T^V range: $400 \text{ GeV} < p_T^V < 600 \text{ GeV}$, $600 \text{ GeV} < p_T^V$.

5.1.1 Event selection and categorization

b-tagging cut optimization

In order to identify("tag") a jet, the b-tagging algorithm provides a single score to represent the confidence of the algorithm in believing a certain jet is a b -jet. Therefore a threshold of this score has to be set so that any jets above such score will be b -tagged, and any jets with lower score will not be b -tagged. This threshold can be set according to fraction of true b -jets passing the b-tagging score threshold. The fraction is called efficiency. In total, there are 4 different efficiency working point values available: 60%, 70%, 77%, 85%. The smaller the efficiency is, the higher the c - and $light$ -jet rejection rate is, where the $light$ -jet is jet originating from light-weight quarks (up,down and strange quarks). Therefore a b -tagged sample is purer in b -jets after a b -tagging requirement with a lower efficiency working point is applied.

In boosted $VH, H \rightarrow bb$ analysis, both jets inside and outside the large-R jet could be true b -jets. For $VH, H \rightarrow bb$ signal events, the two b -jets should be inside the large-R jets and there should be no b -jets out of the large-R jet. For $t\bar{t}$ background event, it is possible that one top quark decays hadronically into a b -quark and a W boson, and that a c -quark is one of the W -boson decay products. In this case, it is possible that the c -quark and one b -quark formed a large-R jet, leaving another b -jet originating from a top quark to be outside the large-R jet. Such kind of $t\bar{t}$ events can be reduced by requiring any jets outside the large-R jet not to be b -tagged. The working point used for this tagging needs to be investigated carefully to maximize the analysis sensitivity. Also, the working point used for b-tagging jets inside the large-R jet should also be investigated. These two investigations shall be carried out together because of correlations to check which combination gives largest gain in analysis overall significance, where analysis significance is defined in section 5.5.1.

This can be done by using the pseudo-continuous b-tagging scheme as introduced in section 4.1 which provides more information on the b-tagging result. In this scheme, the available working point intervals are [0,60%], (60%,70%], (70%,77%], (77%,85%], (85%, 100%] to have exactly two b-tagged truth jets, where truth jets are particle level jets of from Monte Carlo (MC) sample so that the constituent particles are known. Therefore there are two b-tagging scores, one for each truth-jet to be b -tagged. One variable is defined to summarize the two b-tagging scores: trackJetInLeadFatJet, based on the following logic: when both jets are b -tagged to be in [0, 70%] working point interval, the trackJetInLeadFatJet value for this event is chosen to be [0,70%]. Otherwise, if any of the two jet scores is within (70%, 77%], the value of trackJetInLead-

FatJet for this event is defined to be (70%, 77%]. Both considered have to be b -tagged in [0, 77%] working point interval. Another variable, trackJetOutsideLeadFatJet, is defined to represent the b -tagging status of jet outside the large-R jet. The value is set to be equal to the b -tagging working point interval of the track jet outside the large-R jet. In case there is no track-jet outside the large-R jet, the value of trackJetOutsideLeadFatJet is set to (85%,100%], equivalent to the least b -jet like working point interval. This working point interval is renamed to be (85%,100%+] to mark the differences from the normal (85%,100%] working point interval. The expected significance over the background-only hypothesis is calculated by:

$$Z = \sqrt{\sum_i 2((s_i + b_i) \times \ln(1 + \frac{s_i}{b_i}) - s_i)}, \quad (5.1)$$

where b_i represent the yield of background events in bin i , s_i represent the yield of signal events in bin i . This equation gives better estimate of significance compared to $\frac{S}{\sqrt{B}}$ when the number of events in a certain bin is less than 10.

The significances for each analysis region defined by a certain value of trackJetOutsideLeadFatJet and trackJetInLeadFatJet are shown in Figure 5.1 for the low signal purity region and Figure 5.2 in the high signal purity region. It can be seen from the figure that the region having the largest significance is the tightest working point interval for the two track jets inside large-R jet and the loosest (anti-tag) working point interval for the track jet outside large-R jet. This result is expected since this region provides the purest b -tagged jets inside large-R jet, implying a higher signal fraction, and the least $t\bar{t}$ background. The region with the second largest significance is (70%,77%] working point for trackJetInLeadFatJet and (85%, 100%+] for trackJetOutsideLeadFatJet.

The m_{bb} distribution was used only to get a first estimate. In fact, the VH(bb) analysis is multivariate analysis: a set of high level physics variable(not just m_{bb}) is used as training variables for Boosted Decision Tree to provide a multivariate discriminant variable named mva that provides improved signal-vs-background discrimination, to be used in a maximum likelihood fit for measuring the signal strength, cross-section, and extracting the signal significance from the data. Therefore, this study needs to test how the b -tagging working point affects the mva significance. Two b -tagging related variables are used as input training variable, in addition to the other variables already used in the pre-existing BDT. Each one represents the pseudo-continuous b -tagging working point interval for one track jet inside the large-R jet. Another new variable, binTrkJNotInLeadFJMax, represents the working point interval of track-jet outside large-R jet. If there is more than one track-jet outside the

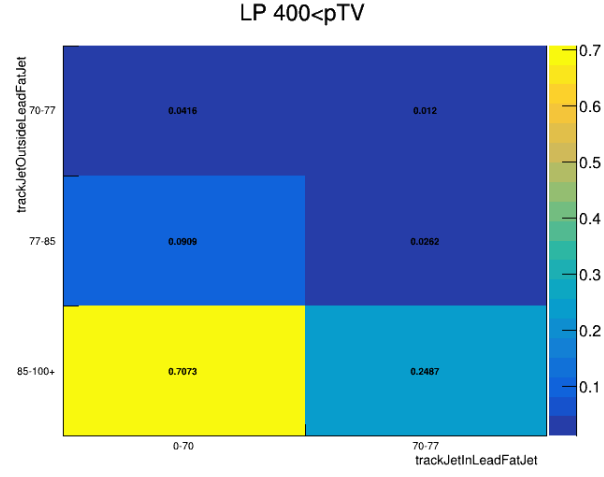


Figure 5.1: Significance scan for VH(bb) boosted low purity $p_T^V > 400 GeV$ region.

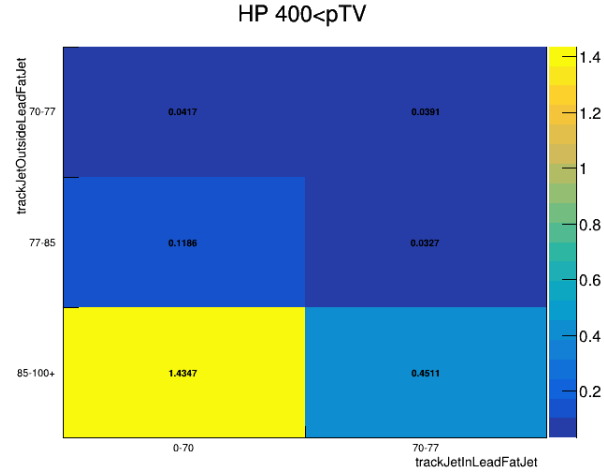


Figure 5.2: Significance scan for VH(bb) boosted high purity $p_T^V > 400 GeV$ region.

large-R jet, the track-jet with the largest b -tagging score is used. Various b -tagging threshold for track jet inside and outside the large-R jet is tested. For each variation, the event selection is changed and also the used analysis BDT is retrained since the input to MVA is changed. The result is shown in Table 5.1, where the b -tagging selection applied is represented by XXinYYout, where XX in XXinYYout represents the b -tagging selection requirement inside leading large-R jet, while YY represent the anti b -tagging(veto) selection requirements outside the leading large-R jet. For the former a higher efficiency implies a looser selection, while for the veto a higher efficiency implies a tighter selection.

	significance	improvement
70in70out(default)	2.33	0.00%
77in70out	2.41	3.43%
77in85out	2.46	5.58%
85in85out	2.57	10.19%
77in70out + binTrkJNotInLeadFJMax	2.47	6.01%
77in85out + binTrkJNotInLeadFJMax	2.43	4.29%
85in70out + binTrkJNotInLeadFJMax	2.55	9.44%

Table 5.1: Signal significance corresponding to different b -tagging selection thresholds for jets inside and outside leading large-R jet. Here the XX in XXinYYout represent the single b -jet efficiency of the b -tagging threshold for track-jet inside leading large-R jet, while YY represent the same efficiency for the anti(veto) b -tagging cut outside the leading large-R jet. All configurations tested include the b -tagging scores of the leading two jets within the large-R jet as input to the mva. Only the last three configurations tested include the variable binTrkJNotInLeadFJMax as input to the mva representing the largest b -tagging score of all VR track jets outside the large-R jet.

The calculation for significance of mva is the same for m_{bb} as described in equation 5.1. The significance scan shows that the b -tagging combination giving the largest significance improvement is 85% for track-jet inside large-R jet and 85% for anti- b -tagging for track jet outside the large-R jet without using the new variable binTrkJNotInLeadFJMax. This is the loosest choice fro the jets inside the large-R jet, and the most strict veto for the jet outside it.

To further check the validity of the new b -tagging working point setup, a comparison of data and Monte Carlo(MC) was needed. This can be seen in Figure 5.3 for high signal purity region and 5.4 for low signal purity region. Figures show that after changing the b -tagging selection from 70in70out to

85in85out, the number of events in the signal sample is increased. The analysis can benefit from higher statistical power especially in the $p_T^V > 600$ GeV region. The agreement between data and MC with 85in85out tagging strategy is good seen from the bottom panel of each figure. As a result of these studies, the setup corresponding to the '85in85out' b -tagging selection has been officially adopted in the legacy Run-2 analysis.

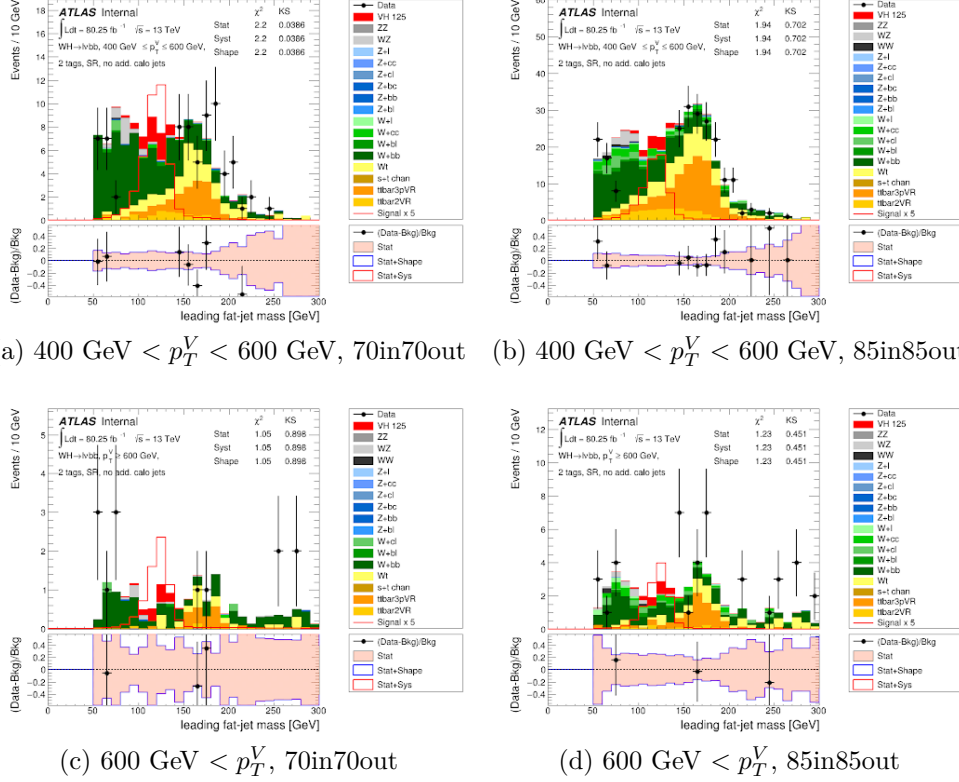


Figure 5.3: Data and Monte Carlo(MC) comparison in the high purity region. Data used is collected from the year 2015,2016 and 2017. 70in70out is the previous default b -tagging selection setting, while 85in85out is the new b -tagging selection proposed in this study. Comparing (a) and (c) with (b) and (d), the size of the data sample is clearly increased with the new selection.

Jet tagging strategy

This section is about the jet tagging strategy for the large-R jet $VH, H \rightarrow bb$ boosted analysis. The old strategy of jet tagging is to require the two highest p_T track jets inside the large-R jet to be b -tagged. However, if the $VH, H \rightarrow bb$

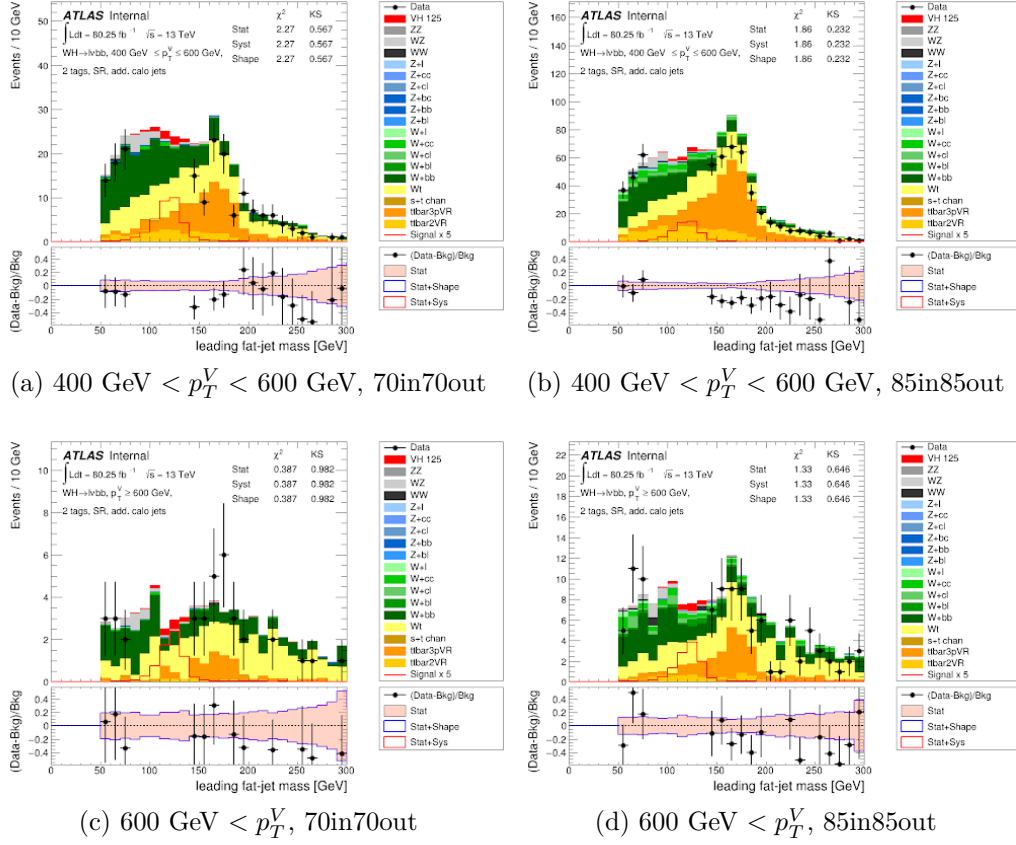


Figure 5.4: Data and Monte Carlo(MC) comparison in the low purity region. Data used is collected from the year 2015,2016 and 2017. 70in70out is the previous default b-tagging selection setting, while 85in85out is the new b-tagging selection proposed in this study. Comparing (a) and (c) with (b) and (d), the size of the data sample is clearly increased with the new selection.

signal events happen to have one b jet not to be among the two highest p_T jets, then with the old tagging strategy this signal events will be lost. Therefore, it is worth to investigate other tagging strategies. There are two options to explore, the first is to b -tag all jets in large-R jet, if there are exactly two b -tagged jets, then this event will be selected. This strategy is called 'AllSignalJets' strategy. The second option is to b -tag the top three highest p_T jet. The event is selected if there are exactly two b -tagged jets. This strategy could potentially reduce $t\bar{t}$ background events which have more than three track-jets within the large-R jet.

The 'AllSignalJets' strategy will consider all signal jets inside the leading large-R jet for tagging. The tagged jets are then ordered by transverse momentum(p_T). The b -tagging scale factors, and inefficiency scale factors are used to correct the difference between b -tagging algorithm's efficiency in Monte Carlo sample and Data as described in more details in section 4.1. Therefore, in the 'AllSignalJets' strategy, the b -tagging efficiency or inefficiency scale factors are applied to all jets.

The 'Leading3SignalJets' strategy is based on the 'AllSignalJets' strategy, but limiting tagging to the three jets with the largest p_T . As a result, if there are one or two or three jets in the event, the tagging strategy is the same as 'AllSignalJets' strategy. For example, if there are 3 track-jets in the event and if there are two tagged jets, then the two tagged jet are selected as leading/subleading jets from $H \rightarrow b\bar{b}$ decay. If there are one or two jets with the large-R jet in the event, then the order of the jets is kept. If there are more than 3 jets within the large-R jet in the event, only the first three jets are considered for tagging. In the 'Leading3SignalJets' strategy, the b -tagging scale factor is applied for the top 3 leading signal jets.

To compare which strategy gives better results, first a comparison of the total expected events yield is carried out. The results show that under the default b -tagging efficiency working point '70in70out', 'LeadingAllSignalJets' strategy allows for a $\sim 10\%$ yield increase in signal at the cost of $\sim 90\%$ background yield increase compared with the default 'Leading2SignalJets' strategy. When comparing the 'AllSignalJets' with 'Leading3SignalJets' strategy, the signal events yield has only 0.5% decrease but the background is $\sim 10\%$ less in the latter strategy. The background decrease in the latter case is $\sim 15\%$ for $t\bar{t}$ events of and $\sim 5\%$ for W+jets events. Therefore 'Leading3SignalJets' is a better strategy compared with 'AllSignalJets'.

To clearly see if there is an overall improvement using 'Leading3SignalJets' compared to default, a test is done to check the improvement in analysis significance using the b -tagging selections as optimized in section 5.1.1, which is '85in85out'. The result is shown in table 5.1, where the significance is cal-

culated based on Equation 5.1 using the full mva information in all analysis regions. The result shows an improvement in analysis significance increased by 4.05%.

	significance
Leading2SignalJets(default)	2.68
Leading3SignalJets	2.78
Improvement	4.05%

Table 5.2: This table shows the significance for old and new large-R tagging strategies, and the related improvement. The b -tagging selection setup at '85in85out' described in section 5.1.1 is used for all tests in the table.

A data and Monte Carlo comparison was performed for the new jet tagging strategy. The comparison results are shown in Figure 5.5 for the high signal purity region and in Figure 5.4 for low signal purity region. The comparison shows that the sample size is increased after moving from the "Leading2SignalJets" strategy to the 'Leading3SignalJets' strategy.

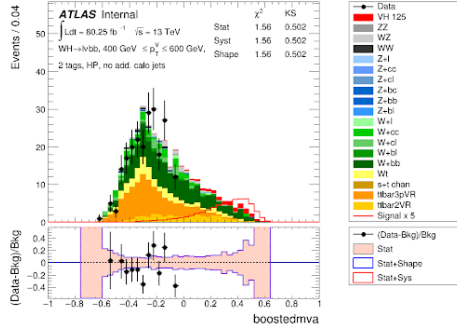
5.2 Analysis Regions

During this thesis work, several options of control regions were considered and tested. The following description will only focus on those that proved successful and which were eventually adopted in the analysis.

