# EUROPEAN ORGANISATION FOR NUCLEAR RESEARCH (CERN)





# A search for dark matter produced in association with a dark Higgs boson decaying into a Higgs boson pair in 3b or 4b final states using pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

## The ATLAS Collaboration

A search is performed for dark matter particles produced in association with a resonant pair of Higgs bosons using  $140 \text{ fb}^{-1}$  of proton–proton collisions at a centre-of-mass energy of 13 TeV recorded by the ATLAS detector at the Large Hadron Collider. This signature is expected in some extensions of the Standard Model predicting the production of dark matter particles, and is interpreted in terms of a dark Higgs model containing a Z' mediator in which the dark Higgs boson s decays into a pair of Higgs bosons. The dark Higgs boson is reconstructed through final states with at least three b-tagged jets, produced by the pair of Higgs boson decays, in events with significant missing transverse momentum consistent with the presence of dark matter. The observed data are found to be in good agreement with Standard Model predictions, constraining scenarios with dark Higgs boson masses within the range of 250 to 400 GeV and Z' mediators up to 2.3 TeV.

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#### 1 Introduction

The existence of dark matter (DM) is widely supported by astrophysical evidence [1–4] including galactic rotation velocities of stars [5–7], gravitational lensing [8–10] and precise measurements of the cosmic microwave background [11, 12]. There is no suitable candidate in the Standard Model (SM), thus its particle nature and interactions remain key open questions in particle physics, motivating many beyond-the-SM (BSM) scenarios.

Complementary approaches are seeking evidence of dark matter particles. These include searches for direct detection of DM scattering from electrons or nuclei [13–18]; indirect searches for the product of DM annihilation or decay [19–24]; gravitational, astrophysical and cosmological probes [25, 26]; and searches for evidence of dark matter production at colliders [27–29] with particle detectors such as the ATLAS experiment [30] at the Large Hadron Collider (LHC) [31].

Collider particle physics experiments have advantages in this endeavour — they are sensitive across a wide range of types and masses of proposed DM candidates, and have the potential to characterise its interactions, making them complementary to other types of searches. One class of DM candidates is stable, electrically neutral, weakly interacting massive particles (WIMPs), motivated by the observation that a candidate with interactions and mass of the order of the weak scale would reproduce the observed relic density [32] via the freeze-out mechanism: a paradigm known as the *WIMP miracle* [33]. Consequently colliders could be a natural place to find evidence for WIMP DM under well-controlled experimental conditions.

At colliders, it is assumed that dark matter interacts via *mediator* particles, which interact with both DM and SM particles. New mediator particles can be searched for directly, via their decay into SM particles, or may decay into DM. DM produced at colliders would not interact with the detector, and its presence must be inferred by an imbalance in the total momentum in the plane perpendicular to the collision axis. This quantity is the missing transverse momentum, with magnitude denoted  $p_{\rm T}^{\rm miss}$  (or  $E_{\rm T}^{\rm miss}$ ). Some visible radiation X must also be present to create this imbalance, creating what is known as an  $X + p_{\rm T}^{\rm miss}$  signature.

This paper presents a search for dark matter produced in association with a new scalar mediator, which decays into a resonant pair of SM Higgs bosons. The decay of each Higgs boson (h) into two b-quark-initiated jets, results in a resonant  $hh(\to b\bar{b}b\bar{b}) + p_{\rm T}^{\rm miss}$  signature. This signature, of large  $p_{\rm T}^{\rm miss}$  consistent with the presence of DM and two Higgs bosons, is sensitive to many DM models with extended Higgs sectors or heavy (pseudo-)scalar mediators [34, 35].

To optimise and interpret the results of the search, a *dark Higgs* model is used [36]. Motivated by the Higgs mechanism for electroweak symmetry breaking in the SM, this model explains massive fermionic dark matter ( $\chi$ ) through a similar mass generation mechanism in the dark sector, positing a *dark Higgs* boson, (s). Such a weak-scale dark Higgs boson, interacting through mixing with the SM Higgs boson, will decay analogously to an SM Higgs boson of that mass. Thus the primary decays are into a pair of b-quarks at lower masses ( $m_s < 150 \, \text{GeV}$ ), with diboson decays (WW, ZZ, hh) dominating at higher masses. Decays of s into a top quark pair can occur at low rate, whilst decays into the dark matter particles may be dominant, if kinematically allowed. An independent motivation for these models is an improved ability to reproduce the observed relic density, due to the presence of additional annihilation channels featuring the dark Higgs boson, such as  $\chi\chi \to ss$ , with subsequent decay of s into SM particles. This avoids the over-population common in simple or simplified models with weak-scale mediators [27]. Thus the relic density depends primarily upon the coupling between DM and s, whose SM couplings can be small, and hard to observe with traditional collider DM signatures.

The specific implementation of this model uses a two-mediator dark Higgs DM scenario, containing the dark Higgs boson, identified through its decay into hh, a new broken U(1)' symmetry yielding an additional massive spin-1 Z' mediator, and a Majorana fermion DM candidate. The model parameters are the DM particle mass  $m_X$ ; the Z' mass  $m_{Z'}$ ; the dark Higgs boson mass  $m_s$ ; the Z' coupling with quarks  $g_q$  and with the DM candidate  $g_\chi$ ; and the mixing angle  $\theta$  between the SM and dark Higgs bosons, which should be small to enable reproduction of the relic density and consistency with measurements of the Higgs boson. The dominant  $q\bar{q} \to Z' \to s\chi\chi$  signal diagram for the large Z' masses explored in this paper can be found in Figure 1.