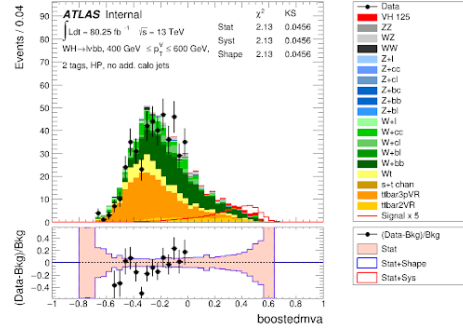
5.2.1 New control region for the top background

The $VH, H \rightarrow bb$ and $VH, H \rightarrow cc$ analyses are designed in such a way to be easy to combine, to be able to determine the rates for $H \rightarrow bb$ and $H \rightarrow cc$ simultaneously. Therefore the two analyses are very similar. The combination of the two analyses, also allows for shared systematic uncertainties, shared control region, etc. This section is mainly focused on defining a shared top control region between $VH, H \rightarrow bb$ and $VH, H \rightarrow cc$ analyses in order to improve the determination of the top background. In the $VH(cc)$ analysis, separate control regions are created for both 2 jets and 3 jets events:

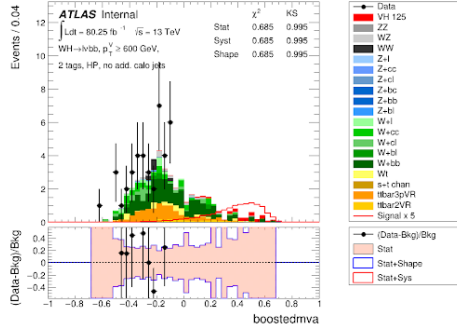
- 2-jet:
 - $topCR_{1A}$: tag category BL
 - $topCR_{1B}$: tag category BT



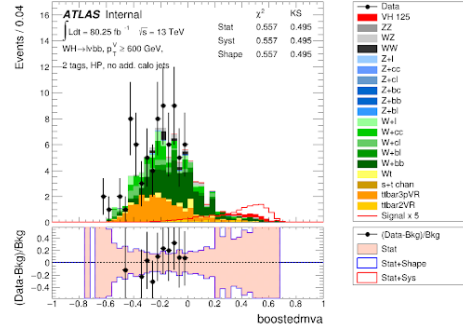
(a) $400 \text{ GeV} < p_T^V < 600 \text{ GeV}$, Leading2SignalJets



(b) $400 \text{ GeV} < p_T^V < 600 \text{ GeV}$, Leading3SignalJets

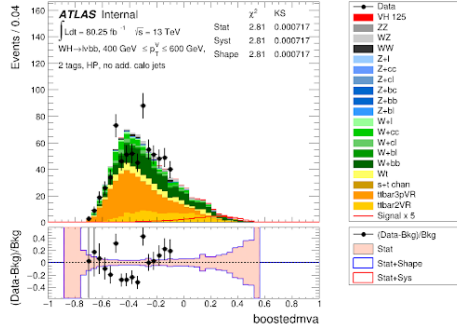


(c) $600 \text{ GeV} < p_T^V$, Leading2SignalJets

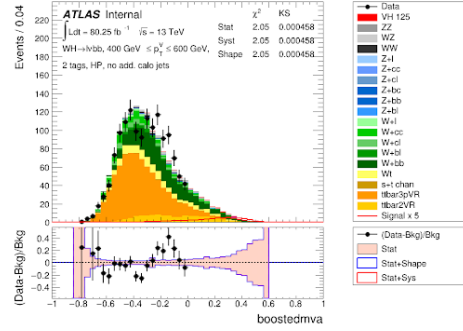


(d) $600 \text{ GeV} < p_T^V$, Leading3SignalJets

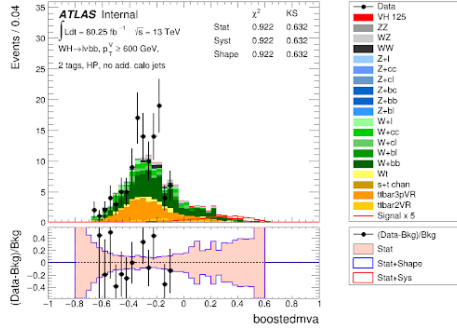
Figure 5.5: Data and Monte Carlo (MC) comparison in the high signal purity region. Data used is collected from the year 2015,2016 and 2017. Leading2SignalJets is the default jet selection strategy, while Leading3SignalJets is the new jet selection strategy. Comparing (a) and (c) with (b) and (d), the amount of data increases after moving from Leading2SignalJets to Leading3SignalJets.



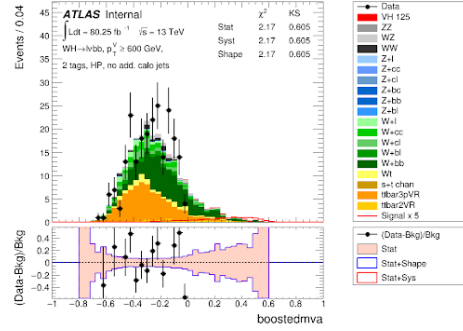
(a) $400 \text{ GeV} < p_T^V < 600 \text{ GeV}$, Leading2SignalJets



(b) $400 \text{ GeV} < p_T^V < 600 \text{ GeV}$, Leading3SignalJets



(c) $600 \text{ GeV} < p_T^V$, Leading2SignalJets



(d) $600 \text{ GeV} < p_T^V$, Leading3SignalJets

Figure 5.6: Data and Monte Carlo (MC) comparison in the low signal purity region. Data used is collected from the year 2015,2016 and 2017. Leading2SignalJets is the default jet selection strategy, while Leading3SignalJets is the new jet selection strategy. Comparing (a) and (c) with (b) and (d), the amount of data increases after moving from Leading2SignalJets to Leading3SignalJets.

- 3-jet:

- $topCR_{2A}$: tag category BLN
- $topCR_{2B}$: tag category $BTT + BTL + BTN + BTB + BBB$

Where in the tag category. B means b -tagged, T means tight c -tagged, L means loose c -tagged and N means not b -tagged and not c -tagged. Notice that, any c -tagged jet is not b -tagged. Tight and loose c -tagged jets are c -tagged with lower and higher c -tagging efficiency working point. The performance of c -tagging is shown in Table 5.3. In order to understand the expected performance of a certain choice of control regions, in the $VH, H \rightarrow bb$ analysis the $t\bar{t}$ sample is split according to the true flavor of two leading jets. It can be split in flavors $t\bar{t} \text{ } bb, bq \text{ and } qq$, where the q represent c - and light-jets. In the $VH, H \rightarrow cc$ analysis, $t\bar{t}$ is split into $bb, bc, bl \text{ and } qq$, where the l here represents light-jets and q represent c - and light-jets. Therefore the $t\bar{t} \text{ } bq$ components as defined in the $VH, H \rightarrow bb$ corresponds to $t\bar{t} \text{ } bc$ and $t\bar{t} \text{ } bl$ components in the $VH, H \rightarrow cc$ analysis.

Name	DL1r b fraction	DL1r cut value	c-eff	b-eff	l-eff
$C\text{Tag}_{Loose}$	0.08	1.275	0.4	0.2	0.04
$C\text{Tag}_{Tight}$	0.02	2.725	0.17	0.05	0.0025

Table 5.3: Table shows the property of the c -tagging algorithm DL1r. In the table c,b,l-eff represents the efficiency of c,b and light-jets with the DL1r c -tagging algorithm. The c -tagging algorithm has two working point, a looser working point $C\text{Tag}_{Loose}$ with higher c -tag efficiency but also higher b,l jet efficiency and a tighter working point $C\text{Tag}_{Tight}$ with lower c -tag efficiency but lower b,l jet efficiency.

The $topCR$ control region is used for constraining the normalization of the different flavor contributions of the $t\bar{t}$ background samples. Two normalisation factors are used for $t\bar{t}$ sample when fitting $VH, H \rightarrow bb$ and cc , one for $t\bar{t} \text{ } bb$, and the other for all other $t\bar{t}$ samples. One might wonder why not create another normalization factor for $t\bar{t} \text{ } qq$. The answer is $t\bar{t} \text{ } qq$ sample only have small number of events. During the process of MC fitting to data (more details of template fit in section 5.5.1), $t\bar{t}$ samples of both $VH, H \rightarrow bb$ and cc share the same normalization factor. However, $t\bar{t}$ events in the $topCR$ control region are not fully representative of the $t\bar{t}$ events in signal region, extrapolation uncertainties are needed to account for the differences. Since the $t\bar{t} \text{ } bq$ and $t\bar{t} \text{ } qq$ normalizations are mainly determined based on the events in control regions, the extrapolation uncertainties are applied directly in signal regions.

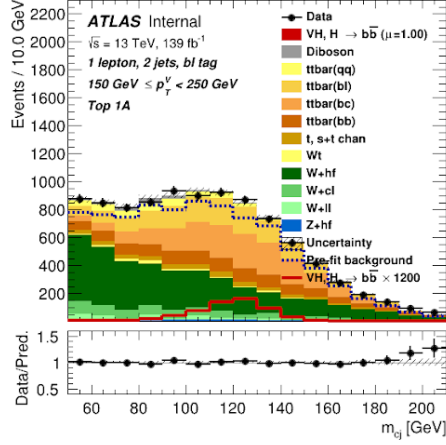
For the same reason, since the $t\bar{t}$ bb normalization is mainly determined in the signal region, the extrapolation uncertainties for $t\bar{t}$ bb are applied to control regions $topCR_{1A}, topCR_{1B}, topCR_{2A}, topCR_{2B}$. Also, since $t\bar{t}qq$ shared the same normalization factor with $t\bar{t}$ bq, bc and bl , and $t\bar{t}$ bq, bc and bl sample cannot fully represent the normalization of $t\bar{t}qq$, an additional extrapolation uncertainty is required to account for this effect. A normalisation uncertainty of 10% is applied to $t\bar{t}$ sample. However, since the sample size of $t\bar{t}qq$ is fairly small leading to this uncertainty becomes fairly small, this uncertainty is finally pruned before the template fit and therefore does not show up in the pull plot Figure 5.10. The uncertainties above are all for $t\bar{t}$ samples. However, the distribution of $topCR$ shown in Figure 5.7 and 5.8 shows that the top control region also contains non-negligible W +jets and Z +jets sample events. These samples are also sharing the same normalization factors between $VH, H \rightarrow bb$ and cc analysis, therefore with the same spirit, an additional uncertainty of 10% on the normalization factor of W +jets and Z +jets in TopCR region are also applied.

After applying the newly added $VH, H \rightarrow cc$ topCR control regions in the $VH, H \rightarrow bb$ 1L analysis, a minimum likelihood fit is applied to data, keeping the $H \rightarrow bb$ signal blinded and post-fit distributions are shown in Figure 5.7, 5.8 and 5.9 for topCR 1A and 1B, topCR 2A and 2B, and Signal region respectively. The post-fit plots shows that the data and fitted MC templates are within the uncertainties.

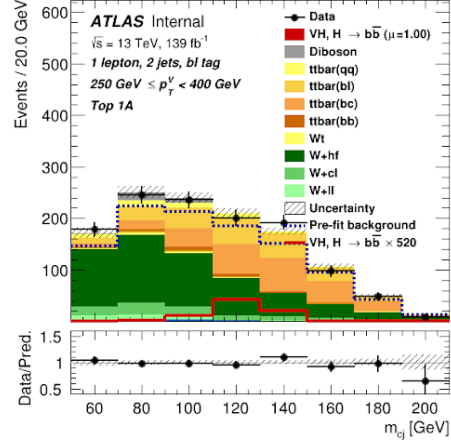
After adding the new topCR control region, the expected $VH.H \rightarrow bb$ signal significance over the background expectation increased from 4.188σ to 4.266σ which corresponds to a 1.8% improvement.

W+HF control region

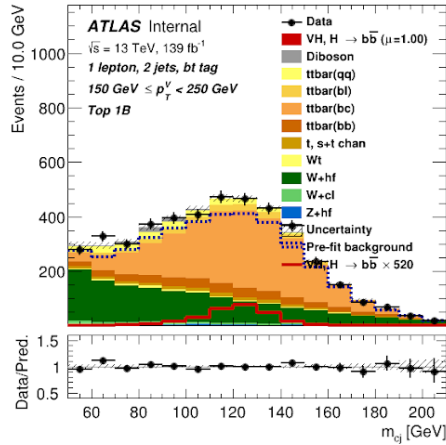
The Control Region Low(CRLow) of the 1-lepton $VH, H \rightarrow bb$ resolved analysis is abundant in both W +jets and $t\bar{t}$ background events. While the normalization of $t\bar{t}$ events is well constrained in CRHigh, which is very pure in $t\bar{t}$ events, it would be desirable to improve the normalization of W +jets, currently the leading uncertainties impacting the resolved $VH, H \rightarrow bb$ analysis in 1-lepton channel as shown in Figure 5.14 (a). The 1st, 3rd, and 4th uncertainties looking from top to bottom are W +jets normalization uncertainties. To achieve this goal, the CRLow region can be purified to better constraint the normalization of the W +jets sample. Therefore in this thesis, a Boosted Decision Tree(BDT) has been developed to separate W +jets events from all other events in CRLow region. The BDT score of the trained Boosted Decision Tree has been defined as $mvaCRLow$. In the distribution of $mvaCRLow$, bins with higher $mvaCRLow$ values contain a higher fraction of W +jets events. These



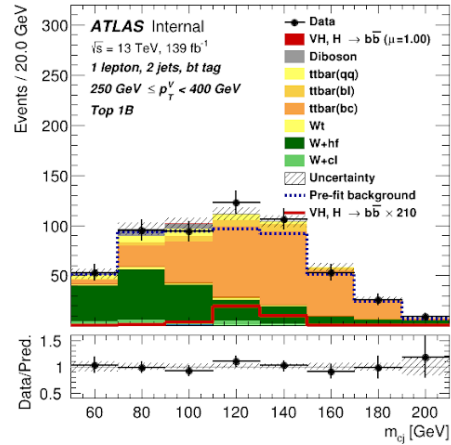
(a) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, 1A



(b) $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$, 1A

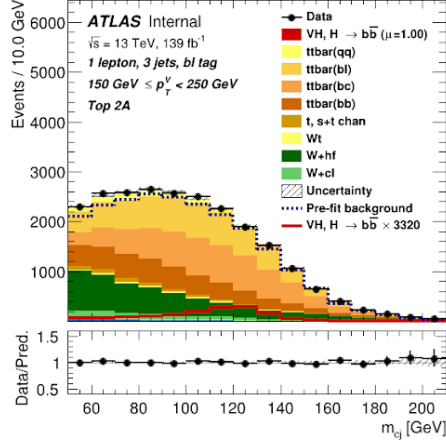


(c) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, 1B

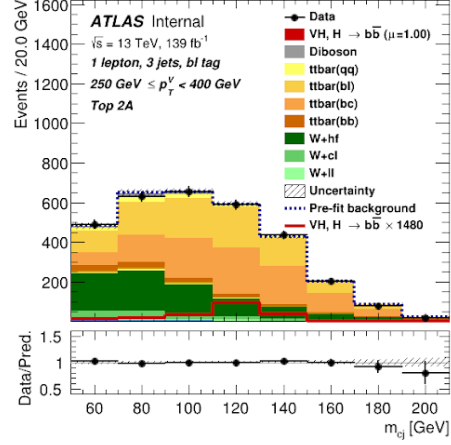


(d) $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$, 1B

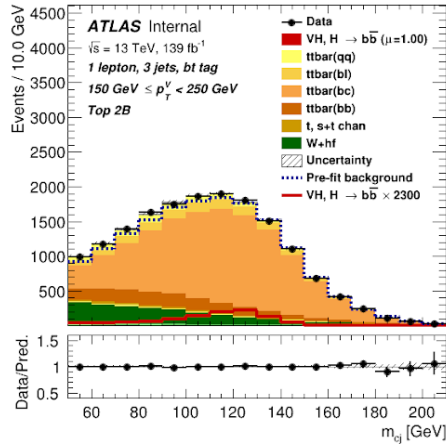
Figure 5.7: Post-fit plot of $VH, H \rightarrow cc$ two candidate jets invariant mass distribution in 1-Lepton Top control region. Figure (a) and (b) shows control region Top 1A, whereas (c) and (d) shows the control region Top 1B.



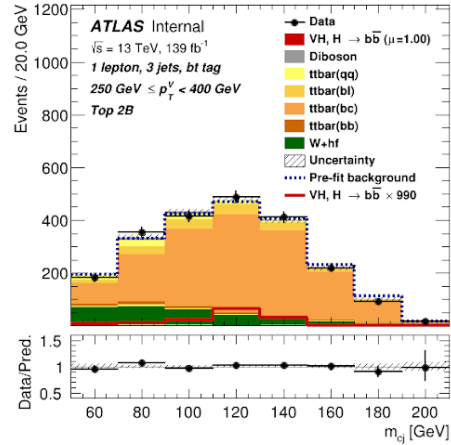
(a) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, 2A



(b) $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$, 2A

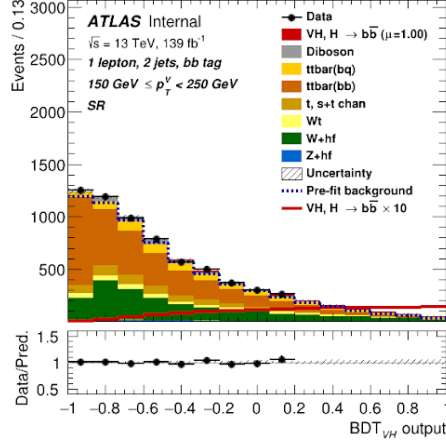


(c) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, 2B

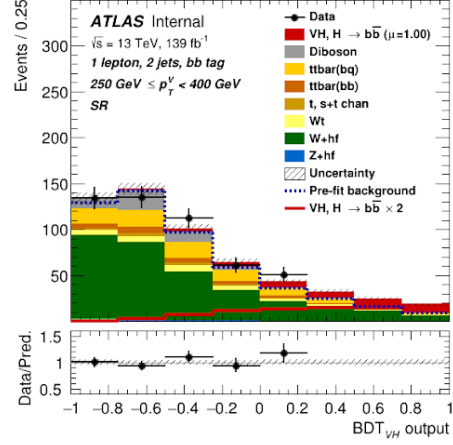


(d) $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$, 2B

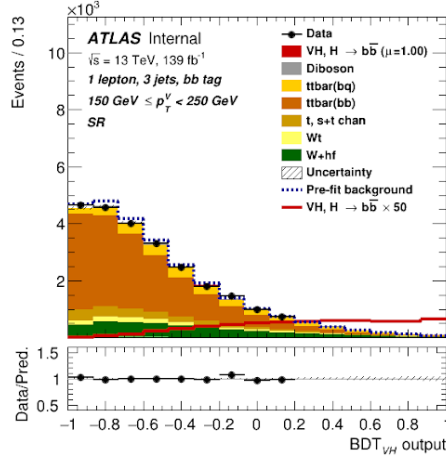
Figure 5.8: Post-fit plot of $VH, H \rightarrow cc$ two candidate jets invariant mass distribution in 1-Lepton Top control region. Figure (a) and (b) shows control region Top 2A, whereas (c) and (d) shows the control region Top 2B.



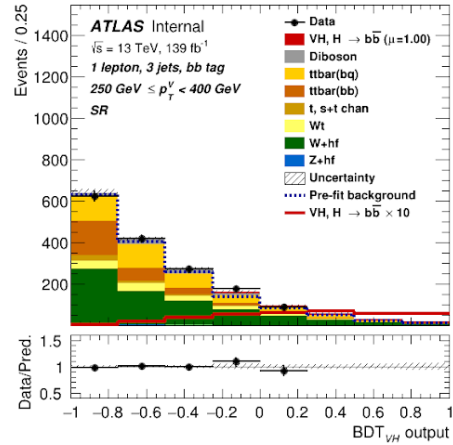
(a) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, SR, 2 jets



(b) $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$, SR, 2 jets



(c) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, SR, 3 jets



(d) $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$, SR, 3 jets

Figure 5.9: Post-fit plot of resolved $VH, H \rightarrow b\bar{b}$ BDT distribution in 1-Lepton signal region (SR). Figure (a) and (b) shows SR 2-jets region, whereas (c) and (d) shows the SR 3-jets region.

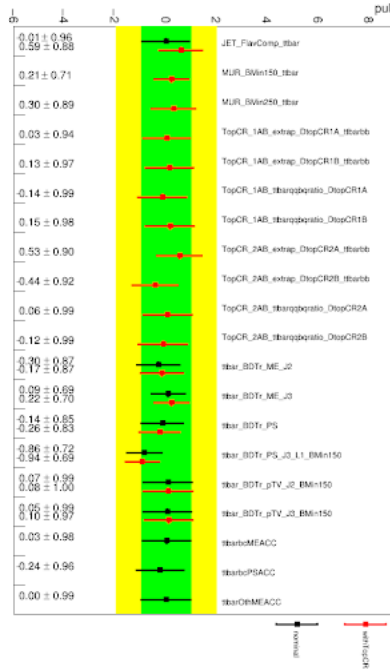


Figure 5.10: Figure shows the pull comparison between VH(bb) 1L resolved analysis fit with VH(bb) 1L resolved analysis fit in addition of VH(cc) topCR control region. The uncertainties start with TopCR are the newly added extrapolation uncertainties.

bins allow for better constraining the W +jets sample normalization. Another advantage is it helps decorrelate the normalization of $t\bar{t}$ and $W + jets$ sample to make the analysis less dependent on the amount of $t\bar{t}$ contamination in CR-Low as predicted by Monte Carlo simulations. The decorrelation could also help making the likelihood minimization step mentioned in section 5.5.1 more likely to converge. This implementation has been derived for the $VH, H \rightarrow b\bar{b}$ resolved 1-lepton channel, but it could be extended to the 0-lepton channel in the future.

First the BDT is trained to classify W +jets samples against all other events. The trained BDT provides an mvaCRLow value for each event. The training results are shown in Figure 5.11 for $75 \text{ GeV} < p_T^V < 150 \text{ GeV}$ and Figure 5.12 for $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$ and $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$. The BDT evaluation shows that the BDT performance on 2 jets events are similar to 3 jets events. Therefore, the training can be done inclusively for 2 jets and 3 jets event and they can share the same trained BDT.

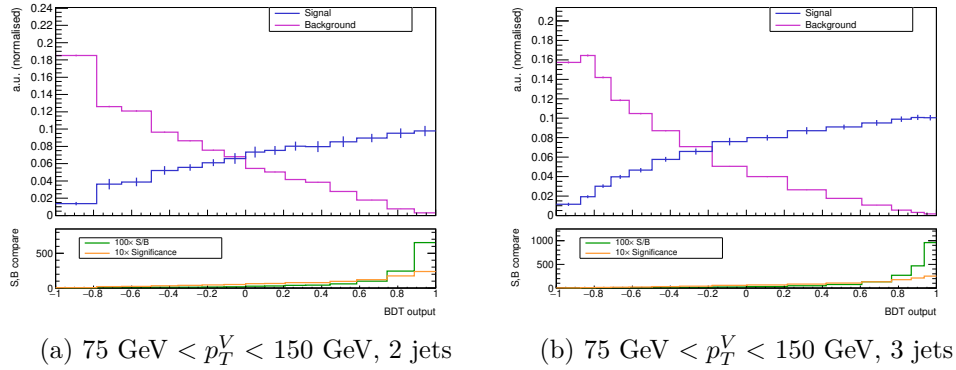
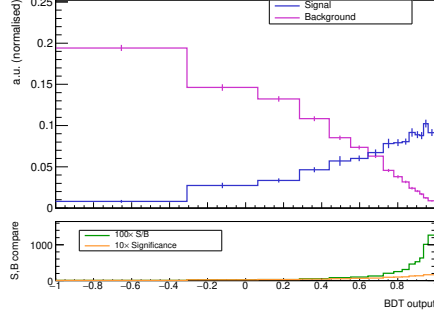
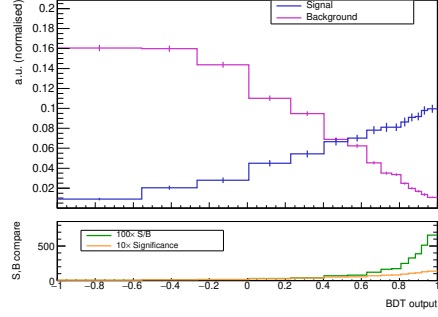


Figure 5.11: The mvaCRLow BDT score is shown for the train sample. For $75 \text{ GeV} < p_T^V < 150 \text{ GeV}$ and separated for 2-jet (a) and 3-jet (b) category. Statistical error is shown as error bar in the plot for both signal and background samples. The background sample size is large so that the statistical uncertainty is very small in the plot.

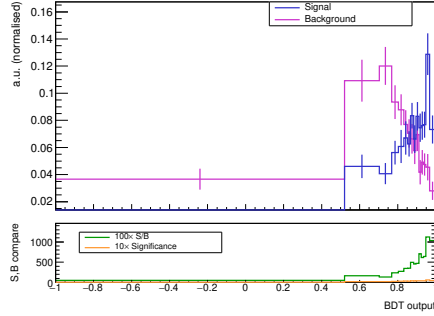
The next step is to apply the mvaCRLow BDT to the analysis. The simplest implementation is to apply a requirement on the mvaCRLow value so that only events with high mvaCRLow value will be kept in the CRLow region, whereas events with low mvaCRLow value will be discarded. To find the mvaCRLow value which gives the best constraint on the W +jets sample normalization, one can scan various mvaCRLow threshold values and re-compute the $VH, H \rightarrow b\bar{b}$ signal significance of the resolved $VH, H \rightarrow b\bar{b}$ analysis using the full



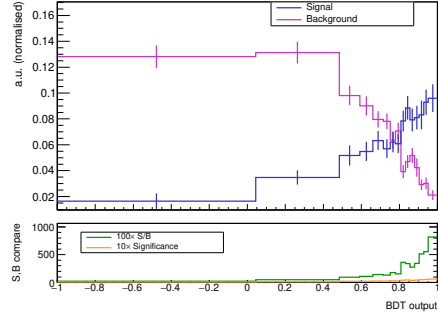
(a) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, 2 jets



(b) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, 3 jets



(c) $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$, 2 jets



(d) $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$, 3 jets

Figure 5.12: The mvaCRLow BDT score is shown for the train sample. For $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$ and separated for 2-jet (a) and 3-jet (b) category. For $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$ and separated for 2-jet (c) and 3-jet (d) category. Statistical error is shown as error bar in the plot for both signal and background samples. The background sample size is large so that the statistical uncertainty is very small in the plot.

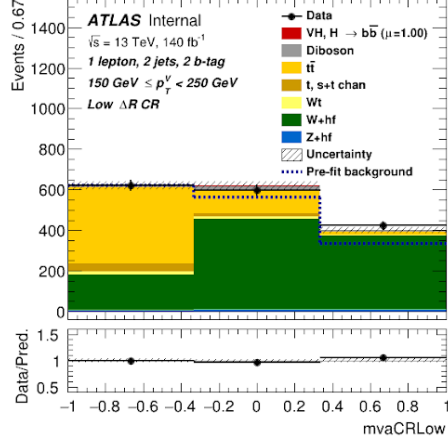
fit machinery as presented in section 5.5.1 and including systematic uncertainties. The significance scan results are shown in Table 5.4. The result shows that the best threshold value for mvaCRLow is 0.9, which gives 3.6% significance improvement. The optimal value 0.9 is not surprising since for events in $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$, the signal and background ratio increases a lot at 0.9 as shown in Figure 5.12.

	default	0.3	0.5	0.6	0.7	0.8	0.9	0.95
significance	3.62	3.64	3.65	3.67	3.69	3.70	3.75	3.66
Improvement	0%	0.8%	0.9%	1.5%	2.0%	2.45%	3.6%	1.35%

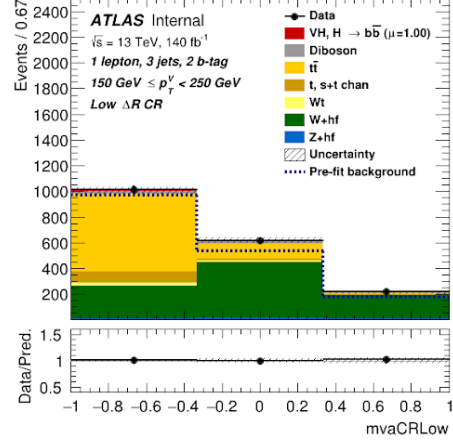
Table 5.4: Table shows how different mvaCRLow threshold value can affect the overall signal significance of $VH, H \rightarrow b\bar{b}$ 1L resolved analysis.

The first implementation discussed above discarded events that have mvaCRLow value smaller than the mvaCRLow threshold value. However, a second implementation has been studied where all events are kept in the CRLow region, but where the mvaCRLow score is used as a fit observable for the CRLow region replacing the previously used p_T^V . The advantage of doing this is that all $W + jets$ events can be kept while effectively giving more weight to those with high mvaCRLow score for stronger constraining power. Also, separating better $W + jets$ from $t\bar{t}$ event helps constraining the $t\bar{t}$ sample normalization as well. However, when using the mvaCRLow score as the fit observable in the CRLow region, the systematic shape uncertainties on the of mvaCRLow distribution do also need to be considered. To minimize the impact of such uncertainties, the number of bins for the mvaCRLow observable has been kept to just 3.

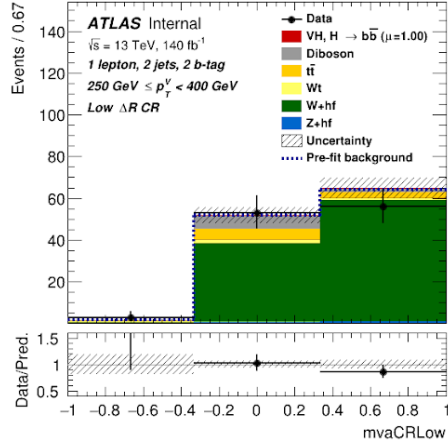
The mvaCRLow is splitted in 3 bins, the binning are chosen to be $[-1, 0.6]$, $(0.6, 0.9]$, $(0.9, 1.0]$. The reason for choosing 0.6 as bin edge is because of the $W + jets$ to background ratio increasing the most at 0.6 for the particularly sensitive medium p_T^V region. The other bin edge, 0.9, is chosen since the overall significance is largest with an mvaCRLow threshold at 0.9. as previously discussed. This second approach has been applied to a full blinded fit to date, and resulting post-fit distributions for the CRLow region are shown in Figure 5.13. The binning in the plot looks different than the binning previous mentioned since there is a monotonic binning transformation done before the fit, but the underlying binning is as previously mentioned. The fit result shows that the data and MC are consistent within uncertainty. Worth mentioning is also that the mvaCRLow bin closest to the right side has a high concentration of $W + jets$ events as expected. The mvaCRLow left side has high concentration of $t\bar{t}$ events yielding better constrain of the $t\bar{t}$ sample normalization.



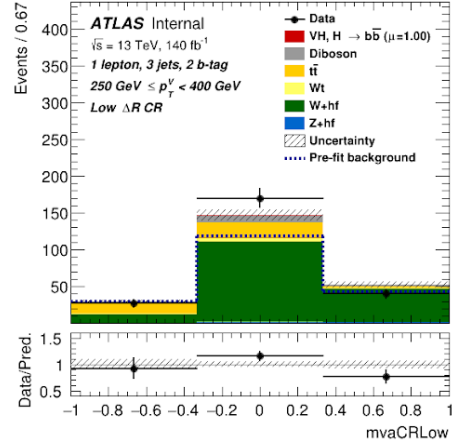
(a) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, 2 jets



(b) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, 3 jets



(c) $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$, 2 jets



(d) $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$, 3 jets

Figure 5.13: The mvaCRLow post-fit distribution of the mvaCRLow score is shown separately for $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$ (top row) and $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$ (bottom row) for 2 (left column) or 3 (right column) jets. The mvaCRLow is splitted into 3 bins. The fitted histograms represent the MC simulations for different processes adjusted in normalization and shape to the result of the blinded fit to data and are stacked on top of each other. The shaded areas represent a projection of the fit uncertainty. The point represent data, with their corresponding statistical uncertainty.

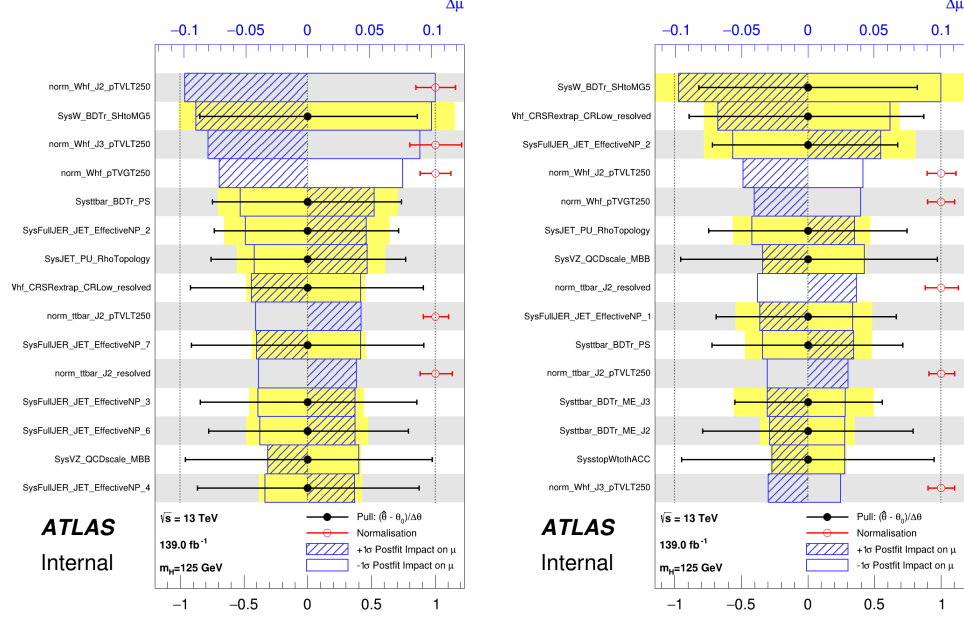
The goal of this study was to reduce the normalization uncertainty of $W + jets$ events. The change in the $W + jets$ normalization uncertainty before and after applying the second implementation of our method as discussed above is shown in Table 5.5. The $W + jets$ normalization uncertainty is successfully decreased by between 14% to 48%, depending on analysis region. The uncertainties are evaluated based on the blinded fit to data. The $t\bar{t}$ normalization uncertainty also decreased by between 3% to 8%, again depending on analysis region.

Sample	Njet	p_T^V region	Normalization uncertainty change
$t\bar{t}$	2	medium p_T^V	-7.8%
$t\bar{t}$	2	high p_T^V	-4.5%
$t\bar{t}$	3	midium p_T^V	-3.3%
$t\bar{t}$	3	high p_T^V	-4.6%
W+jets	3	midium p_T^V	-23%
W+jets	2	midium p_T^V	-48%
W+jets	2&3	high p_T^V	-14%

Table 5.5: The table shows the uncertainty change for the $t\bar{t}$ and W+jets sample normalizations after applying the 3 bin mvaCRLow score as observable in the CRLow region. The 'medium p_T^V ' in the table refers to $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, whereas 'high p_T^V ' refers to $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$.

The uncertainty ranking is also worth reporting. In this plot uncertainties are ranked by their expected impact on the Higgs signal determination, based purely on fit to MC simulations. From the result shown in Figure 5.14. the normalization uncertainties go down being the 1st, 3rd, 4th-leading systematic uncertainty to being the 4th, 15th, 5th-leading uncertainty, with a resulting significant lower impact on the determination of the $VH, H \rightarrow bb$ signal strength. The $VH, H \rightarrow bb$ resolved analysis in 1-lepton channel signal significance is improved for 5% after the mvaCRLow implementation.

As mentioned above, another goal of this study is to reduce the correlation between $t\bar{t}$ and W+jets sample. The correlation between $t\bar{t}$ W+jets normalization before and after applying mvaCRLow is shown in Table 5.6 and 5.7. The correlation are mostly positive before applying mvaCRLow. However, in ideal case when only concerning normalization factors of two sample mixed together in one region, the correlation of normalization factors between two samples should be negative since when one normalization factor goes up, the other normalization factor must go down in order to keep the total number of events unchanged. The reason that the actual correlation is positive could be



(a) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, 2 jets

(b) $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, 3 jets

Figure 5.14: The uncertainty ranking plot before and after applying the mvaCRLow BDT score as observable in the CRLow region. In Figure(a), the largest uncertainty, 'norm_Whf_J2_pTVLT250', is W+jets normalization uncertainty in 2-jet $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$. The 3rd uncertainty, 'norm_Whf_J2_pTVLT250', is is W+jets normalization uncertainty in 3-jet $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$. The 4th uncertainty, 'norm_Whf_pTVGT250', is is W+jets normalization uncertainty in 2,3-jet $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$. The same goes with Figure (b). The meaning of ranking plot is explained in section 5.5.1.

due to uncertainties applied on both $t\bar{t}$ and W+jets samples. For example, if one uncertainty has normalization effect and scale up the normalization of both $t\bar{t}$ and W+jets sample, then the normalization factors of both $t\bar{t}$ and W+jets will scale down in order to keep the total number of events unchanged. In this case, the correlation between two normalization factors is positive. Ideally, if only the normalization effect is considered, the decorrelation between $t\bar{t}$ and W+jets will make the correlation value more positive. This is exactly what is shown in the comparison between Table 5.6 and 5.7.

	$W+jets$ 2-jet medium p_T^V	$W+jets$ 3-jet medium p_T^V	$W+jets$ 2-jet high p_T^V
$t\bar{t}$ 2-jet medium p_T^V	-0.01	0.13	0.02
$t\bar{t}$ 2-jet high p_T^V	0.10	0.16	-0.01
$t\bar{t}$ 3-jet medium p_T^V	0.06	0.08	0.03
$t\bar{t}$ 3-jet high p_T^V	0.09	0.12	-0.03

Table 5.6: Correlation between $t\bar{t}$ and W+jets sample normalization in $VH, H \rightarrow b\bar{b}$ resolved analysis in 1-lepton channel before applying mvaCR-Low. The 'medium p_T^V ' in the table refers to $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, whereas 'high p_T^V ' refers to $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$.

5.3 Signal and background modeling

5.3.1 Signal Modeling

The signal sample VH consists of $Z(\rightarrow \nu\nu)H$, $W(\rightarrow l\nu)H$ and $Z(\rightarrow ll)H$ as discussed in section 5.1. These are the dominant signal contributions selected in the zero, one and two lepton channels, respectively. At leading order in the strong coupling constant(α_S), there are two different production processes: VH could be produced from gluon-gluon initial state(gg) or quark-antiquark($q\bar{q}$). The latter takes place for both WH and ZH: $q\bar{q} \rightarrow WH$ and $q\bar{q} \rightarrow ZH$. However, since the gluon does not carry electric charge, the gluon-gluon initial state can only produce ZH. Therefore for the zero lepton channel, the major

	$W + \text{jets } 2\text{-jet medium } p_T^V$	$W + \text{jets } 3\text{-jet medium } p_T^V$	$W + \text{jets } 2\text{-jet high } p_T^V$
$t\bar{t} \text{ 2-jet medium } p_T^V$	0.12	0.13	0.03
$t\bar{t} \text{ 2-jet high } p_T^V$	0.15	0.14	-0.01
$t\bar{t} \text{ 3-jet medium } p_T^V$	0.18	0.14	0.07
$t\bar{t} \text{ 3-jet high } p_T^V$	0.15	0.12	-0.02

Table 5.7: Correlation between $t\bar{t}$ and $W + \text{jets}$ sample normalization in $VH, H \rightarrow b\bar{b}$ resolved analysis in 1-lepton channel after applying mvaCRLow. All events with mvaCRLow score smaller than 0.6 is discarded. The 'medium p_T^V ' in the table refers to $150 \text{ GeV} < p_T^V < 250 \text{ GeV}$, whereas 'high p_T^V ' refers to $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$.

signal contributions come from the processes $gg \rightarrow Z(\nu\nu)H$. In the one lepton channel the contribution mainly comes from $qq \rightarrow W(l\nu)H$. In the two lepton channel, the contribution mainly comes from $qq \rightarrow Z(ll)H$ and $gg \rightarrow Z(ll)H$. Contributions from gg initial state are suppressed since they only can occur through a top loop, but they are still significant due to the high gluon luminosity at the LHC. The Feynman diagram of $VH, H \rightarrow b\bar{b}$ of three lepton channels are shown in Figure 5.15.

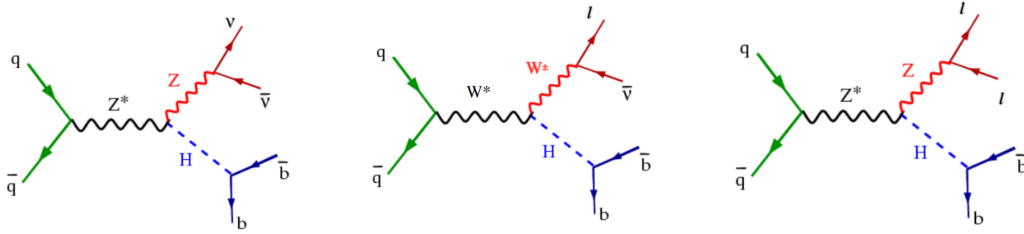


Figure 5.15: Feynman diagram of three lepton channels in $VH, H \rightarrow b\bar{b}$ analysis, all produced from quark-quark interactions. From left to right: 0,1,2-lepton channels.[12].

5.3.2 Background modeling

The major background of the $VH, H \rightarrow bb$ analysis are: $t\bar{t}$, W+jets, Z+jets, diboson, single top. In the one-lepton channel, the leading two backgrounds are $t\bar{t}$ and W+jets. This section is mainly focused on W+jets background modeling, since this has been the focus of this thesis work.

W+jets background modeling

W+jets is one of the two main backgrounds for the $VH, H \rightarrow bb$ one-lepton channel. It is also a sub-dominant background for the $VH, H \rightarrow bb$ zero-lepton channel when the W boson decays to $\tau\nu$ or when to $q\bar{q}$ or when the electron and muon from the W boson decay is not detected.

The nominal W+jets sample is simulated using SHERPA 2.2.11[56]. The sample is simulated with a combination of different parton multiplicities, up to 5 extra partons in the matrix element of the leading order(LO) in QCD and up to 2 extra partons are included at the next-to-leading order(NLO).

Current there is no perfect generator/showering algorithm, therefore uncertainties of these algorithm has to be considered. One way to consider such effect is to use different generator/showering algorithm or different settings of the algorithm to generate a set of alternative sample events. The differences of observables between nominal and alternative samples will be assigned as the systematic uncertainty of nominal generator/showering algorithm. The alternative Monte Carlo sample events are simulated by MADGRAPH5_aMC@NLO[57][58]. The Monte Carlo events are generated in the matrix element at next-to-leading order in QCD with up to three additional partons.