A signal region is defined requiring significant  $p_{\rm T}^{\rm miss}$  and at least three hadronic jets identified to contain b-hadrons (b-tagged jets). The dominant SM background processes in these regions are top quark pair production with additional radiation and Z boson production with multiple additional jets, where the Z boson decays invisibly into neutrinos. Production of W bosons and single top quarks contribute sub-dominantly. Control regions (CRs) are defined to constrain the yields of these processes in a partly data-derived approach. A neural network (NN) is trained to improve the sensitivity through greater discrimination of signal from background processes whilst preserving the shape of the invariant mass distribution of the reconstructed di-Higgs system which is fit in the analysis.

Searches in similar final states have been made for supersymmetric particle cascades in which a pair of new heavy particles decay producing multiple b-quark jets and  $p_{\rm T}^{\rm miss}$ , either from heavy gluino or squark decay cascades [37, 38] or electroweakino decays via the emission of Higgs bosons [39, 40]. The symmetric

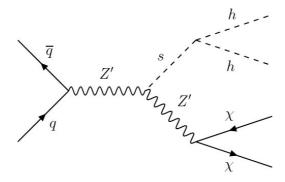


Figure 1: Representative signal diagram for resonant  $q\bar{q} \to Z' \to s\chi\chi$  production with the dark Higgs boson decay  $s \to hh$ .

topology and lack of connection between the four b-quarks differs significantly from the resonant hh topology targeted in this paper. Searches for dark Higgs bosons have been made in the bb signature by the ATLAS Collaboration [41], and in WW final states by the ATLAS [42, 43] and CMS [44] Collaborations. The bb signature is sensitive to  $30 < m_s < 150$  GeV, with WW sensitive from  $m_s = 150$  GeV and growing weaker with increasing  $m_s$ , motivating the exploration of the hh decay for larger  $m_s$  values.

There is complementary sensitivity from spin-1 mediator searches compatible with the Z' mediator present in the standard benchmark model used to facilitate comparisons between signatures and experiments. Care is needed in translating them into the Majorana DM dark Higgs model, but limits from dijet searches [27] are strong and place powerful constraints on TeV-mass Z' mediators, assuming the assumptions underlying the simplified models are fully realised in a more complete model, which may not be the case. Generally, the balance of the resonant and  $p_{\rm T}^{\rm miss}$  signatures depends strongly upon the choice of the couplings  $g_q$  and  $g_\chi$ , and the model is not strongly constrained. Reprodution of the observed relic density tends to favour larger  $g_\chi$  values [36, 41], emphasising the importance of the  $X + p_{\rm T}^{\rm miss}$  signatures.

The paper is organised as follows: Section 2 describes the ATLAS detector, whilst Section 3 details the collision data and simulation used in the analysis. Section 4 documents the object reconstruction and event selections used. The analysis strategy is outlined in Section 5, before Section 6 explains how background processes are estimated. The systematic uncertainties evaluated on data and simulations are detailed in Section 7, and the statistical treatment of the data in Section 8. The analysis results are reported in Section 9; Section 10 provides a conclusion.

## 2 ATLAS detector

The ATLAS experiment [30] at the LHC is a multipurpose particle detector with a forward–backward symmetric cylindrical geometry and a near  $4\pi$  coverage in solid angle. It consists of a tracking inner detector

<sup>&</sup>lt;sup>1</sup> ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the *z*-axis along the beam pipe. The *x*-axis points from the IP to the centre of the LHC ring, and the *y*-axis points upwards. Polar coordinates  $(r, \phi)$  are used in the transverse plane,  $\phi$  being the azimuthal angle around the *z*-axis. The pseudorapidity is defined in terms of the polar angle  $\theta$  as  $\eta = -\ln\tan(\theta/2)$  and is equal to the rapidity  $y = \frac{1}{2}\ln\left(\frac{E+p_z}{E-p_z}\right)$  in the relativistic limit.

(ID) surrounded by a thin superconducting solenoid providing a 2 T axial magnetic field, electromagnetic and hadronic calorimeters, and a muon spectrometer. The inner tracking detector covers the pseudorapidity range  $|\eta| < 2.5$ . It consists of silicon pixel, silicon microstrip, and transition radiation tracking detectors. Lead/liquid-argon (LAr) sampling calorimeters provide electromagnetic (EM) energy measurements with high granularity within the region  $|\eta| < 3.2$ . A steel/scintillator-tile hadronic calorimeter covers the central pseudorapidity range ( $|\eta|$  < 1.7). The endcap and forward regions are instrumented with LAr calorimeters for EM and hadronic energy measurements up to  $|\eta| = 4.9$ . The muon spectrometer surrounds the calorimeters and is based on three large superconducting air-core toroidal magnets with eight coils each. The field integral of the toroids ranges between 2.0 and 6.0 Tm across most of the detector. The muon spectrometer includes a system of precision tracking chambers up to  $|\eta| = 2.7$  and fast detectors for triggering up to  $|\eta| = 2.4$ . The luminosity is measured mainly by the LUCID-2 [45] detector, which is located close to the beampipe. A two-level trigger system is used to select events [46]. The first-level trigger is implemented in hardware and uses a subset of the detector information to accept events at a rate below 100 kHz. This is followed by a software-based trigger that reduces the accepted event rate to 1.25 kHz on average depending on the data-taking conditions. A software suite [47] is used in data simulation, in the reconstruction and analysis of real and simulated data, in detector operations, and in the trigger and data acquisition systems of the experiment.

#### 3 Data and Monte Carlo simulations

The proton–proton collisions analysed were collected by the ATLAS detector between 2015 and 2018, at a centre-of-mass energy of  $\sqrt{s} = 13$  TeV and a 25 ns inter-bunch spacing. They correspond to an integrated luminosity of 140 fb<sup>-1</sup>, with an uncertainty of 0.83% [48] obtained using the LUCID-2 detector [45] for the primary luminosity measurements, complemented by measurements using the inner detector and calorimeters, after requiring all detector systems to be recording good quality data [49].

Unprescaled  $p_{\rm T}^{\rm miss}$  triggers were used [50] to select events for the analysis. The  $p_{\rm T}^{\rm miss}$  thresholds ranged from 70 GeV to 110 GeV, for a  $p_{\rm T}^{\rm miss}$  definition in which muons are treated as invisible. The offline  $p_{\rm T}^{\rm miss}$  selection, which does not treat muons as invisible, was kept more stringent than the trigger-level requirement to ensure that trigger efficiencies are constant.

Dark Higgs Monte Carlo (MC) simulated events were generated, as detailed in Table 1, using consistent parameter choices with other analyses [41–44] and simplified dark matter models: the dark matter mass  $m_{\chi}$  is fixed at 200 GeV, its coupling constant is set as  $g_{\chi}=1$ , the coupling between the SM quarks and the Z' is fixed at  $g_q=0.25$  [51, 52] and the mixing angle between the SM and dark Higgs bosons is set to  $\sin\theta=0.01$ . Samples of MC simulated events are generated for 106 mass points covering a range of  $m_{Z'}$  and  $m_s$  values. To consider the region where the Z' is heavy enough to decay into two dark matter particles and is light enough to have a sufficient production cross-section for sensitivity,  $420 \, \text{GeV} < m_{Z'} < 3300 \, \text{GeV}$  is chosen. The range  $251 \, \text{GeV} < m_s < 435 \, \text{GeV}$  is chosen to probe the region where s is heavy enough to decay into two SM Higgs bosons and light enough that the decay into two dark matter particles in this benchmark is not overwhelming. Larger DM masses will have generally smaller Z' and s production cross-sections, with  $s \to \chi \chi$  decays becoming dominant at larger  $m_s$  and a different predicted relic density. For all generated signal events, the detector response is simulated [53] using a fast parametrised simulation of the calorimeters [54], and the full Geant4 [55] simulation for the other sub-detectors.

Angular distance is measured in units of  $\Delta R \equiv \sqrt{(\Delta y)^2 + (\Delta \phi)^2}$ .

Table 1: Simulated event samples with the corresponding matrix element and parton shower generators, cross-section order in  $\alpha_s$  (and  $\alpha_{EW}$  where corrections are available) used to normalise the event yield, underlying-event set of tuned parameters and the generator PDF sets used. The abbreviation (N)NLO stands for (next-to-)next-to-leading-order, and NNLL stands for next-to-next-to-leading-logarithm.

Physics process	Generator (ME)	Parton shower (PS)	Order in $\alpha_{\rm S}(+\alpha_{\rm EW})$	Tune	PDF (ME)	PDF (PS)
Dark Higgs signals	MadGraph5_aMC@NLO 2.9.9 [65]	. ,	LO	A14 [67]	NNPDF2.3LO [63]	NNPDF2.3LO
$Z(\rightarrow \nu\nu)$ + jets	Sherpa 2.2.1 [68, 69]	Sherpa 2.2.1	NNLO [70]	Sherpa default [71]	NNPDF3.0NNLO[72]	NNPDF3.0NNLO
$W(\rightarrow \ell \nu)$ + jets	Sherpa 2.2.1	Sherpa 2.2.1	NNLO	Sherpa default	NNPDF3.0NNLO	NNPDF3.0NNLO
Diboson	Sherpa 2.2.1	Sherpa 2.2.1	NLO	Sherpa default	NNPDF3.0NNLO	NNPDF3.0NNLO
Triboson	Sherpa 2.2.14	Sherpa 2.2.14	NLO	Sherpa default	NNPDF3.0NNLO	NNPDF3.0NNLO
$t\bar{t}$	Powheg Box v2 [73-76]	Рутніа 8.230 [77]	NNLO+NNLL [78]	A14	NNPDF3.0NLO [72]	NNPDF2.3LO
Single top	Powheg Box v2	Рутніа 8.230	NLO [79, 80]	A14	NNPDF3.0NLO	NNPDF2.3LO
ttW/ttZ	MadGraph5_aMC@NLO 2.3.3	Рутніа 8.210	NLO	A14	NNPDF3.0NLO	NNPDF2.3LO
Four-top	MadGraph5_aMC@NLO 2.2.2	Рутніа 8.186 [62]	NLO	A14	NNPDF2.3LO	NNPDF2.3LO
ttH	Powheg Box v2	Рутніа 8.230	NLO	A14	NNPDF3.0NLO	NNPDF2.3LO
VH	Рутніа 8.186	Рутніа 8.186	NNLO+NLO [81-87]	A14	PDF4LHC15NLO[88]	PDF4LHC15NLO