5.3.3 Modeling systematic uncertainties

Sherpa 2.2.11 provides NLO accuracy in both QCD and electroweak corrections. It provides electroweak correction for both virtual-loop terms and for the real emission of gauge bosons. The corrections are sizable at high- p_T^V . Therefore it is important to include these corrections in the W+jets samples especially in the $VH, H \rightarrow bb$ boosted analysis selecting events with $p_T^V > 400$ GeV. There are three different schemes for the implementation of the electroweak corrections. This is a reflection of the fact that both QCD and EW corrections have been computed independently on top of the LO predictions but no mixed EW+QCD NLO corrections have been derived. The corrected NLO cross-section represented in the additive scheme is:

$$\sigma_{n,QCD+EW}^{NLO} = \sigma_{n,LO} + \Delta\sigma_{n,QCD}^{NLO} + \Delta\sigma_{n,EW_{virt}}^{NLO} \quad (5.2)$$

where the term $\sigma_{n,LO}$ represents the leading order cross-section, $\Delta\sigma_{n,QCD}^{NLO}$ represents NLO QCD correction and $\Delta\sigma_{n,EW_{virt}}^{NLO}$ represents NLO EW virtual-loop term correction. The multiplicative scheme is defined as:

$$\sigma_{n,QCD+EW}^{NLO} = (\sigma_{n,LO} + \Delta\sigma_{n,QCD}^{NLO}) \times (1 + \Delta\sigma_{n,EW_{virt}}^{NLO}) \quad (5.3)$$

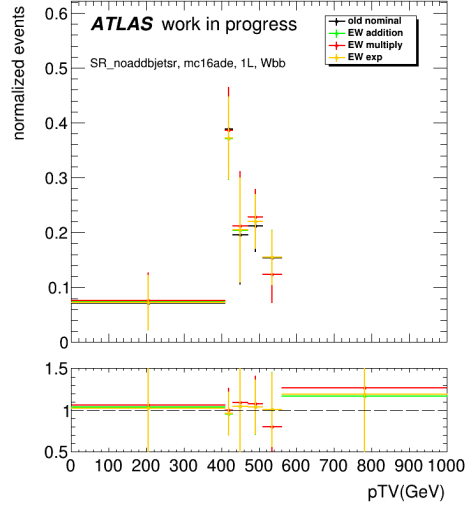
The exponential scheme is:

$$\sigma_{n,QCD+EW}^{NLO} = (\sigma_{n,LO} + \Delta\sigma_{n,QCD}^{NLO}) \times e^{\Delta\sigma_{n,EW_{virt}}^{NLO}} \quad (5.4)$$

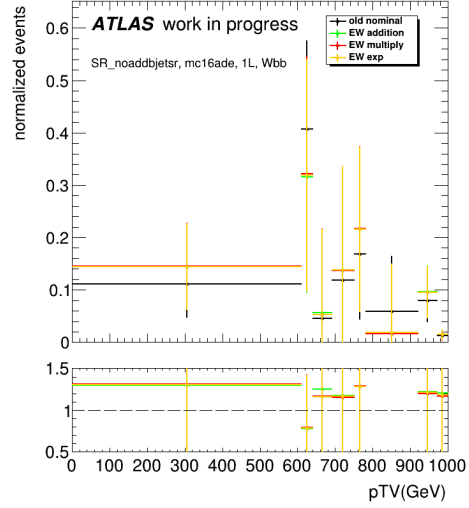
The addition scheme cross-section is chosen to be the new nominal of the W+jets sample since the distribution of observables from addition scheme is closest to those without electroweak correction while from past experiences already proved good data/MC agreement. A new uncertainty is assigned to cover the differences among the three different schemes. The uncertainty will be set to the largest difference among the three schemes. The comparison between the p_T^V distributions without applying electroweak correction and those corrected with the three different schemes in $VH, H \rightarrow bb$ boosted analysis is shown in Figure 5.16. It shows the result from additional scheme is closest to the distribution without applying electroweak correction.

Introduction on BDTr and CARL reweighting technique

Some modeling uncertainties can be evaluated by taking the difference between two samples generated by two different generator/showering algorithms. This approach has the disadvantage of not separating all different effect, but it can be applied easily. However, it requires generating the same samples for each generator/showering algorithm considered. Therefore the evaluation of the modeling systematic uncertainty doubles the computational resources needed. Machine learning method can be used to reduce such computational resources. The idea is to generate an alternative sample with reduced statistical precision and train a machine learning model to learn the difference between the nominal sample and alternative sample, and interpolate between these. The learned differences provide the modeling systematic uncertainties. The main observable for the $VH, H \rightarrow bb$ analysis is the BDT score trained for signal against background. Therefore the modeling systematic uncertainties will also need to be applied to such BDT score. One question the reader might ask her/himself is why not directly evaluate the trained signal-vs-background BDT on the alternative sample and take the difference between such alternative distribution



(a) $400\text{GeV} < p_T^V < 600\text{GeV}$, SR, Wbb



(b) $600\text{GeV} < p_T^V$, SR, Wbb

Figure 5.16: Figure shows p_T^V distribution of the W+bb sample in the signal region (SR). Black shows the distribution without applying electroweak correction. Green, red and yellow show the same distribution after applying electroweak correction with the addition, multiplication and exponential scheme, respectively. The bottom panel shows the ratio between the distribution after applying electroweak corrections and the distribution without applying electroweak corrections. The error bars represent the statistical uncertainty of the samples. The statistical uncertainty is large due to small number of events. Please notice that due to the use of event weights to apply EW correctoins, differences within the statistical uncertainty are still expected to be meaningful.

and the nominal BDT as the systematic uncertainty. The reason is two-fold: on one hand this requires a larger alternative sample, on the other hand the procedure described below is nearly independent on the observable used in the analysis. In order to get the correct $VH, H \rightarrow bb$ signal BDT distribution of an alternative sample, another BDT trained on alternative background against nominal background. The detailed steps to produce the alternative modeling systematic uncertainty are:

- Train a machine learning model(Boosted Decision Tree/Deep Neural Network) to differentiate the nominal sample against an alternative sample. This model will be denoted as BDT_{sys} in the following.
- Take the predicted score (mva score) of BDT_{sys} and evaluate the distribution of this score separated for the nominal sample and for the alternative sample. The two distributions should not be exactly the same.
- Take the ratio of the nominal/alternative sample distribution. This provides an estimate of the ratio of the likelihood functions of alternative and nominal samples, i.e.
- how likely an event with a specific BDT_{sys} score is from alternative sample, rather than from the nominal sample.
- Evaluate the score of BDT_{sys} .
- Use the ratio histogram to look-up the corresponding value of the ratio.
- Modify the original MC event weight by multiplying it by the value of the ratio.

Once the ratio histogram is obtained, this can be applied to each event in the nominal sample to get the systematic uncertainty. The distribution of any observable with the weights applied is defined as the alternative distribution. Note in this step, no alternative sample is processed. The difference between nominal and alternative distribution of any observable will be used as the systematic modeling uncertainty of the sample. The amount of simulated events needed is to be enough to let the machine learning model learn the differences between the nominal and alternative samples. There are two options developed within ATLAS for the machine learning model used for the systematic re-weighting, one is Boosted Decision Tree (BDT), the other is Deep Neural Network (DNN). The method of evaluating modeling systematic uncertainty using BDT is called BDTr, the one using DNN is called CARL. CARL has a

conceptual advantage compared with BDTr. Since CARL is based on a DNN, the value output by the DNN has a statistical meaning if is the posterior probability that of the given event is either alternative or the nominal sample. These two probabilities sum up to 1 by construction.

Proof: The used loss function of the CARL DNN is:

$$\text{Loss} = w[Y \log S(x) + (1 - Y) \log(1 - S(x))] \quad (5.5)$$

where w is the event weight, Y is a truth label which can take a value of either 0 or 1, specifying nominal or alternative sample respectively. $S(x)$ is the neural network output, expressed as a function of the input. When neural network has been trained and optimized, the loss function value will be corresponding to a local or global minimum. Let X be a random vector and x the value of vector X of a certain event. In this case, the form of function $S(x)$ is:

$$S(x) = \arg \min_{S(x)} E_{Y|X=x}[wY \log S(x) + w(1 - Y) \log(1 - S(x))] \quad (5.6)$$

$$= \arg \min_{S(x)} E_{Y|X=x}[wY] \log S(x) + \quad (5.7)$$

$$E[w] \log(1 - S(x)) - E[wY] \log(1 - S(x)) \quad (5.8)$$

The equation above means that with many form of the function $S(x)$, $S(x)$ take the form which can minimize the loss function. Since the neural network is already trained and optimized, the loss function is in a minimum, therefore the functional derivative with respect to $S(x)$ should be 0:

$$\frac{d}{dS(x)} (E[wY] \log \frac{S(x)}{1 - S(x)} + E[w] \log(1 - S(x))) = 0 \quad (5.9)$$

$$E[wY] \left(\frac{1}{S(x)} + \frac{1}{1 - S(x)} \right) - \frac{E[w]}{1 - S(x)} = 0 \quad (5.10)$$

$$E[wY] \frac{1}{S(x)} = E[w] \quad (5.11)$$

$$E[wY] = E[w] S(x) \quad (5.12)$$

$$\frac{E[wY]}{E[w]} = \frac{W_{Y=1}}{W} = P(Y = 1|X = x) = S(x) \quad (5.13)$$

Therefore, with a fully optimized DNN trained using the given loss function and with an event having a certain event weight, the neural network output is the posterior probability for the event to be in one category. The derivation is based on appendix in [59].

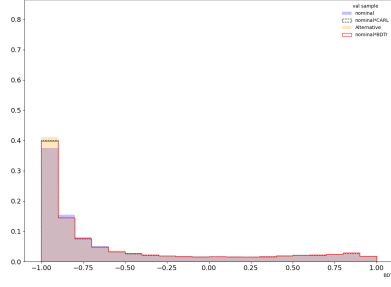
If the probability given by the trained DNN is $P(y = \text{nominal}|\text{event})$, then

the ratio can be derived as:

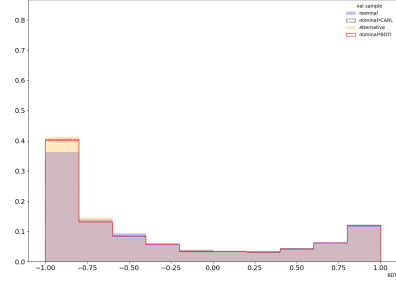
$$r(\text{event}) = \frac{P(y = \text{alternative}|\text{event})}{P(y = \text{nominal}|\text{event})} = \frac{1 - P(y = \text{nominal}|\text{event})}{P(y = \text{nominal}|\text{event})} \quad (5.14)$$

Therefore the ratio value can be obtained directly based on a single neural network score without relying on the ratio between nominal and alternative sample BDT distribution. This is better since it avoids the need to separate the BDTr distribution into a discrete number of bins in order to derive the ratio, whereas with the DNN in CARL, the ratio is no longer depending on histogram binning. Another advantage is that the DNN provides state-of-the-art modern machine learning methods that can provide better training results compared with a BDT.

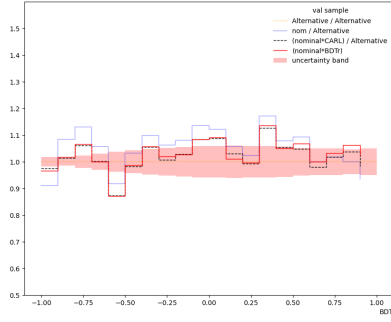
BDTr and CARL reweighting technique comparison For both BDTr and CARL, the input training variables are the same as those used in the $VH, H \rightarrow bb$ signal-vs-background BDT, except for the b-tagging information of the leading two jets since the b-tagging information is based on the lower level variables and does not provide more information on the modeling. The set of training events used are events for 2-jet W+bb sample of the whole p_T^V range and the sample events used for both BDTr and CARL are exactly the same. The comparison between BDTr and CARL are done on both resolved and boosted $VH, H \rightarrow bb$ analyses and are shown in Figure 5.17 and 5.18 respectively. In the result, nominal and alternative sample is generated by SHERPA 2.2.11 and Madgraph5 respectively. The bottom two plots shows the quality of CARL BDTr reweighting by showing the ratio of CARL/BDTr reweighted nominal sample distribution. Ideally, if the CARL/BDTr reweighting is perfect, then the ratio should be equals to one in all analysis BDT bin. The plots show that although the ratio does not stay at one exactly, it is mostly relies in the statistical red nominal sample uncertainty band. Also, the result shows the performance of CARL is similar to BDTr and sometimes CARL reweighted distribution is closer to the nominal distribution in both resolved and boosted analyses. Given the various advantage of using CARL stated above, $VH, H \rightarrow bb$ analysis group eventually adopted CARL instead of BDTr.



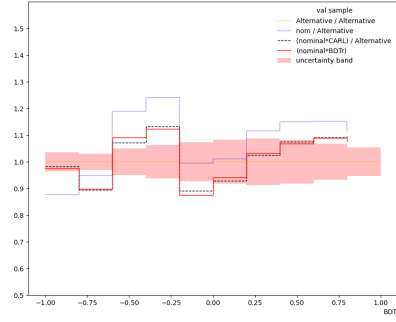
(a) $150\text{GeV} < p_T^V < 250\text{GeV}$



(b) $250\text{GeV} < p_T^V < 400\text{GeV}$

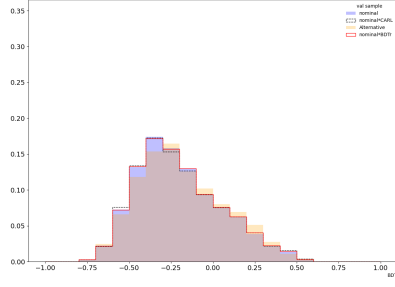


(c) $150\text{GeV} < p_T^V < 250\text{GeV}$ ratio

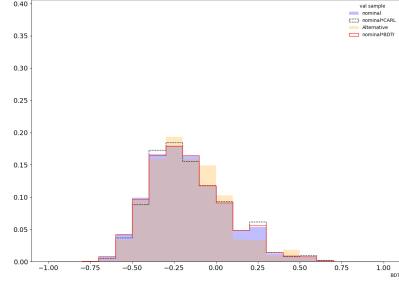


(d) $250\text{GeV} < p_T^V < 400\text{GeV}$ ratio

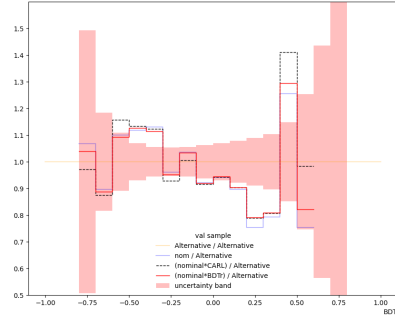
Figure 5.17: Figure shows the comparison on the distribution of 2-jet $W+bb$ $VH, H \rightarrow bb$ signal-versus-background BDT between BDTr and CARL reweighting in the resolved analyses. The nominal and alternative sample is generated by SHERPA 2.2.11 and Madgraph5 respectively. Plots on top (a) (b) shows the distribution of $VH, H \rightarrow bb$ analysis BDT. Bottom two plots (c) (d) shows the ratio of the distribution of various sample over alternative sample. The left two plots (a) and (c) and the right two plots (b) and (d) shows the analysis BDT distribution in different p_T^V region, $150\text{GeV} < p_T^V < 250\text{GeV}$ and $250\text{GeV} < p_T^V < 400\text{GeV}$ respectively. Blue dashed line and red line shows the ratio of CARL and BDTr reweighted nominal sample over alternative sample respectively. Red shadow shows the statistical uncertainty of nominal sample.



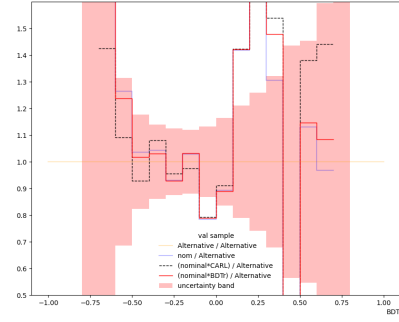
(a) $400\text{GeV} < p_T^V < 600\text{GeV}$



(b) $600\text{GeV} < p_T^V$



(c) $400\text{GeV} < p_T^V < 600\text{GeV}$ ratio



(d) $600\text{GeV} < p_T^V$ ratio

Figure 5.18: Figure shows the comparison on the distribution of 2-jet $W+bb$ $VH, H \rightarrow bb$ signal-versus-background BDT between BDTr and CARL reweighting in the resolved analyses. The nominal and alternative sample is generated by SHERPA 2.2.11 and Madgraph5 respectively. Plots on top (a) (b) shows the distribution of $VH, H \rightarrow bb$ analysis BDT. Bottom two plots (c) (d) shows the ratio of the distribution of various sample over alternative sample. The left two plots (a) and (c) and the right two plots (b) and (d) shows the analysis BDT distribution in different p_T^V region, $250\text{GeV} < p_T^V < 400\text{GeV}$ and $400\text{GeV} < p_T^V < 400\text{GeV}$ respectively. Blue dashed line and red line shows the ratio of CARL and BDTr reweighted nominal sample over alternative sample respectively. Red shadow shows the statistical uncertainty of nominal sample.

5.4 Multivariate discriminants

Both the resolved and boosted $VH, H \rightarrow bb$ analyses utilize information from multiple physics observables to magnify the sensitivity of the Higgs boson signal. This allows summarising multiple physics observables into One single multivariate discriminant, as defined by the machine learning score from a Boosted Decision Tree trained with Monte-Carlo events.

5.4.1 Boosted decision trees

A boosted decision tree is based on the concept of decision/regression tree. A decision tree has a data structure of a tree. Each node of the tree has a criteria to split the event based on an input variable. The criteria of each node is set to maximize the information gain or minimize the entropy of signal-versus-background events in the child node. Each leaf node has an output corresponding to a class label or probability. If the target of the events is a continuous variable, the tree is called regression tree. A number of trees will be trained and the output of all trees will be combined to give a more accurate prediction of the event label. This step is called "Boosting". To combine all the outputs of the trees, each tree is given a weight representing the accuracy of the prediction. The more accurate the tree can predict, the larger weight it will have. The output of each tree times the corresponding weight will be summed up and give the final output of the boosted decision tree. The boosted decision tree will be optimized by minimizing the loss function and penalized by a higher complexity of the trees.

5.4.2 Input variables

The input variables of the boosted decision tree used in $VH, H \rightarrow bb$ boosted analysis are listed in Table 5.8.

input variable	explanation
mJ	mass of the fat jet
$\Delta R(b_1, b_2)$	ΔR between two b-tagged track-jets inside the leading fat jet.
p_T^{b1}	transverse momentum of the leading b-tagged track-jet.
p_T^{b2}	transverse momentum of the sub-leading b-tagged track-jet.
p_T^V	transverse momentum of the reconstructed vector boson.
$\Delta\phi(V, bb)$	$\Delta\phi$ between the vector boson and two b-tagged jets.
$DL1r(b1)$	DL1r b-tagging score of leading b-tagged jet.
$DL1r(b2)$	DL1r b-tagging score of sub-leading b-tagged jet.
m_{eff}	sum of scalar sum of transverse momentum of all jets and missing transverse energy
$\Delta y(V, bb)$	Rapidity difference between vector boson and two b-tagged jets.
NAddCaloJets	number of additional calorimeter jets outside leading fat jet.
NMatchedTrackJet	number of track-jets matching the leading fat jet.

Table 5.8: List of input variables used in the boosted $VH, H \rightarrow bb$ BDT to separate the $VH, H \rightarrow bb$ signal and background.

5.4.3 BDT setup and training

In the BDT training, one potential problem is overtraining. This occurs when the machine learning model learned "too much" from the training events. i.e. about futures corresponding to sample statistical fluctuations that as such only exist in the training sample, but not in the testing sample. This often harms the accuracy of the prediction. To prevent this from happening, the training so called "hyper-parameters" are tuned and chosen carefully. For examples of such parameters are the number of trees used in training, the maximum depth of each decision tree, and the minimum percentage of training events in a leaf node. Parameters as such will be set prior to training and will remains constant. These hyper-parameters control the complexity of the BDT model. The more complex the model is, the easier it is for the training to result in overtraining.

The hyper parameters are set such that the BDT training will not result in overtraining. Several different sets of hyper-parameters are tested, and both perfomance and overtraining are evaluated. The goal is the best signal-versus-background separation, while keeping differences between BDT score distribution in training and testing sample small. The finally chosen hyper-parameters are listed in Table 5.9.

Hyper parameter	value
Number of decision trees used in BDT	200
Max depth of the tree	3
Boost method	AdaBoost
AdaBoost beta parameter	0.35
separation measure evaluating the node purity	Gini Index
the number of steps in the optimisation of the cut for a node	60
minimum percentage of training events in a leaf node	5%
Pruning method	No pruning

Table 5.9: List of hyper parameters and the corresponding value used for boosted $VH, H \rightarrow bb$ BDT training.

The comparison of the BDT score distribution between training and testing events is shown in Figure 5.19 (a). For both background and signal samples, training and testing BDT score distributions are roughly consistent, meaning there is no sign of overtraining. The overtraining can also be judged based on the ROC curve. The ROC curve is a curve of background inefficiency vs. signal efficiency where the inefficiency is defined by $1 - \text{efficiency}$. The ROC curve can be used as a measure on how well is the separation between signal and background by BDT at different BDT score threshold. Also, the area

under the ROC curve can be used as a single value measure on the effectiveness of BDT. The ideal case when signal and background is fully separated by BDT has background inefficiency stay at constant equals to 1 for all signal efficiency value and gives area under the curve equals to 1. Training results are only shown for one category of the 1-lepton channel in the boosted $VH, H \rightarrow bb$ analysis, but a similar procedure is followed in both resolved and boosted analyses, and in all categories. The thesis work involves training on the signal-versus-background BDT for boosted $VH, H \rightarrow bb$ 1-lepton channel when optimizing the b -tagging strategy as mentioned in section 5.1.1 and the result was adopted by analysis group.