The dominant SM background processes are  $t\bar{t}$  production with additional radiation, and  $Z(\to \nu\nu)$  + jets. Subdominant background processes are single top (Wt) production and  $W(\to \ell \nu)$  + jets. Smaller background processes include other multi-top processes hereinafter grouped as  $t\bar{t} + X$  (ttW, ttZ, ttH, four-top production), and diboson (WW, WZ, ZZ) production. Triboson production and VH production were also considered and found to be negligible. All SM processes are modelled using MC simulations, processed through a full simulation of the ATLAS detector [53] based on Geant [55]. All samples used (signal and SM) are listed in Table 1 along with the relevant parton distribution function (PDF) sets used for the matrix element (ME) and parton shower (PS), the configuration of underlying-event and hadronisation parameters (tune), and the cross-section order in  $\alpha_s$  (and  $\alpha_{\rm EW}$  where corrections are available) used to normalise the event yields for these samples. Further information about the ATLAS simulations of  $t\bar{t}$ , single top, multi-boson and vector-boson plus jets processes can be found in Refs. [56–60]. The decays of bottom and charm hadrons were simulated using the EvTGEN 1.6.0 program [61] for the samples not generated with SHERPA. The effect of pile-up in the same and neighbouring bunch crossings was modelled by overlaying the simulated hard-scattering event with inelastic proton–proton events generated with PYTHIA8.186 [62] using the NNPDF2.3LO leading-order PDF set [63] and the A3 set of tuned parameters [64]. The MC samples were reweighted so that the distribution of the average number of interactions per bunch crossing reproduces the observed distribution in the data.

The  $t\bar{t}$  processes are categorised based on the true flavour content of the jets in the events. An event is labelled as  $t\bar{t} + \ge 1b$  if three or more jets are associated with b-hadrons. Events with two b-jets and at least one c-hadron are labelled as  $t\bar{t} + \ge 1c$  while all remaining events are categorised as  $t\bar{t} + \text{light}$ .

#### 4 Event reconstruction

For the particle candidate objects used in this analysis, two distinct categories are defined. These differ in the stringency of their reconstruction requirements, and have different uses in the analysis. Baseline objects are used to construct the events'  $p_{\rm T}^{\rm miss}$ . After this, an overlap removal procedure is applied to deal with potential ambiguities between particle candidates. Finally Signal objects are defined with additional reconstruction requirements, which are used for the analysis region selections.

All events are required to have a primary vertex. Primary vertices are reconstructed from at least two charged-particle tracks with transverse momentum  $p_T > 0.5$  GeV, measured in the ID [89]. The hard-scatter

vertex is defined as the primary vertex with the largest sum of squared track momenta.

Hadronic jets are reconstructed from particle flow objects [90], using the anti- $k_t$  algorithm [91, 92] with a radius parameter of R=0.4. These are calibrated using a multi-step procedure as outlined in Ref. [93]. Baseline jets are required to have  $p_T>20\,\mathrm{GeV}$  and  $|\eta|<2.8$  to be considered in the analysis. To suppress jets originating from pile-up, a Jet Vertex Tagger (JVT) is used; this is a likelihood-based algorithm described in Ref. [94]. Baseline jets with  $20< p_T<60\,\mathrm{GeV}$  and  $|\eta|<2.4$  are required to satisfy a selection on the JVT with a 0.90-0.96 probability of correctly identifying hard-scatter jets depending on the  $p_T$ . Outside of this  $p_T$  range, no JVT requirement is applied. Signal jets are formed from the Baseline jets which pass the overlap removal procedure, and are additionally required to satisfy an increased  $p_T$  requirement of  $25\,\mathrm{GeV}$ .

For both Baseline and Signal jets, those likely to originate from a b-quark are identified using a deep neural network-based algorithm (DL1r) [95]. This is applied to jets with  $p_T > 20 \,\text{GeV}$  and  $|\eta| < 2.5$ , with a 77% probability to identify jets containing b-hadrons, as measured in MC simulations of  $t\bar{t}$  processes. The algorithm has a probability of 0.5% (18%) of misidentifying light-flavour (charm) jets, as determined in a sample of simulated  $t\bar{t}$  events. The b-tagging efficiencies in simulated events are corrected to match those measured in data [96–98].

Baseline electrons (muons) are required to have  $|\eta| < 2.47$  ( $|\eta| < 2.7$ ) and  $p_T > 8$  GeV, and to satisfy the Loose likelihood-based identification working point defined in Ref. [99] (Medium identification working point as defined in Ref. [100]). Signal electron and muon candidates are defined to place a stringent veto on events with any prompt leptons, to reduce SM backgrounds, and Signal muons are used in the estimate of the Z-boson background. These are required to fulfil the following additional requirements and the overlap removal procedure must be passed. The significance of the transverse impact parameter  $d_0$  must obey  $d_0/\sigma(d_0)$  less than 5 (3), for electrons (muons). Signal electrons are required to satisfy the Loose isolation working point of Ref. [99] to reduce contamination from semileptonic hadron decays and jets misidentified as electrons. Signal muons are required to satisfy the Tight isolation working point of Ref. [100] to reduce contamination from semileptonic heavy flavour and hadron decays.

The overlap removal procedure is applied to Baseline electrons (e), muons  $(\mu)$  and jets (j). Individual overlap removals are done in the following sequence of steps, in which objects are considered at a given step only if they were not removed in a previous step. Firstly, if a muon shares an ID track with an electron, the electron is removed. Secondly, if  $\Delta R(j,e) < 0.2$  the jet is removed. For any surviving jets, if  $\Delta R(j,e) < \min(0.4, 0.04 + 10 \, \text{GeV}/p_T^e)$ , the electron is removed. Penultimately, if  $\Delta R(j,\mu) < 0.2$  or the muon ID track is ghost associated with the jet, then the jet is removed if the jet has less than three associated tracks with  $p_T > 0.5$  GeV. Finally, for any surviving jets, if  $\Delta R(j,\mu) < \min(0.4, 0.04 + 10 \, \text{GeV}/p_T^\mu)$ , the muon is removed.

The missing transverse momentum ( $p_T^{miss}$ ) of the event is defined as the negative vector sum of the  $p_T$  of all selected and calibrated Baseline physics objects in the event before the overlap removal procedure, with an extra term added to account for soft energy in the event which is not associated with any of the selected objects. This soft term is calculated from inner detector tracks matched to the primary vertex. The magnitude of the missing transverse momentum vector is denoted  $p_T^{miss}$ . The Loose  $p_T^{miss}$  working point is used, as defined in Ref. [101]. The object-based  $p_T^{miss}$  significance ( $S(p_T^{miss})$ ), defined in Ref. [101], is also used in the analysis. This is an estimate of how genuine the  $p_T^{miss}$  in the event is, originating from neutrinos or potential dark matter candidates, in contrast to 'fake'  $p_T^{miss}$  originating from the finite detector

<sup>&</sup>lt;sup>2</sup> Ghost association consists of repeating the anti- $k_t$  jet clustering process with the addition of 'ghost' versions of the muon's track with the same direction but infinitesimal  $p_T$ . A muon is ghost-associated if it is contained within the re-clustered jet.

Table 2: Definition of the event	preselection requirements	s, used to select the final states of interest.
	P	.,

Variable	Requirement
$n_{ m leptons}$	0
$n_{ m jets}$	[4, 7]
$n_{b-\mathrm{jets}}$	≥ 3
$p_{\rm T}^{\rm miss}$ [GeV]	> 200
$\Delta\phi_{ m min}^{4j}$	> 0.4
$m_{\mathrm{T,min}}^{b}$ [GeV]	> 80
$\mathcal{S}(p_{\mathrm{T}}^{\mathrm{miss}})$	> 7
$m_{\mathrm{T}}^{4b}$ [GeV]	> 300

acceptance and resolution, pile-up and object mismeasurement. It is calculated by dividing the  $p_{\rm T}^{\rm miss}$  by a measure of its resolution, built from the resolutions of the objects from which the  $p_{\rm T}^{\rm miss}$  is constructed.

# 5 Analysis strategy

#### **5.1** Event selection

The signal is characterised by large  $p_{\rm T}^{\rm miss}$  from the DM particle production and substantial hadronic activity from  $s\to hh$  decays resulting in four b-quark jets with an invariant mass consistent with  $m_s$ . Events considered for the search must fulfil a set of 'preselection' requirements summarised in Table 2. To target the signal's final state, events are required to contain no Signal leptons ( $n_{\rm leptons}$ ) and between four and seven Signal jets ( $n_{\rm jets}$ ), at least three of which must be b-tagged. The loose upper requirement on  $n_{\rm jets}$  reduces backgrounds with many additional jets, including top quark processes. Requiring the events'  $p_{\rm T}^{\rm miss}$  to be greater than 200 GeV ensures the selected trigger is fully efficient over the complete data-taking period, and effectively targets the high  $p_{\rm T}^{\rm miss}$  signature for the range of DM masses considered. To reduce background contributions from QCD multijet processes,  $\Delta \phi_{\rm min}^{4j}$  — the minimum azimuth between any of the event's four highest  $p_{\rm T}$  jets and the  $p_{\rm T}^{\rm miss}$  is required to be greater than 0.4. The variable  $m_{\rm T,min}^b$ , defined as:

$$m_{\text{T,min}}^b = \min_{1 \le i \le 3} \sqrt{(p_{\text{T}}(b_i) + p_{\text{T}}^{\text{miss}})^2 - (p_{\text{x}}(b_i) + p_{\text{x}}^{\text{miss}})^2 - (p_{\text{y}}(b_i) + p_{\text{y}}^{\text{miss}})^2},$$

where i indexes the three highest- $p_{\rm T}$  b-tagged jets in the event, has an approximate upper bound at the mass of a particle with decay products including a b-tagged jet and  $p_{\rm T}^{\rm miss}$ , such as a semileptonic top quark decay in which the lepton is not reconstructed. It is thus generally smaller for SM background processes than the signal. The optimal event requirement was found to be  $m_{\rm T,min}^b$  larger than 80 GeV. To reduce backgrounds with fake  $p_{\rm T}^{\rm miss}$  such as QCD multijet processes, events must have a  $\mathcal{S}(p_{\rm T}^{\rm miss})$  greater than 7. Finally, the transverse mass of the di-Higgs system and  $p_{\rm T}^{\rm miss}$  must exceed 300 GeV to target events consistent with a heavy Z' decay.

To discriminate further between the signals and SM backgrounds, an NN classifier is used, as detailed in Section 5.3, which produces a probability score for events ranging from 0 (highly background compatible)

Table 3: Search region event requirements supplementing the preselection defined in Table 2.

Region	Variable requirement		
	NN score	$m_{hh}$ [GeV]	
SR	≥ 0.95	[100, 900]	
DRa		[100, 250)	
DRb		[200, 300)	
DRc		[250, 350)	
DRd	≥ 0.95	[300, 400)	
DRe		[350, 450)	
DRf		[400, 900)	
DRg		[500, 900)	

to 1 (highly signal compatible). For all the search regions in the analysis, the events' NN output score is required to be greater than 0.95 to maximise sensitivity to the dark Higgs signals whilst keeping sufficient event yields to maintain the clear resonant peak signature expected in the signal in the di-Higgs invariant mass  $(m_{hh})$ . For the dark Higgs model this corresponds to the reconstructed  $m_s$ , and has a resonance peak in its distribution.