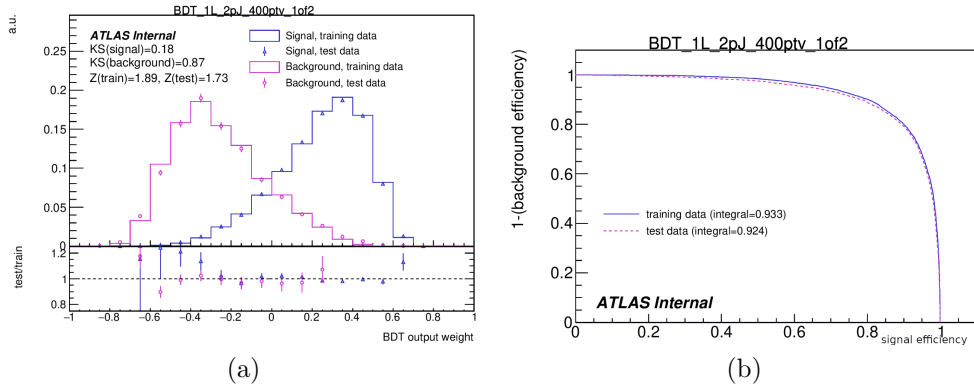


Figure 5.19: Figure shows the overtraining check result of the $VH(bb)$ boosted 1L training. The training used the input variable listed in Table 5.8 and hyper parameter values listed in Table 5.9. Figure (a) shows the overtraining check on events with $p_T^V > 400$ GeV and at least two jets. The top panel of Figure (a) shows the distribution of signal (blue) and background (red) in training (box) and test (point) data. The bottom panel shows the ratio between the test data and training data for signal and background. Figure (b) shows ROC curve in terms of background inefficiency vs. signal efficiency, for the training sample (blue, continuous line) and the testing sample (violet, dashed line), in the $p_T^V > 400$ GeV with at least two jets category of the boosted $VH, H \rightarrow bb$ analysis.

5.5 Statistical analysis

The goal of the analysis is to measure the $VH, H \rightarrow bb$ signal strength both inclusively and differentially vs. p_T^V , where signal strength is the ratio of measured cross-section of signal over predicted cross-section of signal. The measurement performed on data is from LHC collisions with centre-of-mass

energy of 13 Tev and collected by ATLAS during Run-II (2015-2018), corresponding to an integrated luminosity of approximately $L=139 \text{ fb}^{-1}$. The analysis also relies extensively on the detailed Monte Carlo (MC) simulations. The MC samples are generated based on known physics no BSM contributions and provide predictions for the signal and most of the backgrounds except multijet prediction. A model that varies as a function of a certain number of physics parameters can be built based on MC. By fitting the model to data using a maximum likelihood fit, one can get the best estimate of these measured physics parameters their associated uncertainties. The likelihood parameters include both parameters of interest, the ultimate goal of the measurement, such as signal strength and cross-section, and nuisance parameters, usually related to auxiliary measurement that constraint systematic uncertainties and to normalization factors for the background processes.

5.5.1 Statistical analysis method

Maximum likelihood and template fit

The statistical analysis of the data is mainly based on a maximum likelihood fit. The BDT score is used as main analysis observable in the likelihood to discriminate signal and background. The likelihood function encodes the expectation value for the number of events in each bin of the physics observable histogram. Additional analysis categories are just treated as additional set of observable bins. The number of events effectively seen on data is assumed to be randomly distributed according to a Poisson distribution around the respective expectation value. The number of expected events for both signal and background in the likelihood is mainly fixed to MC predictions, except for the signal strength and overall normalization factors of the main background which are determined directly in the fit. The expected number of events in each bin is:

$$N_i^{exp} = \mu s_i + b_i \quad (5.15)$$

where N_i^{exp} denotes the expected number of events, μ denotes the signal strength to be determined via maximum likelihood fit and s_i denotes the nominal number of predicted signal events in bin i , and b_i represent the number of background events in bin i . Considering a number M of analysis bins, a Poisson probability distribution of events in each bin, the likelihood can be constructed by the product of the Poisson probabilities:

$$L(\mu) = \prod_{i=1}^M \frac{(\mu s_i + b_i)^{N_i^{data}}}{N_i^{data}!} e^{-(\mu s_i + b_i)}, \quad (5.16)$$

where N^{data_i} represents the number of events observed in data in bin "i". This likelihood only include statistical uncertainties. The systematic uncertainties can be included by parametrizing the number of expected events in each sample as a function of additional nuisance parameters θ . For example, the number of events are parametrized into:

$$N_i^{exp}(\theta) = \mu s_i(\theta) + b_i(\theta) \quad (5.17)$$

To explain how a single nuisance parameter θ works, let's consider a single bin of the binned observable distribution. For example, let's assume there is a systematic uncertainty which has an impact on the expected number of events. Since the expected number of events cannot be perfectly known/simulated, one needs to give this model flexibility to vary the "true" value of the number of expected events within the allowed uncertainty. To do this, one can assume the "true" value of the number of expected events not to be just the nominal value but to be distributed according to a Gaussian centered around the nominal value. The width of the Gaussian is given by the predicted 1σ variation on the number of expected events due to that systematic uncertainty. In practice, in order to take correlations in how a common systematic uncertainty affects multiple analysis bins into account, a common nuisance parameter θ is used to parametrize this systematic uncertainty: the deviations on expected number of events in all bins is parametrized such that when $\theta = 0$, the systematic uncertainty does not have any impact, while for $\theta = \pm 1$ the systematic uncertainty corrects the nominal prediction by $\pm 1\sigma$. The nuisance parameters θ is then constrained by an auxiliary Gaussian constraint, with expected value of 0 and $\sigma=1$. Once the nominal prediction and $\pm 1\sigma$ deviations are given, the number of expected events in bin i, $b_i(\theta)$ can be expressed by interpolating linearly between the given points:

$$b_i(\theta) = b_i^0 + \theta * \Delta b_i, \quad (5.18)$$

where Δb_i denotes the $\pm 1\sigma$ deviation for a specific systematic uncertainty. Note that due to the linear interpolation, the b_i defined in the equation above are not exactly the real $b_i(\theta)$. The reason to do this linear interpolation is mainly to save computational resources as it takes significant extra effort to evaluate the value of $b_i(\theta)$ for each θ value. The number of signal events is also parametrized in the same way. The final likelihood function can be expressed as:

$$L(\mu, \theta) = \prod_{i=1}^M \frac{(\mu s_i(\theta) + b_i(\theta))^{N_i^{data}}}{N_i^{data}!} e^{-(\mu s_i(\theta) + b_i(\theta))} \times \prod_{j \in syst} \mathcal{N}(\theta_j, \Delta\theta_j), \quad (5.19)$$

where the signal and background expectation values for each bin i are parametrized by a set of nuisance parameters $\boldsymbol{\theta}$. Systematic deviations are constrained by the last term on the right-hand side of the equation, providing a penalty for deviations that are too far away from the nominal predictions. Once the likelihood model including both statistical and systematic uncertainties is defined, the likelihood function is maximized (or negative log likelihood as $-\log L$ is minimized) over the signal strength μ , any other parameter of interest. However, the values of θ for which the likelihood is maximal may depend on the value of μ , and this has an impact on evaluating confidence intervals for μ . This effect can be taken into account in the so called "profile likelihood" approach by using as test statistics the likelihood ratio λ expressed as:

$$\lambda(\mu) = \frac{L(\mu, \hat{\boldsymbol{\theta}})}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})} \quad (5.20)$$

where $\hat{\mu}, \hat{\boldsymbol{\theta}}$ denote the combined value of μ and $\boldsymbol{\theta}$ that maximize the likelihood, while vector $\hat{\boldsymbol{\theta}}$ are the values of $\boldsymbol{\theta}$ after maximizing the likelihood for a certain value of μ . In this way, the nuisance parameters are "profiled" out of the estimation of the parameter of interest μ , and they act in such a way to broaden the likelihood distribution as a function of the parameter of interest, increasing its associated uncertainty estimate.

The test statistics is then defined as:

$$t_\mu = -2 \log \lambda(\mu) = \left(\frac{\mu - \hat{\mu}}{\sigma_\mu} \right)^2 \quad (5.21)$$

The test statistics t_μ is independent of the nuisance parameter $\boldsymbol{\theta}$ and has a parabolic shape. The fitted signal strength is the μ value that maximizes the test statistics t_μ . According to Wilks' theorem, when the sample size is large enough, the test statistics t_μ asymptotically approaches a χ^2 distribution. The number of degrees of freedom of the χ^2 distribution is equal to the difference between the number of free parameters in the denominator and numerator of the likelihood function. In the case of the example where there is only one μ , the degree of freedom for the χ^2 is one. Based on this property, both confidence intervals for μ and the significance/p-value a signal-like excess can be calculated without the use of computationally expensive toy Monte Carlo fits.

There are also various ways to test the fit on MC. The first option is called pre-fit (meaning with pre-fit background normalizations), which allows the fit to be performed on the MC sample without any prior adjustment. The second option is called post-fit (meaning with post-fit background normaliza-

tions), where the fit is applied to a MC sample with the main background normalization rescaled as follows. First, a fit is performed to data to determine the normalization scale factors for the main backgrounds, $W+\text{jet}$ and $t\bar{t}$. In this fit, the signal strength parameter is kept blinded, to avoid introducing any interpretation bias. Then all $W+\text{jets}$ and $t\bar{t}$ events in the Monte Carlo samples are rescaled according to their respective scale factors.

Uncertainties as nuisance parameters

In the $VH, H \rightarrow bb$ analysis, the fit can be applied separately to each 0-,1- or 2-charged lepton channels, and separately to the resolved or boosted analysis, or combined fit over all regions can be performed. Tests with separate region help understand how uncertainties or changes to the analysis strategy affect the fit result. One example of nuisance parameters values after profile likelihood fit to either 'pre-fit' MC or data is shown in Figure 5.20 for the 1-lepton channel boosted $VH, H \rightarrow bb$ fit. Note that the extrapolation uncertainties evaluated in section 4.3 also shown up in the Figure. There are two extrapolation uncertainties for b-jets and one for c-jets. All the others are pruned away due to their limited effect on MVA score and p_T^V distributions entering the $VH, H \rightarrow bb$. For all nuisance parameters including both those related to the in-situ b -tagging calibration and the high- p_T extrapolation, the fitted values are all close to zero, meaning that the profiling the flavour tagging uncertainties provides nearly no correction to the shape and normalization likelihood function as determined on MC. The error bars of the fitted nuisance parameters are close to one, meaning that profiling does not significantly reduce b -tagging uncertainties compared to their pre-fit size. Freely floating normalizations such as for the $W+\text{jet}$ and $t\bar{t}$ background are also considered as nuisance parameters, but their associated uncertainty is purely determined from data.

Ranking of systematics and breakdown into categories To understand the importance of a certain systematic uncertainty, its impact on the parameter of interest is evaluated. In practice, the nuisance parameter value related to that systematics is set to ± 1 sigma, then the profile likelihood fit is repeated, resulting in a modified best-fit values for the parameter of interest. The difference between the original and new value for the parameter of interest represents the impact of that specific uncertainty. The impact is measured separately for both ± 1 sigma variations. After performing this procedure for all nuisance parameters, the uncertainties are ranked by their impact on μ and the top 15 uncertainties are illustrated in the so called "ranking plot". Such plot is very helpful in guiding analysers to focus on certain uncertainties rather

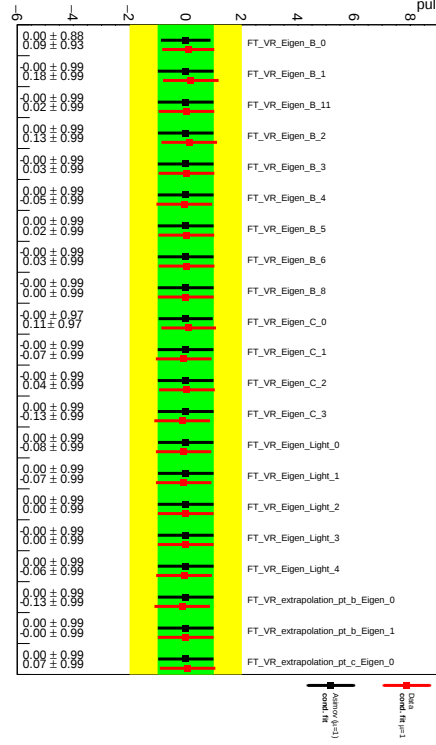


Figure 5.20: The flavor tagging nuisance parameters values and related uncertainties after the $VH, H \rightarrow bb$ likelihood fit is applied to either data (red) or to 'pre-fit' MC (black). The name of the nuisance parameters can be decoded as follows: FT is the abbreviation for flavour tagging, 'VR' represents the variable radius jet to which b -tagging is applied. 'B', 'C' and 'Light' represents b -, c - and *light*-jet. The suffix 'extrapolation_pt' denotes the b -tagging extrapolation uncertainties as introduced in section 4.3. The green and yellow bands determine the $\pm 1\sigma$ and $\pm 2\sigma$ regions, respectively

than others. If a certain nuisance parameter is top-ranked, then it is especially important to understand if that nuisance parameter acquires a non-negligible value after the profile likelihood fit to data, since such deviation from zero can potentially lead to a bias on the best-fit value of the signal strength.

The ranking plot for the 1-lepton channel of the boosted $VH, H \rightarrow bb$ analysis is shown in Figure 5.21. The nuisance parameter giving the largest impact on the parameter of interest (signal strength) is the normalization of the W+jets sample for events above 400 GeV. The 2nd ranked nuisance parameter is acceptance uncertainty of $t\bar{t}$ sample. The 3rd ranked nuisance parameter is modeling uncertainty of W+jets sample. The 4th ranked nuisance parameter is the largest b -tagging eigenvector uncertainty for b -jet.

The ranking plot shows the importance of such single uncertainty but sometimes it is also helpful to know the contribution to the overall uncertainty of a group of uncertainties. For example, flavor tagging uncertainties are decomposed into $O(10)$ eigenvector uncertainties, and, rather than checking the impact of a certain eigenvector uncertainty, it is also important to know how the whole set of eigenvector uncertainties contributes to the fit uncertainty on the parameter of interest. This can be done by fixing all nuisance parameters in the group to their nominal value and performing the profile likelihood fit again. The difference in quadrature between the original and new uncertainty on the parameter of interest provides an estimate of the contribution to the uncertainty of that specific group of systematic uncertainties. Uncertainties are calculated for both upward and downward variations of the parameter of interest. The impact of the statistical uncertainty is calculated easily by just fixing all nuisance parameters to their value from the original profile likelihood fit and then performing a new profile likelihood fit. Since the nuisance parameters are not allowed to vary, systematic uncertainties will not affect the fit result and the new uncertainty on the parameter of interest can be directly interpreted as the statistical uncertainty. Table 5.10 shows the breakdown table for the 1-lepton channel of the boosted $VH, H \rightarrow bb$ analysis, highlighting the contribution to the signal strength uncertainty of different groups of systematics and just due to statistical effect. Sum in quadrature of the statistical uncertainty and of the total systematic uncertainty is equal to the total uncertainty since these two are uncorrelated. However, the sum in quadrature of all individual groups of uncertainties is not equal to the total uncertainty because of correlations. In fact, in the profile likelihood fit to data, correlations between systematic uncertainties are introduced due to how the data constrains the nuisance parameters. In the presence of correlations, the sum in quadrature of the individual uncertainties will in general not be equal to the total uncertainty. The extrapolation uncertainties derived in section 4.3

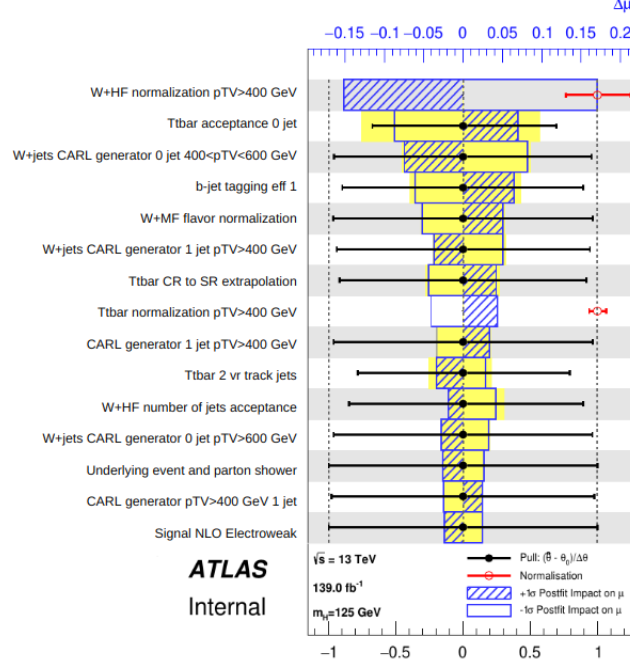


Figure 5.21: This figure illustrates the impact of systematic uncertainties on the fitted Higgs boson signal strength μ in the 1-lepton channel for the $VH, H \rightarrow bb$ boosted analysis from Run-2 data, using the nominal MVA analysis. The systematic uncertainties are arranged in decreasing order of their impact on μ . The blue boxes represent the variations of μ along the top x-axis. To obtain these variations, we fix the corresponding individual nuisance parameter θ to its fitted value $\hat{\theta}$ and modify it upwards or downwards by its fitted uncertainty. We then perform the fit again, allowing all other parameters to vary, ensuring proper consideration of correlations between systematic uncertainties. The hatched and open areas on the plot correspond to the upwards and downwards variations, respectively. On the other hand, the filled circles, referencing the bottom x-axis, indicate the deviations of the fitted nuisance parameters $\hat{\theta}$ from their nominal values θ_0 , expressed in terms of standard deviations with respect to their nominal uncertainties $\Delta\theta$. The associated error bars on the plot represent the fitted uncertainties of the nuisance parameters relative to their nominal uncertainties.

contributes to 0.2% of the total systematic uncertainty. The reason for such small impact is that the majority of events contains jets with $p_T < 250$ GeV, therefore this uncertainty has negligible impact on the 1-lepton channel of the $VH, H \rightarrow bb$ boosted analysis.

Source of uncertainties	Avg. Impact
Total	0.475
Statistical	0.419
Systematic	0.223
Theoretical and modelling uncertainties	
Signal	0.040
Background	0.143
$\hookrightarrow$ MultiJet	0.000
$\hookrightarrow$ Single top quark	0.014
$\hookrightarrow t\bar{t}$	0.088
$\hookrightarrow$ W+jets	0.103
$\hookrightarrow$ Z+jets	0.001
$\hookrightarrow$ Diboson	0.013
MC statistical	0.036
Experimental uncertainties	
Leptons	0.001
E_T^{miss}	0.010
Small-R jets	0.034
Large-R jets	0.036
b -tagging b-jet	0.068
b -tagging c-jet	0.011
b -tagging l-jet	0.002
b -tagging extrapolation	0.012
Pile-up	0.003
Luminosity	0.006

Table 5.10: The breakdown table shows the absolute contributions to the uncertainty on the signal strength of the $VH, H \rightarrow bb$ 1-lepton channel, for each category of uncertainty source. The impact on the signal strength μ determined for both upward and downward variations, of the parameter of interest. The average impact is computed as the square root of half of the sum in quadrature the signed impacts.

5.6 Combined VH , $H \rightarrow bb$ Results

As mentioned in section 5.1, the $VH \rightarrow bb$ analysis is separated into a resolved and a boosted analysis, into the 0-,1-,2-lepton channels. These can all be combined while measuring the cross-section times branching ratio of $VH, H \rightarrow bb$. Since the $VH \rightarrow bb$ analysis to which this thesis contributed is still ongoing, this section presents the current status of the analysis in terms of expected sensitivity and measurement uncertainties. The result of the fit to data is kept blinded to reduce the experimenter's potential bias while the internal ATLAS review of the analysis is ongoing. The result in this section refers to the combined measurement of the $VH, H \rightarrow bb$ signal in both resolved and boosted analyses, and in the three 0-,1- and 2-lepton channels. Note that the analysis fit integrates the top control region based on the $VH, H \rightarrow cc$ analysis selection, as described in detail in section 5.2.1.

5.6.1 Signal sensitivity and measurement uncertainty

In particle physics, the signal sensitivity is a measurement of how well is the signal can be disentangled from the background. To be more precise, this is usually quantified in the p-value, i.e. the probability, in a background only experiment, to see a signal-like excess that is equal or larger to that observed in data. The expected significance for the combined $VH, H \rightarrow bb$ is 8.36σ .

The expected signal strength is determined to be:

$$\mu = 1.00^{+0.10}_{-0.10}(\text{stat.})^{+0.09}_{-0.09}(\text{syst.}) = 1.00^{+0.13}_{-0.13}(\text{tot.}) \quad (5.22)$$

Table 5.11 shows the breakdown of expected contributions to the uncertainties for the combined $VH, H \rightarrow bb$ signal strength measurement. The total expected uncertainty of $\pm 13\%$ represents a reduction of $\sim 30\%$ compared to the previous result[60] that was based on the same dataset.