Two sets of search regions are defined in Table 3, which both exploit  $m_{hh}$  to distinguish the signals from the SM backgrounds. Firstly, a binned signal region (SR), optimised for sensitivity to the dark Higgs signal resonances, is used to test the signal hypotheses in multi-bin profile likelihood fits over  $m_{hh}$ . The  $m_{hh}$  distribution is binned with the set of lower edges: [100, 200, 250, 300, 350, 400, 450, 500, 700] GeV, with the final bin ending at 900 GeV. The binning is chosen to reflect the mass resolution of the dark Higgs signal and there are no yields in data or MC simulation above 900 GeV. The overall acceptance times efficiency for the dark Higgs signals to enter the SR varies from 1.5% to 6.9% across the parameter space considered. Secondly, a set of single bin regions (DRa-DRg) is used to perform individual discovery fits testing the SM-only hypothesis and set limits on the possible number of BSM events with this detector signature. These are each defined in a given range of  $m_{hh}$ . These overlapping regions are chosen to cover a range of possible BSM particle masses, contain sufficient expected event yields, and reflect the expected mass resolution. Whilst the 4b final state is the most sensitive at preselection level, the larger event samples in the 3b regions benefit most from the NN discrimination, such that both contribute and a categorisation in b-tagged jet multiplicity does not enhance the sensitivity.

#### 5.2 Higgs boson reconstruction

The fully visible final state of the dark Higgs boson decay allows its mass to be reconstructed, providing an effective discriminant between the signal process and SM backgrounds. This relies first on selecting the four jets from the two SM Higgs boson decays from which the invariant mass  $(m_{4j} = m_{hh})$  can be calculated. If there are at least four *b*-tagged jets in the event, the four *b*-tagged jets with the largest transverse momenta are selected. If there are three *b*-tagged jets, and the mass of one of these is greater than 100 GeV, then it is assumed to be a 'merged' jet formed from two Higgs boson decay products being collimated, and used in addition to the other two *b*-tagged jets. If the mass threshold is not met by any of the *b*-tagged jets, then the fourth jet is chosen from the remaining untagged jets. This jet is chosen to

minimise the mass of the heaviest possible Higgs boson candidate constructed from any two of the set containing the three b-tagged jets  $(\alpha, \beta, \gamma)$  and the considered light jets (j):

$$\min_{j} \left[ \max_{\alpha,\beta,\gamma} \left( m_{\alpha\beta}, m_{\gamma j} \right) \right].$$

The kinematic properties of the SM Higgs boson candidates are also useful for discriminating between the signal and backgrounds and are used as input features to the NN. To reconstruct these, the four jets must be paired to form two Higgs bosons. When there is a merged jet present, it is chosen as one Higgs boson candidate, whilst the other two jets form the second Higgs boson candidate. Otherwise, the four jets (j = 1, 2, 3, 4) are paired to minimise the greatest angular separation between the Higgs boson candidates decay products (jets i, k, l, m). This is expressed as:

$$\min(\Delta R_{\max}(b,b)) = \min_{i,k,l,m \in I} (\max(\Delta R(i,k), \Delta R(l,m))).$$

The two Higgs boson candidates are then numbered in descending  $p_T$ .

#### 5.3 Neural network classifier

The supervised NN classifier is trained on events satisfying the preselection requirements defined in Table 2. For the signal training set, simulated MC events for all signal models are combined (using the same number of events per model, randomly sampled such that the  $4.3 \times 10^5$  signal training set size is equal to that of the background training set), to maintain sensitivity across the model parameter space of interest. For the background training set, all MC simulated events of the SM background processes were used as they provided a good match to the expected weighted background composition satisfying the analysis preselection. To avoid overtraining and benefit from the full set of available events, orthogonal training and testing/validation datasets are used, through a k-fold splitting procedure with k = 5 [102]. The datasets are split randomly into five subsets and five NNs are trained, such that the network trained on four fifths of the events is applied to the other fifth of the events in the analysis, and the full statistical power of the simulated MC datasets can be conserved.

The kinematic input features used in the NN are listed and defined in Table 4. These were selected from a wider set as the kinematic variables that provided the best signal-background discrimination and improved the NN performance, either alone or in combination with other variables. The NN can exploit correlations between variables to enhance discrimination power, particularly when the correlations between the variables are different for signal and background events. The impact of each variable was also quantified using Shapley values [103] (a common measure to assess how impactful an input feature is on the classifier output). Variables which had high Shapley values, and led to a reduced NN performance if they were removed from training, were retained. Finally, more complex compound kinematic variables were considered and evaluated, again using their Shapley values. These variables were generated using the Python featuretools [104] package, which combines pairs of variables from the existing list using basic arithmetic operations. The compound variables with high Shapley values, and which improved NN performance if they were added, were included in the training. Whilst these variables are correlated with the existing input features, they can help the NN to converge more quickly, focus more on more important properties, and learn finer details in the data sample.

A feed-forward neural network architecture is used. The NN has 8 fully connected hidden layers, with 1024 hidden nodes in the first layer and the number of hidden nodes halving repeatedly in each

Table 4: Neural network input features and their definitions.

Variable	Definition
$p_{\mathrm{T}}^{\mathrm{miss}}$	Missing transverse momentum.
$\mathcal{S}(p_{\mathrm{T}}^{\mathrm{miss}})$	Object-based $p_{\rm T}^{\rm miss}$ significance.
$m_{\mathrm{T.min}}^{b}$	Minimum transverse mass of $p_T^{\text{miss}}$ and any of the <i>b</i> -jets in the event.
$m_{ m T,min}^b \ m_{ m T}^{4b}$	Transverse mass of the di-Higgs system and $p_{\rm T}^{\rm miss}$ .
$m_{h1}$	Mass of the higher- $p_T$ Higgs boson candidate.
$m_{h2}$	Mass of the lower- $p_T$ Higgs boson candidate.
$H_{ m T}$	Scalar sum of $p_T$ of Signal jets.
$p_{\mathrm{T}}^{4b}$	$p_{\mathrm{T}}$ of the reconstructed di-Higgs system.
$p_{\mathrm{T}}(b_1)$	Transverse momentum of the highest $p_T$ $b$ -jet.
$p_{\mathrm{T}}(b_2)$	Transverse momentum of the second-highest $p_T$ $b$ -jet.
$p_{\mathrm{T}}^{j4}$	Transverse momentum of the fourth-highest $p_{\rm T}$ jet.
$\Delta R(b_{h1}^1, b_{h1}^2)$	$\Delta R$ between the two jets associated with the higher- $p_{\rm T}$ Higgs boson candidate.
$\Delta R(b_{h2}^1, b_{h2}^2)$	$\Delta R$ between the two jets associated with the lower- $p_T$ Higgs boson candidate.
$\Delta R_{\min}(b,b)$	min $\Delta R(b_i, b_j)$ for all b-jet pairs i and j in the event.
$\Delta\eta_{\max}(b,b)$	max $\Delta \eta(b_i, b_j)$ for all <i>b</i> -jet pairs <i>i</i> and <i>j</i> in the event.
$n_{ m jets}$	Number of Signal jets in the event.
$n_{b-\mathrm{jets}}$	Number of <i>b</i> -jets in the event.
$p_{\mathrm{T}}^{\mathrm{miss}}/\sqrt{H_{\mathrm{T}}}$	Event-based (rather than object-based) estimate of $\mathcal{S}(p_{\mathrm{T}}^{\mathrm{miss}})$ .
$p_{\mathrm{T}}^{\mathrm{miss}}/p_{\mathrm{T}}^{4b}$	The ratio of $p_{\rm T}^{\rm miss}$ and $p_{\rm T}^{4b}$ .
$n_{\rm jets}/n_{b-{ m jets}}$	The ratio of the Signal jet and <i>b</i> -jet multiplicities.
$n_{\text{jets}} - n_{b-\text{jets}}$	The number of Signal jets in the event not $b$ -tagged.
$p_{\rm T}(b_1)/n_{\rm jets}$	The ratio of the $p_T$ of the highest $p_T$ jet and the event's Signal jet multiplicity.
$S(p_{\mathrm{T}}^{\mathrm{miss}})/n_{b-\mathrm{jets}}$	The ratio of $p_{\rm T}^{\rm miss}$ significance and the number of $b$ -jets in the event.
$S(p_{\mathrm{T}}^{\mathrm{miss}}) \times p_{\mathrm{T}}^{4b}$	The product of $p_{\rm T}^{\rm miss}$ significance and the $p_{\rm T}$ of the di-Higgs system.
$\Delta R_{\min}(b,b)/p_{\mathrm{T}}^{\mathrm{miss}}$	The ratio of $\Delta R_{\min}(b, b)$ and $p_{\mathrm{T}}^{\mathrm{miss}}$ .
$\Delta\eta_{\rm RMS}(b,b) \times \Delta\eta_{\rm max}(b,b)$	The product of RMS $\Delta \eta(b_i, b_j)$ and max $\Delta \eta(b_i, b_j)$ for all <i>b</i> -jet pairs <i>i</i> and <i>j</i> in the event.
$\Delta R_{\min}(b,b) \times p_{\mathrm{T}}(b_2)$	The product of $\Delta R_{\min}(b, b)$ and the second-highest <i>b</i> -tagged jet $p_{\mathrm{T}}$ .
xwt	min $\sqrt{\left(\frac{m_W^i - 80.4 \text{ GeV}}{0.1 m_W^i}\right)^2 + \left(\frac{m_t^i - 172.5 \text{ GeV}}{0.1 m_t^i}\right)^2}$ , for $i$ in the top quark and $W$ -boson
	candidates in the event. Top quark candidates are defined through a <i>W</i> -boson candidate and <i>b</i> -tagged jet such that each jet from a Higgs boson decay represents
	the $b$ -jet from the top decay. $W$ -boson candidates are defined from pairs of
	the event's remaining jets, where at most one is associated with a Higgs
	boson (as hadronic W decays are likely to produce at least one light jet). The
	0.1 approximates the fractional mass resolution for the reconstructed particle candidate hypotheses.

subsequent layer. Training is performed in batches, with a batch size of 4096. Rectified linear unit (ReLU) activation [105, 106], batch normalisation [107], an Adam [108] optimiser with weight decay, and dropout regularisation [109] (with a dropout rate of 0.2) are used between layers. An initial learning rate of  $5 \times 10^{-6}$  is used, with a learning rate scheduler that halves the learning rate every five epochs. The network is trained for 25 epochs; that with the lowest validation loss is used in the analysis. As the signal regions in the analysis rely on the  $m_{hh}$  distribution alongside high NN score values, it is important that the NN does not sculpt or bias the background  $m_{hh}$  distribution to a more signal compatible shape. To prevent this, the loss function used contains not only a standard binary cross-entropy term  $L_{\rm BCE}$ , but also a distance correlation term  $\mathcal{R}$  defined between vectors X and Y as:

$$\mathcal{R}^{2}(X,Y) = \begin{cases} \frac{\mathcal{V}^{2}(X,Y)}{\sqrt{\mathcal{V}(X,X)\mathcal{V}(Y,Y)}}, & \text{if } \mathcal{V}^{2}(X)\mathcal{V}^{2}(Y) > 0, \\ 0, & \text{otherwise,} \end{cases}$$

where

$$\mathcal{V}^2(X,Y) = \langle |X - X'||Y - Y'|\rangle + \langle |X - X'||\rangle\langle |Y - Y'|\rangle - 2\langle |X - X'||Y - Y''|\rangle,$$

following Refs. [110] and [111]. These are combined thus [111]:

$$L_{\text{total}}(\hat{Y}, Y) = \alpha L_{\text{BCE}}(\hat{Y}, Y) + (1 - \alpha) \mathcal{R}(\hat{Y}, m_{hh}),$$

where Y is the vector of true signal or background labels for the events, and  $\hat{Y}$  the predictions. The optimal value of  $\alpha$  was found to be 0.7, providing successful mass decorrelation and good training and classification performance.