Since this thesis is mainly focused on the $VH, H \rightarrow bb$ in 1-lepton channel, the expected signal strength measurement in the $VH, H \rightarrow bb$ resolved and boosted 1-lepton channel is also reported. The expected significance is 5.04σ . The expected signal strength is:

$$\mu = 1.00^{+0.15}_{-0.15}(\text{stat.})^{+0.14}_{-0.13}(\text{syst.}) = 1.00^{+0.21}_{-0.20}(\text{tot.}) \quad (5.23)$$

The expected uncertainty of $\pm 21\%$ represent a reduction of $\sim 25\%$ compared to the previous result (± 0.18) [60], and the sensitivity to WH production is expected for the first time to exceed 5σ of the 25% improvement, the following stem directly from this thesis work: $\sim 10\%$ from b -tagging optimization (section

Source of uncertainties	Avg. Impact
Total	0.132
Statistical	0.100
Systematic	0.087
Theoretical and modelling uncertainties	
Signal	0.021
Background	0.067
$\hookrightarrow$ MultiJet	0.005
$\hookrightarrow$ Single top quark	0.015
$\hookrightarrow t\bar{t}$	0.020
$\hookrightarrow$ W+jets	0.034
$\hookrightarrow$ Z+jets	0.022
$\hookrightarrow$ Diboson	0.040
MC statistical	0.018
Experimental uncertainties	
Leptons	0.007
E_T^{miss}	0.018
Small-R jets	0.029
Large-R jets	0.009
b -tagging Calorimeter b-jet	0.019
b -tagging Calorimeter c-jet	0.009
b -tagging Calorimeter l-jet	0.005
b -tagging Track b-jet	0.006
b -tagging Track c-jet	0.002
b -tagging Track l-jet	0.001
b -tagging Track jet extrapolation	0.002
Pile-up	0.010
Luminosity	0.007

Table 5.11: The breakdown table shows the absolute contributions to the uncertainty on the signal strength of the combined $VH, H \rightarrow bb$, for each category of uncertainty source. The impact on the signal strength μ determined for both upward and downward variations, of the parameter of interest. The average impact is computed as the square root of half of the sum in quadrature the signed impacts.

5.1.1), $\sim 2\%$ from jet selection 5.1.1, $\sim 2\%$ from new $t\bar{t}$ CR (section 5.2.1), and $\sim 3\%$ from new W+jets optimization (section 5.2.1).

5.6.2 Simplified template cross sections(STXS)

When measuring the overall signal strength or the inclusive cross-section, the $VH, H \rightarrow bb$ signal is rescaled by a common factor μ across all reconstruction-level categories. However, many beyond the standard model(BSM) physics theories predict enhancement only in certain phase space regions such as at high Higgs boson transverse momentum. Therefore it is beneficial to measure a differential cross-section. However, there are not enough $VH, H \rightarrow bb$ data events for measuring the differential cross-section continuously. One option is to group truth-level phase space regions depending on kinematic features (number of jets, number of leptons, transverse momentum of the Higgs boson, etc) and production mode, and then measure them simultaneously across appropriately defined reconstruction-level regions. This is the so called simplified template cross section(STXS) approach. STXS categories/templates are defined for each production mode[61] and are implemented as uniformly as possible across all analyses so that it is easier for future combined Higgs measurements to use previous analysis results. Table 5.12 shows the expected uncertainties for one possible STXS measurement of VH production, based on the new $VH, H \rightarrow bb$ analysis. The STXS template is set depending on the vector boson type produced in association with the Higgs boson ($W^\pm$ or Z^0), and the transverse momentum of same vector boson (p_T^V). The expected uncertainty on the signal strength ($\frac{\sigma_{meas}}{\sigma_{pred}}$) is larger in the high p_T^V STXS region due to smaller amount of data, but this can be compensated by the higher signal enhancement expected in certain BSM models. It should be noted that high p_T^V correlates with high m_{VH} , the effective energy being exchanged by the colliding protons to produce VH. Comparing this STXS template with the latest result [60], the $400 \text{ GeV} < p_T^V$ bin in WH and ZH production channel is split into two bins: $400 \text{ GeV} < p_T^V < 600 \text{ GeV}$ and $600 \text{ GeV} < p_T^V$ since many BSM physics is sensitive to Higgs boson with high transverse momentum. Apart from the high p_T^V region, comparison between expected result shown in table 5.12 and the latest result measured on data is shown in Table 5.13. The uncertainty reduction is between 3-47%.

Higgs production channel	p_T^V	Expected signal strength
WH	$150 < p_T^V < 250$ GeV	1.00 ± 0.39
WH	$250 < p_T^V < 400$ GeV	1.00 ± 0.35
WH	$400 < p_T^V < 600$ GeV	1.00 ± 0.63
WH	$600 \text{ GeV} < p_T^V$	1.00 ± 0.91
ZH	$75 < p_T^V < 150$ GeV	1.00 ± 0.60
ZH	$150 < p_T^V < 250$ GeV	1.00 ± 0.27
ZH	$250 < p_T^V < 400$ GeV	1.00 ± 0.32
ZH	$400 < p_T^V < 600$ GeV	1.00 ± 0.61
ZH	$600 \text{ GeV} < p_T^V$	1.00 ± 1.02

Table 5.12: Expected uncertainties for the simplified template cross sections (STXS) measurement in the combined $VH, H \rightarrow bb$ analysis. In this STXS scheme, the signal strength is measured in different p_T^V ranges and different Higgs production modes depending on the type of vector boson. In total, nine signal strengths are measured.

Higgs production channel	p_T^V	Uncertainty reduction
WH	$150 < p_T^V < 250$ GeV	47%
WH	$250 < p_T^V < 400$ GeV	3%
WH	high p_T^V	-9%
ZH	$75 < p_T^V < 150$ GeV	29%
ZH	$150 < p_T^V < 250$ GeV	16%
ZH	$250 < p_T^V < 400$ GeV	20%
ZH	high p_T^V	80%

Table 5.13: STXS measurement relative uncertainty reduction for STXS bins. The comparison is between expected STXS measurement of the ongoing analysis with previous result[60] measured based on same set of data. In the new STXS scheme in the ongoing analysis, region $p_T^V > 400$ GeV is splitted into two STXS bins: $400 \text{ GeV} < p_T^V < 600$ GeV and $600 \text{ GeV} < p_T^V$, while in the previous result there is only one STXS bins. Therefore, in $p_T^V > 400$ GeV region, the comparison of uncertainty is done between the single STXS bin in previous analysis and $400 \text{ GeV} < p_T^V < 600$ GeV STXS bin in the ongoing analysis. The reason for choosing $400 \text{ GeV} < p_T^V < 600$ GeV is because it is the much more sensitive. The comparison result is shown in row labeled with high p_T^V in the table.

Chapter 6

Summary and conclusion

This thesis focused on new methods for flavor tagging in ATLAS and on the study of $H \rightarrow bb$ decays in VH production based on $L = 139fb^{-1}$ of LHC collision data.

On the flavor tagging side, the methodology and the validation of a novel "eigenvector recomposition" approach was produced. This method uses information from the flavor-tagging eigenvector uncertainties and "recomposes" them back into the original sources of uncertainty of the flavor-tagging calibration analysis. This allows analyses having different flavor-tagging setups to properly correlate their flavor-tagging uncertainties by a simple modification of the final likelihoods used in the signal extraction fits. This is useful, for example, to take the correlated impact of the flavor-tagging uncertainties in combination analyses properly into account, e.g. in the combination of all Higgs boson measurements [62], where the flavor-tagging uncertainties can play a non negligible role. In addition, by reverting to the original sources of uncertainty in the flavor tagging calibration, the method also enables the correlation of systematic effects impacting directly the physics analysis with those that have and indirect impact due to changes induced in the flavor-tagging scale factors.

A careful validation has been performed both at histogram level, as well as at the level of the final maximum likelihood fit. The checks performed at histogram level show that the recomposed uncertainties match the original source uncertainties within numerical accuracy. At the maximum likelihood fit level, no significant difference is observed in terms of fit results and pulls of nuisance parameters between the original and the recomposed likelihoods. The software tool implementing the new method is thus ready to be deployed more widely in ATLAS physics analyses, and a public ATLAS note has been released that describes the new approach [52].

Also, a new method has been developed to evaluate the high- p_T extrapola-

tion uncertainties for the pseudo-continuous b -tagging calibration for variable radius track jets. The pseudo-continuous b -tagging calibration is a simultaneous calibration of a binned version of the b -tagging score distribution, allowing analyses to use multiple b -tagging criteria simultaneously. The new method is purely based on Monte-Carlo and leverages high p_T events generated from a $Z' \rightarrow bb/cc/ll$ sample. Its formalism preserves the sign of the systematic variations across the various kinematic bins and b -tagging score bins, providing a better preservation of the total number of jets even when systematic variations are applied. In addition, this thesis explains how the high- p_T extrapolation uncertainties are decomposed into an additional set of eigenvectors and additionally pruned to remain within $\mathcal{O}(5)$ while keeping deviations in the description of the correlation factors across p_T and tag weight bins compared to their nominal value to below 12%. The sum in quadrature of the selected eigenvector uncertainties represents 99.5% of the total uncertainties. The high- p_T extrapolation uncertainties have been implemented in the official ATLAS b -tagging calibration framework and carefully validated, so that they are now available for use in ATLAS physics analyses.

This thesis also contributed to setting up and performing the final ATLAS Run-2 analysis of $VH, H \rightarrow bb$, including introducing several improvements. The b -tagging working points are optimized for the boosted $VH, H \rightarrow bb$ analysis specifically for the 1-lepton channel. For the track jets inside the large-R jet, the b -tagging working point selection is loosened from 70% to 85% b -jet efficiency. For track jets outside the large-R jet, the anti- b -tagging selection cut is moved from 70% to 85% to reduce the $t\bar{t}$ background. The analysis significance improved by $\sim 10\%$ after such optimization. The jet tagging strategy in terms of which jets to tag within the large-R jet is also revised. The old default strategy was to tag the two track jets with highest p_T inside the large-R jet. Two new strategies were tested: 1. Tagging the three track jets with highest p_T inside the large-R jet. 2. Tagging all track jets inside the large-R jet. The best strategy turns out to be option 1, which improves the analysis significance by $\sim 4\%$.

Apart from the improvements introduced in the boosted $VH, H \rightarrow bb$ 1-lepton analysis, several studies were also performed in the resolved $VH, H \rightarrow bb$ 1-lepton analysis. The first improvement is the additional of control region for the top background based on the c -tagging selection of the $H \rightarrow cc$ analysis, to help constrain the normalization factor of the $t\bar{t}$ background in $VH, H \rightarrow bb$ analysis. This result in a 1.8% improvement to the signal significance. Second improvement is achieved in tightening the constrain on the normalization factor for the W +jets background. In a dedicated control region(CRLow), a BDT is trained to separate events from $t\bar{t}$ and W +jets production. After ex-

exploiting such BDT in the likelihood fit, the uncertainties on the W+jets and $t\bar{t}$ normalization factors are reduced by 14-48% and 3-8% respectively, leading to an improvement in the signal significance of around 5%. The new approach also reduces the correlation between the $t\bar{t}$ and W+jets normalization factors, leading to a more robust result.

Another area where several improvements were introduced is the background modeling for both the resolved and the boosted $VH, H \rightarrow b\bar{b}$ analysis. To model the W+jet events distributions more accurately, electroweak corrections are now applied. Also, a new technique called CARL for estimating the modeling uncertainty was tested and is now implemented in both resolved and boosted analyses. This technique is based on deep neural networks thus it has conceptual advantages over the previous BDT-based method.

The expected significance of the $H \rightarrow b\bar{b}$ signal in the combined $VH, H \rightarrow b\bar{b}$ analysis is 8.36σ and the signal strength is expected to be measured as:

$$\mu = 1.00^{+0.10}_{-0.10}(\text{stat.})^{+0.09}_{-0.09}(\text{syst.}) = 1.00^{+0.13}_{-0.13}(\text{total}) \quad (6.1)$$

with an uncertainty of $\pm 13\%$, an improvement of $\sim 30\%$ compared to the $\pm 18\%$ uncertainty on the previous result[60], based on the same data set. This thesis work is mainly focused on $VH, H \rightarrow b\bar{b}$ 1-lepton channel, where the signal strength is expected to be measured as:

$$\mu = 1.00^{+0.15}_{-0.15}(\text{stat.})^{+0.14}_{-0.13}(\text{syst.}) = 1.00^{+0.21}_{-0.20}(\text{total}) \quad (6.2)$$

With an uncertainty of $\pm 21\%$, an improvement of $\sim 25\%$ compared to the previous result. While the analysis is currently under ATLAS internal review and the result on data is thus kept blinded to avoid any procedural and/or interpretation bias, the work in this thesis has contributed significantly towards the above mentioned improvement in expected sensitivity to the $H \rightarrow b\bar{b}$ signal.

The analysis is also interpreted in the STXS scheme in terms of a differential measurement of $VH, H \rightarrow b\bar{b}$ in bins of p_T^V and separately for WH and ZH production.

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Appendices

Appendix .1 describes the mathematical derivation of the covariance matrix. Appendix .2 proves how to mathematically transform the likelihood function in Eq. 4.17 to Eq. 4.18, and vice versa. Appendix .3 summarises pruning studies performed on the original b - and c -jet calibration uncertainties before they even enter the eigenvector decomposition, and thus the recomposition method. Appendix .4 shows concrete examples of the U and the $\tilde{U}_{\text{right}}^{-1}$ matrices to illustrate the level of complexity of these operations. Appendix .5 shows additional high- p_T extrapolation uncertainties. Appendix .6 proves how to restore eigenvalue after extending the in-situ calibration uncertainties into the high- p_T region. Appendix .7 proves how to restore eigenvector after extending the in-situ calibration uncertainties into the high- p_T region. Appendix .8 shows the detailed information of MC samples used for evaluating high- p_T extrapolation uncertainties.

.1 Derivation of the covariance matrix

Let i and j be two different p_T bins, the covariance of the total systematic uncertainty between these two bins is calculated as follows. Denoting T_i the total systematic variation in bin i , and denoting $\mathcal{N}(\sigma)$ the normal distribution centered at 0 with variance σ^2 :

$$\begin{aligned}
V_{ij} &= E[T_i T_j] - E[T_i]E[T_j] \\
&= E\left[\sum_{k=1}^M \mathcal{N}(u_{ik}) \sum_{l=1}^M \mathcal{N}(u_{jl})\right] - E\left[\sum_{k=1}^M \mathcal{N}(u_{ik})\right]E\left[\sum_{l=1}^M \mathcal{N}(u_{jl})\right] \\
&= E\left[\sum_{k=l} \mathcal{N}(u_{ik})\mathcal{N}(u_{jl}) + \sum_{k \neq l} \mathcal{N}(u_{ik})\mathcal{N}(u_{jl})\right] - \\
&\quad \sum_{k=1}^M E[\mathcal{N}(u_{ik})] \sum_{l=1}^M E[\mathcal{N}(u_{jl})] \\
&= \sum_{k=1}^M E[\mathcal{N}(u_{ik})\mathcal{N}(u_{jk})] + \sum_{k \neq l} E[\mathcal{N}(u_{ik})]E[\mathcal{N}(u_{jl})] \\
&= \sum_{k=1}^M u_{ik}u_{jk}
\end{aligned} \tag{3}$$

Where the last step used the property that a single source of uncertainty is fully correlated between two bins, i.e. $E[\mathcal{N}(u_{ik})\mathcal{N}(u_{jk})] = u_{ik}u_{jk}$. Also, during the derivation, the following assumptions were made:

- The systematic uncertainties are distributed according to a Gaussian with central values set to zero by construction.
- The different sources of uncertainty are independent between each other.

.2 Proof of the equivalence of the likelihood functions involving the θ or the η parameters

This section aims at demonstrating the equivalence between the likelihood function before the eigenvector decomposition in Eq. 4.17, expressed as a function of η nuisance parameters constrained by Gaussian priors, and the likelihood function shown in Eq. 4.18, after eigenvector decomposition, expressed as a function of the θ nuisance parameters also constrained by Gaussian priors. We will demonstrate first how to get from the likelihood function $\mathcal{L}(\mu, \eta)$ to the likelihood function $\mathcal{L}(\mu, \theta)$, i.e. following the eigenvector decomposition step (Section .2.1), and then how to get back from $\mathcal{L}(\mu, \theta)$ to $\mathcal{L}(\mu, \eta)$ (Section .2.2), which is the operation performed by the eigenvector decomposition method.

.2.1 Transforming $\mathcal{L}(\mu, \eta)$ into $\mathcal{L}(\mu, \theta)$

First, let us re-introduce the likelihood function before applying the eigenvector decomposition. In this case, the b -tagging systematic uncertainties are encoded into the nuisance parameters η . These parameters η are defined in such a way that their priors have mean 0 and variance equal to 1. To simplify the notation the implicit summation over indices will be used through the appendix. The analysis likelihood was shown in Eq. 4.18 to be:

$$\mathcal{L} = L(\mu, \eta_1, \eta_2, \dots, \eta_M) \exp \left[-\frac{\eta_i (V_\eta^{-1})_{ij} \eta_j}{2} \right] \quad (4)$$

where:

$$\exp \left[-\frac{\eta_i (V_\eta^{-1})_{ij} \eta_j}{2} \right] = \prod_{i=1}^M \exp \left[-\frac{(\eta_i)^2}{2} \right]. \quad (5)$$

Since the parameters η encode independent sources of systematic uncertainties and their variance is chosen to be 1, their covariance matrix is diagonal, i.e. $V_\eta = I$.

The analysis likelihood $\mathcal{L}$ is only dependent on variations of the b -tagging scale factors in the N kinematic bins of the calibration. There can therefore

only be up to N independent linear combinations of the η nuisance parameters that induce variations of the scale factors. In practice, once accounting for the additional kinematic bins introduced by the smoothing procedure, only up to L ($L \leq N$) independent combinations induce variations of the b -tagging scale factors, while all other $M - L$ combinations of the η nuisance parameters, with M being the number of η parameters, have to be orthogonal to these and do not have any impact on the scale factors, and thus on the analysis likelihood.

The easiest way to derive this set of L independent variations of the scale factors and associated nuisance parameters is to compute the covariance matrix of the b -tagging calibration scale factors in the space of the N kinematic bins, and diagonalize it, getting a set of L ($L \leq N$) independent eigenvector variations with non-zero eigenvalues, as described in detail in Section 4.2.2. This set of L scale factor eigenvector variations, once normalized through their eigenvalues, is described by the nuisance parameters θ .

The expression of the θ nuisance parameters as a function of the η nuisance parameters has been derived in this document (see Eq. 4.15) and has been shown to be:

$$\theta_i = \eta_j \cdot \left(U \cdot \tilde{U}_{\text{right}}^{-1} \right)_{ji} = \text{Re}_{ij}^T \eta_j, \quad (6)$$

where the index i runs from 1 to L , while the index j runs from 1 to M .

As demonstrated later in this appendix in Section 2.1, $\text{Re}^T \text{Re} = I_L$. This means that the rows of the matrix Re^T represent an orthonormal set of vectors. This is not too surprising since the transformation of Eq. 6 transforms orthogonal (i.e. independent) directions in $\boldsymbol{\eta}$ into orthogonal directions of $\boldsymbol{\theta}$. However, it is a transformation from a higher-dimensional space to a lower-dimensional space, and is thus not directly invertible. We can make it invertible adding the missing dimensions, i.e. those directions of the subspace $M - L$ that have no impact on the b -tagging scale factors, and thus on the analysis likelihood.

We can define a new matrix A^T with number of rows $M - L$ and number of columns M , such that the $M - L$ rows contain a set of orthonormal vectors representing all $M - L$ directions that are orthogonal to those represented by the row vectors of the matrix Re^T . The matrix A^T will thus need to respect the orthogonality relation $A^T \text{Re} = 0$, or equivalently $\text{Re}^T A = 0$. Since we chose a set of orthonormal vectors, the condition $A^T A = I$ needs to be imposed as well. Note that it is always possible to find an orthonormal basis to span this $M - L$ -dimensional sub-space of the η parameters, and therefore it is always possible to define such matrix A^T .

We can define a new set of nuisance parameters $\boldsymbol{\kappa}$, such that:

$$\kappa_i = A_{ij}^T \eta_j, \quad (7)$$

where the index i runs from 1 to $M - L$, while the index j runs from 1 to M .

We can now consider the nuisance parameters θ (of dimension L) and κ (of dimension $M - L$) as part of a single M -dimensional vector of nuisance parameters x :

$$x = \begin{pmatrix} \theta \\ \kappa \end{pmatrix} = \begin{bmatrix} \text{Re}^T \\ A^T \end{bmatrix} \eta = \mathcal{O} \eta \quad (8)$$

Because of the orthonormality and orthogonality conditions previously imposed, the transformation matrix $\mathcal{O}$ composed by Re^T and A^T is an $M \times M$ orthogonal matrix, representing a simple rotation. It can be therefore inverted, with $\mathcal{O}^{-1} = \mathcal{O}^T$:

$$\eta = \mathcal{O}^T \begin{pmatrix} \theta \\ \kappa \end{pmatrix} = [\text{Re} \ A] \begin{pmatrix} \theta \\ \kappa \end{pmatrix} = \text{Re} \theta + A \kappa \quad (9)$$

Starting from the likelihood of Eq. 4 expressed in the space of the parameters η , we can now replace η with θ everywhere:

$$\begin{aligned} \mathcal{L} &= L(\boldsymbol{\mu}, \eta_1(\theta), \dots, \eta_M(\theta)) \exp \left[\sum_{i=1}^M -\frac{(\eta_i(\theta, \kappa))^2}{2} \right] \\ &= L(\boldsymbol{\mu}, \theta_1, \dots, \theta_L) \exp \left[-\frac{(\theta \ \kappa) \begin{bmatrix} \text{Re}^T \\ A^T \end{bmatrix} [\text{Re} \ A] \begin{pmatrix} \theta \\ \kappa \end{pmatrix}}{2} \right] \\ &= L(\boldsymbol{\mu}, \theta_1, \dots, \theta_L) \exp \left[-\frac{(\theta \ \kappa) \begin{bmatrix} \text{Re}^T \text{Re} & \text{Re}^T A \\ A^T \text{Re} & A^T A \end{bmatrix} \begin{pmatrix} \theta \\ \kappa \end{pmatrix}}{2} \right]. \end{aligned} \quad (10)$$

Here we already made use of the information that the b -tagging scale factors, and thus the analysis likelihood, does only vary under variations of the parameters $\boldsymbol{\theta}$, but not of the parameters $\boldsymbol{\kappa}$. Using the orthonormality and orthogonality relations $\text{Re}^T \text{Re} = I$, $A^T A = 1$ and $\text{Re}^T A = 0$, we can factorize the constraint term in $\boldsymbol{\theta}$ from the constraint term in $\boldsymbol{\kappa}$, so that the final likelihood in the space of the $\boldsymbol{\theta}$ becomes:

$$\mathcal{L} = L(\boldsymbol{\mu}, \theta_1, \dots, \theta_L) \prod_{i=1}^L \exp \left[-\frac{(\theta_i)^2}{2} \right] \prod_{j=1}^{M-L} \exp \left[-\frac{(\kappa_j)^2}{2} \right] \quad (11)$$

Note that since the analysis likelihood L does not depend on $\boldsymbol{\kappa}$, the maximization of the likelihood will not be affected by the constraint term in $\boldsymbol{\kappa}$,

which can be thus safely removed, yielding:

$$\mathcal{L} = L(\boldsymbol{\mu}, \theta_1, \theta_2, \dots, \theta_L) \exp \left[-\frac{\theta_i (V_{\theta}^{-1})_{ij} \theta_j}{2} \right], \quad (12)$$

with constraint term:

$$\exp \left[-\frac{\theta_i (V_{\theta}^{-1})_{ij} \theta_j}{2} \right] = \prod_{i=1}^L \exp \left[-\frac{(\theta_i)^2}{2} \right]. \quad (13)$$

When applying the eigenvector decomposition, and moving from Eq. 4 to Eq. 12, effectively we are applying a rotation in the space of the $\boldsymbol{\eta}$ (Eq. 9) to separate the directions that induce a variation in the b -tagging scale factors (spanned by the $\boldsymbol{\theta}$), from those that leave them invariant (spanned by the $\boldsymbol{\kappa}$), and then we are dropping the $\boldsymbol{\kappa}$ directions since they do not have any impact on the analysis.

Proof that $\text{Re}^T \text{Re} = I_L$

From Appendix .1, the covariance matrix can be expressed as:

$$V = U^T U \quad (14)$$

where $U \in R^{M \times N}$, $V \in R^{N \times N}$. Applying the eigenvector decomposition to the covariance matrix (V):

$$V = P \Lambda P^T \quad (15)$$

Where P is an orthogonal matrix and Λ is diagonal matrix in which the diagonal terms are eigenvalues of V.

$$\Lambda = \begin{pmatrix} \lambda_1^2 & & \\ & \ddots & \\ & & \lambda_N^2 \end{pmatrix}, P = (\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N) \quad (16)$$

Therefore

$$\tilde{U} = \sqrt{\Lambda} P^T = \begin{pmatrix} \lambda_1 \mathbf{v}_1^T \\ \vdots \\ \lambda_N \mathbf{v}_N^T \end{pmatrix} \rightarrow \begin{pmatrix} \lambda_1 \mathbf{v}_1^T \\ \vdots \\ \lambda_L \mathbf{v}_L^T \end{pmatrix} \quad (17)$$

In the last step above, the rows in matrix $\tilde{U}$ have been discarded as explained

in section 4.2.2. Writing it in compact form:

$$\tilde{U}_{\text{right}}^{-1} = \left(\frac{1}{\lambda_1} \mathbf{v}_1 \quad \dots \quad \frac{1}{\lambda_L} \mathbf{v}_L \right) \quad (18)$$

Following from the properties of $\text{Re}^T \text{Re}$ one obtains:

$$\begin{aligned} \text{Re}^T \text{Re} &= [\tilde{U}_{\text{right}}^{-1}]^T \cdot U^T U \cdot \tilde{U}_{\text{right}}^{-1} \\ &= [\tilde{U}_{\text{right}}^{-1}]^T \cdot V \cdot \tilde{U}_{\text{right}}^{-1} \\ &= [\tilde{U}_{\text{right}}^{-1}]^T \cdot P \Lambda P^T \cdot \tilde{U}_{\text{right}}^{-1} \\ &= \begin{pmatrix} \frac{1}{\lambda_1} & & 0 & \dots & 0 \\ & \ddots & 0 & \vdots & 0 \\ & & \frac{1}{\lambda_L} & 0 & \dots & 0 \end{pmatrix} \begin{pmatrix} \lambda_1^2 & & & & \\ & \ddots & & & \\ & & \lambda_N^2 & & \end{pmatrix} \begin{pmatrix} \frac{1}{\lambda_1} \\ & \ddots & \\ 0 & \dots & \frac{1}{\lambda_L} \\ \vdots & & \vdots \\ 0 & \dots & 0 \end{pmatrix} \\ &= I_L, \end{aligned} \quad (19)$$

where I_L is a unit diagonal matrix of size $L \times L$. As a consequence, the rows of the matrix Re^T represent an orthonormal set of L vectors of dimension M .

.2.2 Transforming $\mathcal{L}(\boldsymbol{\mu}, \boldsymbol{\theta})$ back into $\mathcal{L}(\boldsymbol{\mu}, \boldsymbol{\eta})$

We can also perform explicitly the inverse transformation starting from the likelihood function in the $\boldsymbol{\theta}$ space:

$$\mathcal{L} = L(\boldsymbol{\mu}, \theta_1, \theta_2, \dots, \theta_L) \prod_{i=1}^L \exp \left[-\frac{(\theta_i)^2}{2} \right], \quad (20)$$

and transforming it back to the likelihood in the $\boldsymbol{\eta}$ space.

First, we re-add explicitly the additional nuisance parameters $\boldsymbol{\kappa}$ that the analysis likelihood function L does not depend on, yielding the expression:

$$\mathcal{L} = L(\boldsymbol{\mu}, \theta_1, \dots, \theta_L) \prod_{i=1}^L \exp \left[-\frac{(\theta_i)^2}{2} \right] \prod_{j=1}^{M-L} \exp \left[-\frac{(\kappa_j)^2}{2} \right] \quad (21)$$

Then we replace $\boldsymbol{\theta}$ and $\boldsymbol{\kappa}$ as a function of $\boldsymbol{\eta}$, using equations 6 and 7,

obtaining:

$$\mathcal{L} = L(\boldsymbol{\mu}, \theta_1(\eta), \dots, \theta_L(\eta)) \exp \left[-\frac{\eta^T \text{Re} \text{Re}^T \eta}{2} \right] \exp \left[-\frac{\eta^T A A^T \eta}{2} \right] \quad (22)$$

$$= L(\boldsymbol{\mu}, \eta_1, \dots, \eta_M) \exp \left[-\frac{\eta^T [\text{Re} \text{Re}^T + A A^T] \eta}{2} \right] \quad (23)$$

The constrain term in $\boldsymbol{\eta}$ originating from the $\boldsymbol{\theta}$ space, and the one originating from the $\boldsymbol{\kappa}$ space are not diagonal in the $\boldsymbol{\eta}$ space. However, as we have seen already in Eq. 9, we can define a rotation matrix $\mathcal{O}$ merging the rows of matrix Re^T with the rows of matrix A^T . We can thus re-express the likelihood as a function of $\mathcal{O}$:

$$\mathcal{L} = L(\boldsymbol{\mu}, \eta_1, \dots, \eta_M) \exp \left[-\frac{\eta^T \mathcal{O}^T \mathcal{O} \eta}{2} \right], \quad (24)$$

but since $\mathcal{O}^T = \mathcal{O}^{-1}$, we trivially get:

$$\begin{aligned} \mathcal{L} &= L(\boldsymbol{\mu}, \eta_1, \dots, \eta_M) \exp \left[-\frac{\eta^T \eta}{2} \right] \\ &= L(\boldsymbol{\mu}, \eta_1, \dots, \eta_M) \prod_{i=1}^M \exp \left[-\frac{(\eta_i)^2}{2} \right], \end{aligned} \quad (25)$$

When applying the recomposition method to revert back from the likelihood function of Eq. 20 expressed in the space of the $\boldsymbol{\theta}$, to the likelihood function of Eq. 25 expressed in the space of the $\boldsymbol{\eta}$, it is therefore important to remember that the latter can only be recovered after adding back the constraint term in the $\boldsymbol{\kappa}$. In the eigenvector recomposition method described in Section 4.2.2, this step is accomplished by simply removing the (diagonal) priors in $\boldsymbol{\theta}$ (from Eq. 20), and then just adding back all (diagonal) priors in the $\boldsymbol{\eta}$ (see Eq. 25), which will thus effectively include both the directions spanned by the $\boldsymbol{\theta}$ and by the $\boldsymbol{\kappa}$.

In addition, the formalism just presented allows for the derivation of an explicit expression of the η as a function of the θ nuisance parameters. Since the analysis likelihood L does not depend on the $\boldsymbol{\kappa}$, the full likelihood $\mathcal{L}$ is maximized over the $\boldsymbol{\kappa}$ by setting $\boldsymbol{\kappa} = \mathbf{0}$ (see Eq. 21), regardless of the value of the θ that maximizes the likelihood. This implies that Eq. 9 simplifies to:

$$\boldsymbol{\eta} = \text{Re } \boldsymbol{\theta} \quad (26)$$

which proves explicitly the uniqueness of the relation between the $\boldsymbol{\eta}$ and the

θ nuisance parameters. Multiplying both terms of Eq. 26 by their transpose the expression becomes $\boldsymbol{\eta}^T \boldsymbol{\eta} = \boldsymbol{\theta}^T (\text{Re}^T \text{Re}) \boldsymbol{\theta} = \boldsymbol{\theta}^T I_L \boldsymbol{\theta}$, which after considering the likelihood maximization leads to:

$$\sum_{k=1}^L \theta_k^2 = \sum_{j=1}^M \eta_j^2 \quad (27)$$

.3 Pruning the original sources of uncertainty

In order to speed up the fitting time, the calibration uncertainty sources can be pruned "a priori", even before entering the eigenvector diagonalization step (e.g. the *decomposition* step described in section 4.2.2). A dedicated study on the b -jet calibration uncertainty sources of both Fixed cut and Pseudo-Continuous working points is reported in Figure 1. The plot shows the ratio between the uncertainty calculated keeping only a certain number of original NPs over the total b -jet uncertainty as a function of p_T . The uncertainty sources have been ranked summing in quadrature their variation (systematic-nominal) in all p_T bins (or all combinations of p_T and b -tagging score bins for the pseudo-continuous calibration), divided by the number of bins¹. Both statistical and systematic sources of uncertainty have been considered for this study. The dashed line shows the 98% threshold. For the current b -jet calibration, one can reconstruct 98% of the total b -jet uncertainty considering only the first 26 original NPs for the Fixed Cut 70% working point (44 for the pseudo-continuous calibration), over a total of 127 NPs.

The correlations across p_T bins before and after pruning are also checked. A dedicated study performed on the Fixed Cut WP, shown in Figure 2, confirms that with this threshold the correlation pattern remains largely similar to the full NPs scenario.

Analogously, a similar study has been performed with the c -jet calibration uncertainties. Figure 3 shows the ratio between the uncertainty calculated keeping only a certain number of original NPs over the total c -jet uncertainty as a function of p_T . The uncertainty sources have been ranked as described above. The dashed line shows the 98% threshold. It is possible to reconstruct 98% of the total c -jet uncertainty considering the first 13 original NPs for the Fixed Cut 70% working point (33 for the pseudo-continuous calibration), over a total of 95 NPs.

¹This method gives more importance to variations having a high impact on a small number of bins. However most of the uncertainty sources are distributed over all the kinematic bins, so these scenarios are limited.

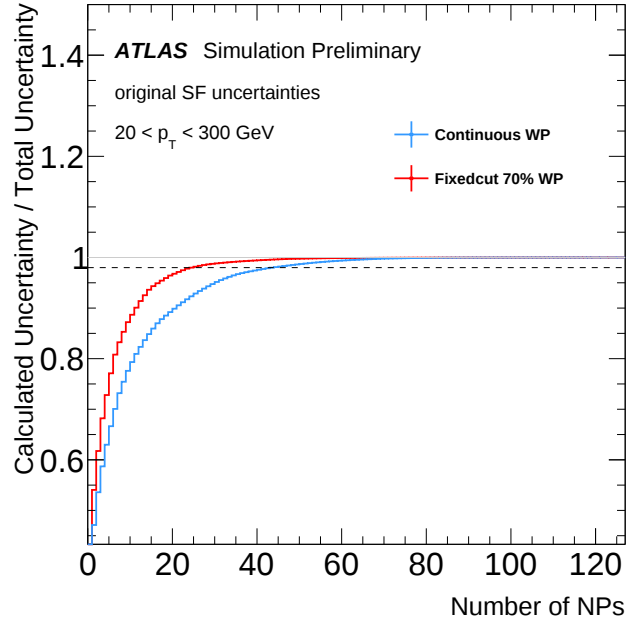
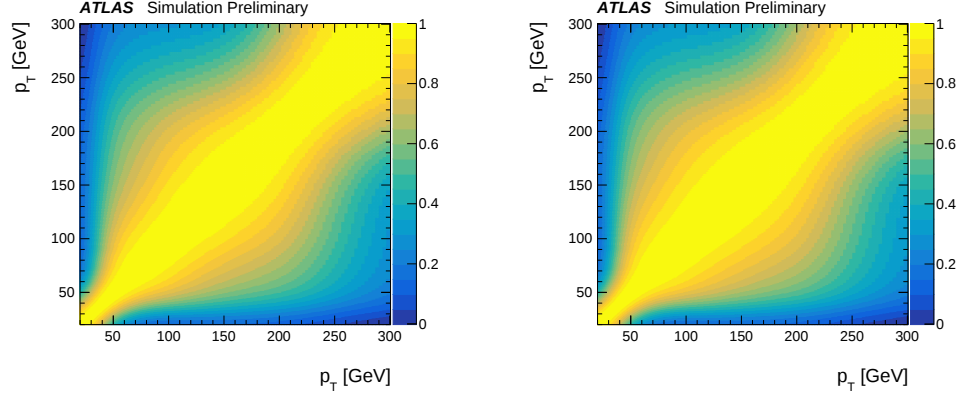
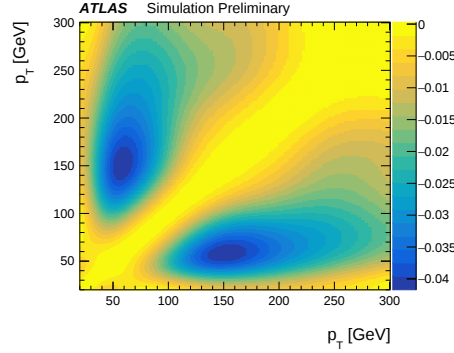


Figure 1: Ratio between the sum in quadrature of the uncertainty calculated using a certain number of *original* NPs over the sum in quadrature of the *total* b -jet uncertainty. The transverse momentum is restricted within the validity range of the calibration ($20 < p_T < 300 \text{ GeV}$). The horizontal dashed line marks the 98% threshold, while the solid line marks the 100% limit.



(a) 127 uncertainty sources (full set)

(b) 26 uncertainty sources



(c) Difference

Figure 2: Plots showing the correlation matrix of the b -jet sources of uncertainty on the scale factor as a function of p_T before (a) and after (b) pruning them. Figure (c) shows the difference between the two correlation matrices. Pruning has been applied computing the sum in quadrature of the variance of each uncertainty source over all p_T bins and keeping only the first N uncertainty sources that summed together give 98% of the total uncertainty. The absolute difference between the full matrix and the pruned matrix is at most 4% around the darkest region.

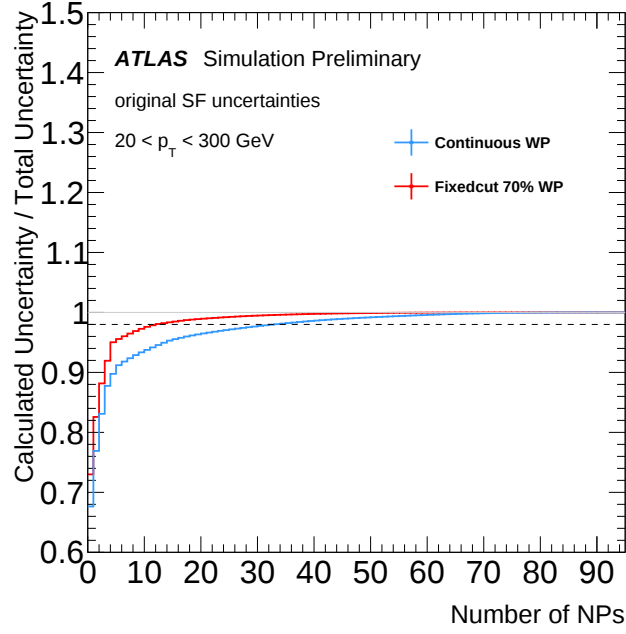


Figure 3: Ratio between the sum in quadrature of the c -jet uncertainty calculated using a certain number of *original* NPs over the sum in quadrature of the *total* c -jet uncertainty. The transverse momentum is restricted within the validity range of the calibration ($20 < p_T < 300 \text{ GeV}$). The horizontal dashed line marks the 98% threshold, while the solid line marks the 100% limit.

.4 Examples of U and $\tilde{U}_{\text{right}}^{-1}$ matrices

In order to illustrate the complexity behind the recomposition tool, this Appendix reports a concrete example of U and $\tilde{U}_{\text{right}}^{-1}$ matrices for the pseudo-continuous WP case. Figure 4 shows the U matrix, while Figure 5 shows the $\tilde{U}^{-1}$ matrix. Without pruning $L = N$, so in this case $\tilde{U}$ is a square matrix. Therefore $\tilde{U}_{\text{right}}^{-1}$ is simply $\tilde{U}^{-1}$. The bin index, from 1 to 45, corresponds to the kinematic bin index considering both b -tagging score bin and p_T dependence. In total, 45 combinations are considered in the pseudo-continuous calibration, obtained from 5 b -tagging score bins and 9 p_T bins.

Figure 4 shows the top 22 largest uncertainties contribution to the U matrix, the original U used in this case has dimension 127x45. The eigenvector decomposition is used to compactify U into a 45x45 diagonal matrix carrying the same information.

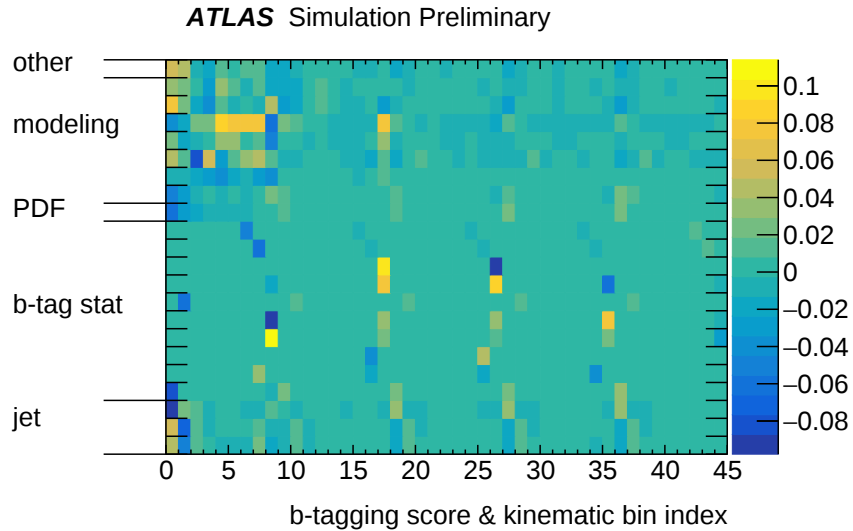


Figure 4: The U matrix in the pseudo-continuous WP case. The 22 largest uncertainties (out of 127) which add up to about 90% of the total uncertainty. Uncertainties are categorized into different categories as shown on the y axis.

.5 Uncertainty evaluation plots

The additional b -tagging high- p_T extrapolation uncertainties are shown in Figure 6, 7 8.

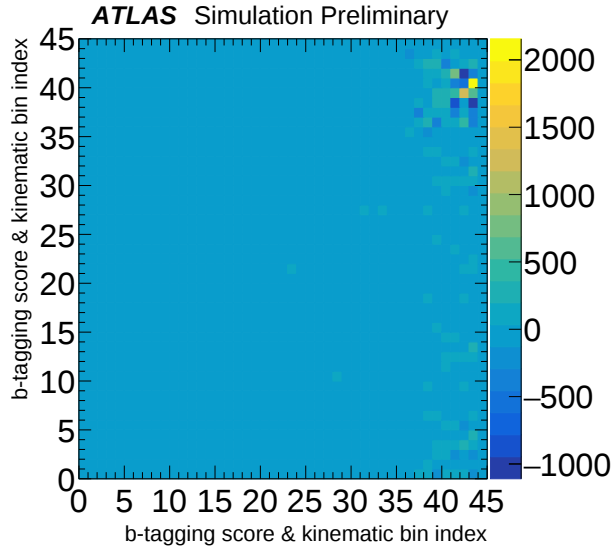


Figure 5: The $\tilde{U}^{-1}$ matrix in the pseudo-continuous WP case. The z-axis indicates the coefficient of each entry of the $\tilde{U}^{-1}$ matrix. The meaning of the z-axis value is explained in Eq. 18.

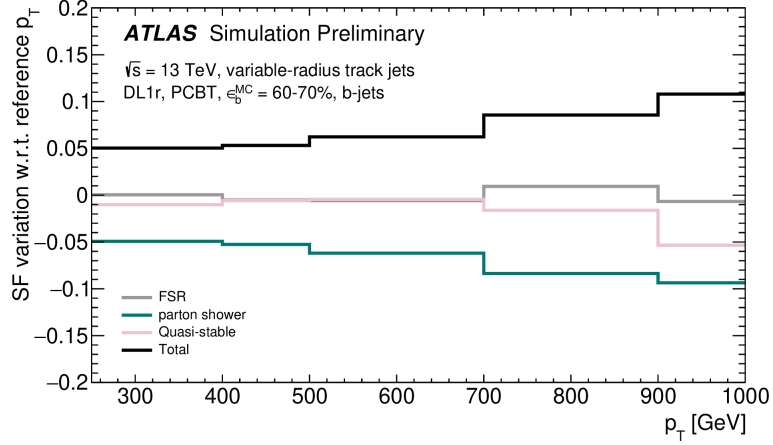


Figure 6: Modeling related scale factor variations used to extract the Monte Carlo based extrapolation uncertainties for the DL1r tagger applied to Variable Radius track jets as a function of the reconstructed b -jet p_T . The figure refers to the 60-70% Working Point interval of the pseudo-continuous b -tagging calibration, which is a simultaneous calibration of a binned version of the continuous b -tagging score distribution, expressed in intervals of the b -tagging efficiency [10]. The uncertainties are evaluated on $Z' \rightarrow \bar{q}$ samples, largely following the method described in Ref.[11]. The monotonic requirement described in Ref. [11] is now dropped and the extrapolation uncertainties are applied to reconstructed $pT \geq 250$ GeV jets. The events are required to have b -hadron $pT \leq 1000$ GeV. The contribution from final state radiation is shown in grey, variations pertaining to the parton shower modeling are shown in blue, while the pink curve accounts for the effect of simulating the hits in the detector before the charged b -hadron decay, which is usually not included in the current ATLAS detector simulations. The total variation (black curve) is obtained as the sum in quadrature of the single contributions.

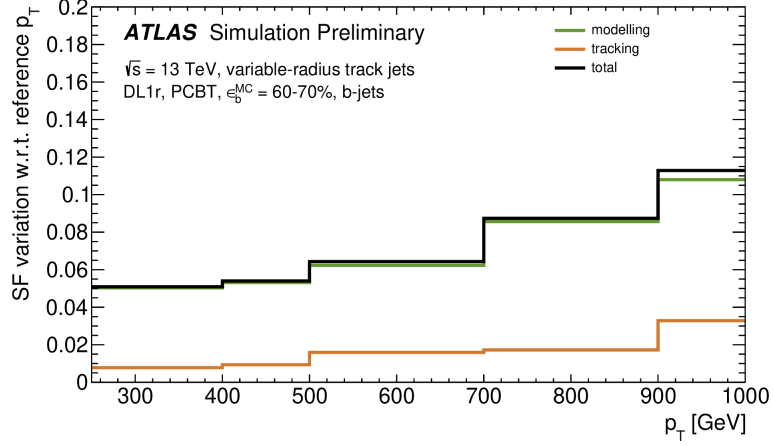


Figure 7: Monte Carlo based extrapolation uncertainties for the DL1r tagger applied to Variable Radius track jets as a function of the reconstructed b -jet p_T (black curve). The contribution from experimental uncertainties affecting the reconstruction of tracks is shown in orange. Theoretical uncertainties on the modeling of the jet fragmentation are drawn in green. The total variation is obtained summing in quadrature the single contributions. The figure refers to the 60-70% Working Point interval of the pseudo-continuous b -tagging calibration, which is a simultaneous calibration of a binned version of the continuous b -tagging score distribution, expressed in intervals of the b -tagging efficiency [10]. The uncertainties are evaluated on $Z' \rightarrow q\bar{q}$ samples, largely following the method described in Ref. [11]. The events are required to have b -hadron $p_T \leq 1000$ GeV. The monotonic requirement described in Ref. [11] is now dropped and the extrapolation uncertainties are applied to $p_T \geq 250$ GeV jets.

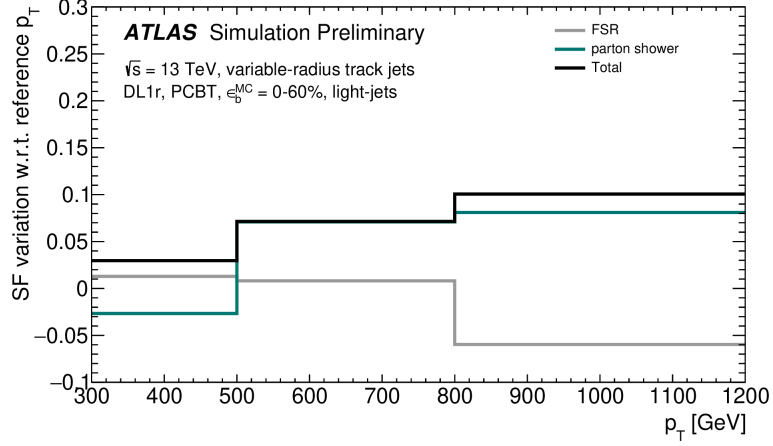


Figure 8: Modeling related scale factor variations used to extract the Monte Carlo based extrapolation uncertainties for the DL1r tagger applied to Variable Radius track jets as a function of the reconstructed *light*-jet p_T . The figure refers to the 0-60% Working Point interval of the pseudo-continuous b-tagging calibration, which is a simultaneous calibration of a binned version of the continuous b-tagging score distribution, expressed in intervals of the *b*-tagging efficiency [10]. The uncertainties are evaluated on $Z' \rightarrow q\bar{q}$ samples, largely following the method described in Ref. [11]. The monotonic requirement described in Ref. [11] is now dropped and the extrapolation uncertainties are applied to reconstructed $p_T \geq 300$ GeV jets. The contribution from final state radiation is shown in grey, variations pertaining to the parton shower modeling are shown in blue. The total variation (black curve) is obtained as the sum in quadrature of the single contributions.

.6 Restoring uncertainty eigenvalues after p_T extension on uncertainties

This section intended to prove the eigenvalue from uncertainty eigenvector decomposition can be restored after uncertainty p_T extension. First, there is a property that AA^T and $A^T A$ share the same non-zero eigenvalue. It can be proved as follows: Assume λ and $\mathbf{v}$ are the eigenvalue and eigenvector of $A^T A$ then

$$A^T A \mathbf{v} = \lambda \mathbf{v} \quad (28)$$

Then multiply A on left of both sides of the equation above and regroup the elements:

$$AA^T(A\mathbf{v}) = \lambda(A\mathbf{v}) \quad (29)$$

Therefore it shows λ and $A\mathbf{v}$ are the eigenvalue and eigenvector of AA^T . Therefore AA^T and $A^T A$ shares the same non-zero eigenvalue λ .

With this property in hand, one can move to scale factor uncertainties. The original uncertainty from j th source, denoted as $\mathbf{u}_j$, can be written as:

$$\mathbf{u}_j = \begin{pmatrix} \Delta x_0^j \\ \vdots \\ \Delta x_i^j \\ \vdots \\ \Delta x_N^j \end{pmatrix} \quad (30)$$

where x_j^i denote the uncertainty value in the i th p_T bin of j th uncertainty source. Next constructing the covariance matrix of original uncertainties without p_T extension:

$$COV = \Delta S F \Delta S F^T \quad (31)$$

$$= (\mathbf{u}_0 \ \mathbf{u}_1 \ \dots \ \mathbf{u}_M) (\mathbf{u}_0 \ \mathbf{u}_1 \ \dots \ \mathbf{u}_M)^T \quad (32)$$

Now proving that $\Delta SF \cdot \Delta SF^T$ and $\Delta SF^T \cdot \Delta SF$ share the same eigenvalues:

$$\Delta SF^T \cdot \Delta SF = \begin{pmatrix} \mathbf{u}_0^T \\ \mathbf{u}_1^T \\ \vdots \\ \mathbf{u}_M^T \end{pmatrix} (\mathbf{u}_0 \quad \mathbf{u}_1 \quad \dots \quad \mathbf{u}_M) \quad (33)$$

$$= \begin{pmatrix} \mathbf{u}_0^T \mathbf{u}_0 & \mathbf{u}_0^T \mathbf{u}_1 & \dots \\ \mathbf{u}_1^T \mathbf{u}_0 & \dots & \dots \\ \dots & \dots & \mathbf{u}_M^T \mathbf{u}_M \end{pmatrix} \quad (34)$$

Then the original uncertainty $\mathbf{u}_0$ can be extended in p_T to be $\mathbf{u}_{j,EXT}$:

$$\mathbf{u}_{j,EXT} = \begin{pmatrix} \Delta x_0^j \\ \vdots \\ \Delta x_i^j \\ \vdots \\ \frac{\Delta x_N^j}{\sqrt{n}} \\ \frac{\Delta x_{N+1}^j}{\sqrt{n}} \\ \vdots \\ \frac{\Delta x_{N+n-1}^j}{\sqrt{n}} \end{pmatrix} \quad (35)$$

Where $\Delta x_k^j \equiv \Delta x_N^j$ and k is integer such that $(N \leq k \leq N + n - 1)$. This means the value of the first $N - 1$ elements stays the same and the N th, i.e. the uncertainty of the last p_T bin (reference point) before the p_T extension is scaled by factor of $1/\sqrt{n}$ and this value is copied to the $n - 1$ new p_T bins of the uncertainty. The reason of scaling the last element by $1/\sqrt{n}$ is because this will ensure the eigenvalue won't change after p_T extension and will be explained below. With the extended original uncertainty $\mathbf{u}_{j,EXT}$:

$$\mathbf{u}_{a,EXT}^T \cdot \mathbf{u}_{b,EXT} = \Delta x_0^a \Delta x_0^b + \dots + \Delta x_{N-1}^a \Delta x_{N-1}^b + \quad (36)$$

$$\frac{\Delta x_{N-1}^a \Delta x_{N-1}^b}{n} + \dots + \frac{\Delta x_{N-1}^a \Delta x_{N-1}^b}{n} \quad (37)$$

$$= \sum_{d=1}^{d=N} \Delta x_d^a \Delta x_d^b \quad (38)$$

$$= \mathbf{u}_a^T \cdot \mathbf{u}_b \quad (39)$$

Therefore, after p_T extension $\Delta SF^T \Delta SF$ stays the same. Also, since $COV = \Delta SF \Delta SF^T$ share the same eigenvalues with $\Delta SF^T \Delta SF$, this means the non-zero eigenvalues of the covariance matrix before and after the p_T extension

stays the same. Thus by extending uncertainties in p_T like the description above, the eigenvalues stays the same after the p_T extension.

.7 Restoring uncertainty eigenvectors after p_T extension on uncertainties

Original scale factor uncertainties can be expressed as an uncertainty matrix ΔSF :

$$\Delta SF = \begin{pmatrix} x_1^1 & x_1^2 & \dots & x_1^M \\ x_2^1 & x_2^2 & \dots & x_2^M \\ \vdots & \vdots & \dots & \vdots \\ x_N^1 & x_N^2 & \dots & x_N^M \end{pmatrix} \quad (40)$$

where in the matrix it includes M original uncertainties sources and N p_T bins. The element in the matrix, x_i^j , denote the uncertainty value in the i th pT bin of j th uncertainty source. For convenience, rewrite the notation of the last row in the matrix by y as follows:

$$\Delta SF = \begin{pmatrix} x_1^1 & x_1^2 & \dots & x_1^M \\ x_2^1 & x_2^2 & \dots & x_2^M \\ \vdots & \vdots & \dots & \vdots \\ y_1^1 & y_1^2 & \dots & y_1^M \end{pmatrix} = \begin{pmatrix} X \\ \gamma^T \end{pmatrix} \quad (41)$$

The last row is denoted as γ^T , where γ is a column vector $\begin{pmatrix} y_1^1 \\ y_1^2 \\ \vdots \\ y_1^M \end{pmatrix}$. With matrix ΔSF , the covariance matrix can be constructed as:

$$COV = \Delta SF \Delta SF^T = \begin{pmatrix} X \\ \gamma^T \end{pmatrix} (X^T \gamma) = \begin{pmatrix} XX^T & X\gamma \\ \gamma^T X^T & \gamma^T \gamma \end{pmatrix} \quad (42)$$

The eigenvalue and eigenvector could be expressed as:

$$\begin{pmatrix} XX^T & X\gamma \\ \gamma^T X^T & \gamma^T \gamma \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ a \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{v} \\ a \end{pmatrix} \quad (43)$$

Here λ is the eigenvalue of the covariance matrix and $\begin{pmatrix} \mathbf{v} \\ a \end{pmatrix}$ is an eigenvector of the covariance matrix. The a in the eigenvector is a scalar value. Next,

writing out the equation as two equations below:

$$XX^T \mathbf{v} + aX\boldsymbol{\gamma} = \lambda \mathbf{v} \quad (44)$$

$$\boldsymbol{\gamma}^T X^T \mathbf{v} + a\boldsymbol{\gamma}^T \boldsymbol{\gamma} = \lambda a \quad (45)$$

Now, One can extend each original uncertainty so that the uncertainty of the last p_T bin is copied $k - 1$ times. The expanded ΔSF , denoted as $\Delta SF'$, can be expressed as:

$$\Delta SF' = \begin{pmatrix} X \\ \frac{1}{\sqrt{k}}\boldsymbol{\gamma}^T \\ \frac{1}{\sqrt{k}}\boldsymbol{\gamma}^T \\ \vdots \\ \frac{1}{\sqrt{k}}\boldsymbol{\gamma}^T \end{pmatrix} = \begin{pmatrix} X \\ \frac{1}{\sqrt{k}}\Gamma \end{pmatrix} \quad (46)$$

Where $\Gamma = \begin{pmatrix} \boldsymbol{\gamma}^T \\ \boldsymbol{\gamma}^T \\ \vdots \\ \boldsymbol{\gamma}^T \end{pmatrix} \in R^{k \times M}$ is a matrix represents the last and extended p_T

bin uncertainties. Then the new covariance matrix COV' after p_T extension can be expressed as:

$$COV' = \Delta SF' \Delta SF'^T = \begin{pmatrix} X \\ \frac{1}{\sqrt{k}}\Gamma \end{pmatrix} \begin{pmatrix} X^T & \frac{1}{\sqrt{k}}\Gamma^T \end{pmatrix} = \begin{pmatrix} XX^T & \frac{1}{\sqrt{k}}X\Gamma^T \\ \frac{1}{\sqrt{k}}\Gamma X^T & \frac{1}{k}\Gamma\Gamma^T \end{pmatrix} \quad (47)$$

The eigenvalue and eigenvectors of new covariance matrix after extension can be expressed as:

$$\begin{pmatrix} XX^T & \frac{1}{\sqrt{k}}X\Gamma^T \\ \frac{1}{\sqrt{k}}\Gamma X^T & \frac{1}{k}\Gamma\Gamma^T \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ b\hat{1} \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{v} \\ b\hat{1} \end{pmatrix} \quad (48)$$

Here for simplicity, denoting $\hat{1} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$. And b is a scalar. Also, it is assumed

that the eigenvector of the new covariance matrix can be written as $\begin{pmatrix} \mathbf{v} \\ b\hat{1} \end{pmatrix}$, where $\mathbf{v}$ is the same vector used for covariance matrix before extension in Eq. 43. This will be proved to be true in the following part of the proof by finding the value of b and showing the two equations are valid. Next, expanding Eq.

48 to get:

$$XX^T \mathbf{v} + \frac{1}{\sqrt{k}} X \Gamma^T b \hat{\mathbf{1}} = \lambda \mathbf{v} \quad (49)$$

$$\frac{1}{\sqrt{k}} \Gamma X^T \mathbf{v} + \frac{1}{k} \Gamma \Gamma^T b \hat{\mathbf{1}} = \lambda b \hat{\mathbf{1}} \quad (50)$$

The goal is to prove both Eq. 49 and 50 are valid. The right hand side of Eq.44 and 49 are exactly the same. Therefore if Eq. 49 is valid, the left hand side of Eq. 44 and 49 should equal as well:

$$XX^T \mathbf{v} + aX\boldsymbol{\gamma} = XX^T \mathbf{v} + \frac{1}{\sqrt{k}} X \Gamma^T b \hat{\mathbf{1}} \quad (51)$$

Cancel $XX^T \mathbf{v}$ on both sides to simplify the equation:

$$aX\boldsymbol{\gamma} = \frac{1}{\sqrt{k}} X \Gamma^T b \hat{\mathbf{1}} \quad (52)$$

Now focusing on the right-hand side.

$$\frac{b}{\sqrt{k}} X \Gamma^T b \hat{\mathbf{1}} = \frac{1}{\sqrt{k}} X (\boldsymbol{\gamma} \quad \dots \quad \boldsymbol{\gamma}) \hat{\mathbf{1}} = \frac{b}{\sqrt{k}} (X\boldsymbol{\gamma} \quad \dots \quad X\boldsymbol{\gamma}) \hat{\mathbf{1}} = b\sqrt{k} X\boldsymbol{\gamma} \quad (53)$$

This need to be equal to the left hand side of Eq. 52. Therefore gives:

$$b = \frac{a}{\sqrt{k}} \quad (54)$$

Now that Eq. 49 is valid with the condition above, the only thing left is to check if Eq. 50 is valid. Simplifying the left hand side of Eq. 50 as:

$$\frac{1}{\sqrt{k}}\Gamma X^T \mathbf{v} + \frac{1}{k}\Gamma \Gamma^T b \hat{1} = \frac{1}{\sqrt{k}} \begin{pmatrix} \gamma^T \\ \gamma^T \\ \vdots \\ \gamma^T \end{pmatrix} X^T \mathbf{v} + \frac{b}{k} \Gamma (\gamma \quad \dots \quad \gamma) \hat{1} \quad (55)$$

$$= \frac{1}{\sqrt{k}} \begin{pmatrix} \gamma^T X^T \mathbf{v} \\ \gamma^T X^T \mathbf{v} \\ \vdots \\ \gamma^T X^T \mathbf{v} \end{pmatrix} + \frac{b}{k} \begin{pmatrix} \gamma^T \\ \gamma^T \\ \vdots \\ \gamma^T \end{pmatrix} k \gamma \quad (56)$$

$$= \frac{1}{\sqrt{k}} \gamma^T X^T \mathbf{v} \mathbf{1} + b \begin{pmatrix} \gamma^T \gamma \\ \gamma^T \gamma \\ \vdots \\ \gamma^T \gamma \end{pmatrix} \quad (57)$$

$$= \frac{1}{\sqrt{k}} \gamma^T X^T \mathbf{v} \mathbf{1} + b \gamma^T \gamma \hat{1} \quad (58)$$

$$= \frac{1}{\sqrt{k}} \gamma^T X^T \mathbf{v} \mathbf{1} + \frac{a}{\sqrt{k}} \gamma^T \gamma \hat{1} \quad (59)$$

where in the last step b is replaced by a . Compare the result with left hand side of Eq. 45:

$$\frac{1}{\sqrt{k}}\Gamma X^T \mathbf{v} + \frac{1}{k}\Gamma \Gamma^T b \hat{1} = \frac{1}{\sqrt{k}} \hat{1} \lambda a = \lambda b \hat{1} \quad (60)$$

Therefore Eq. 49 and 50 are valid under the relation between eigenvectors of standard and new covariance matrix shown in Eq. 54.

.8 High pT extrapolation sample details

Sample name	Sample number	Uncertainty Type
Pythia8EvtGen_A14NNPDF23LO_flatpT_Zprime_Extended	427081	Tracking
Py8EG_A14NNPDF23LO_flatpT_Zprime_Extended	800030	Final state radiation
MGH7EG_NNPDF23ME_Zprime	500567	Parton shower
MGPY8EG_NNPDF23ME_A14_ZPrime	500568	Parton shower

Table 1: A list of Z' samples used for evaluating systematic uncertainties of Monte Carlo events with exact sample name.