Some example distributions of discriminating kinematic variables important to the NN are shown in Figure 2. Figures 2(a) and 2(b) show the  $p_{\rm T}^{\rm miss}$  and  $\mathcal{S}(p_{\rm T}^{\rm miss})$  distributions. The illustrated signals demonstrate the large  $p_{\rm T}^{\rm miss}$  and  $\mathcal{S}(p_{\rm T}^{\rm miss})$  generated by the dark matter production, in comparison with the rapidly dropping distributions for SM processes, particularly  $t\bar{t}$  processes. The  $\Delta\eta_{\rm max}(b,b)$  distribution in Figure 2(c) demonstrates the discrimination resulting from the closer proximity of the b-tagged jets in the signal process compared with those in the background processes. The  $m_{\rm T,min}^b$  distribution (Figure 2(d)) connects the  $p_{\rm T}^{\rm miss}$  and b-tagged jets: for semileptonic top quark decays it is constrained to lie within  $m_t$ , whereas at high values processes with additional or independent sources of  $p_{\rm T}^{\rm miss}$  are increasingly dominant.

# 6 Background estimation

After the preselection and search region NN score requirements, the dominant SM background processes remaining include  $t\bar{t}$  with additional radiation and Z + jets production with multiple additional jets. The  $t\bar{t}$  backgrounds are divided into distinct processes depending on the flavour of the jets produced in association with the  $t\bar{t}$  process:  $t\bar{t}$  + light,  $t\bar{t}$  +  $\geq 1b$  (which are both large) and  $t\bar{t}$  +  $\geq 1c$  (which is smaller). The Z + jets,  $t\bar{t}$  + light and  $t\bar{t}$  +  $\geq 1b$  backgrounds are estimated by using MC simulated events and dedicated control regions are defined to improve their modelling and provide normalisation factors derived from data. These control regions are designed to be kinematically similar to the search regions, reasonably pure in the relevant background processes and low in signal contamination.<sup>3</sup> Sub-dominant background contributions come from W+ jets, single top,  $t\bar{t}$  + X and diboson production processes. These, and the

<sup>&</sup>lt;sup>3</sup> A signal contamination below 10% for dark Higgs models not excluded by other searches is achieved in all control and validation regions.

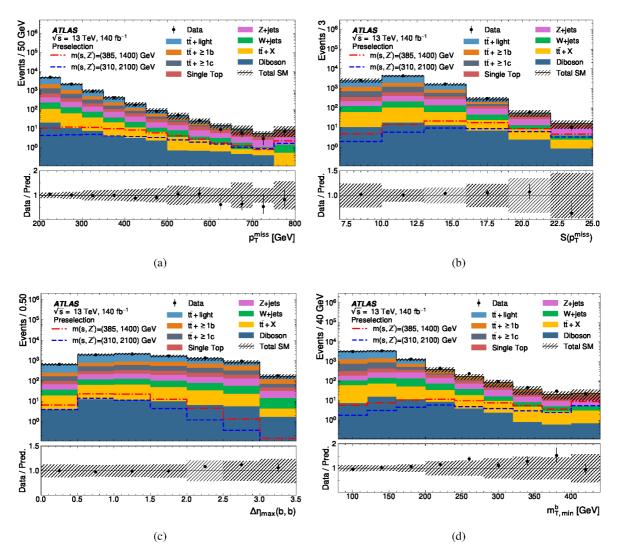


Figure 2: In the top panel of each plot, distributions of important kinematic variables in the NN training are given: (a)  $p_{\rm T}^{\rm miss}$ , (b)  $p_{\rm T}^{\rm miss}$  significance, (c)  $\Delta\eta_{\rm max}(b,b)$  and (d)  $m_{\rm T,min}^b$ . The preselection requirements (defined in Table 2) are applied and the background, benchmark signals and data distributions are shown, before any fit is performed. The uncertainty band on the background includes all systematic and MC statistical uncertainties. In the bottom panels the ratio of data to background is shown. The final bin in each distribution includes overflow.

 $t\bar{t} + \geq 1c$  background, are estimated with MC simulated events. The QCD multijet background satisfying the preselection requirements is negligible.

The Z+jets process entering the search regions consists primarily of  $Z \to \nu\nu$  decays. To obtain a high purity control region, a  $Z \to \mu\mu$  selection is used. This event sample is kinematically analogous to the signal process, contains high- $p_T$  Z bosons orthogonal to the signal regions, and is treated identically by the  $p_T^{\text{miss}}$  triggers, which consider muons to be invisible. So that the  $Z \to \mu\mu$  events emulate the  $Z \to \nu\nu$  events in the search regions, their missing transverse momentum is calculated treating the muons as invisible, termed  $p_T^{\text{miss}-\mu}$ . The control region definition starts by altering the standard preselection to require two Signal muons, and using  $p_T^{\text{miss}-\mu}$  instead of  $p_T^{\text{miss}}$  for the 200 GeV selection and  $m_{T,\text{min}}^b$  calculation

Table 5: Selection for Z + jets control region.

Variable	CRZ Requirement
$n_{\mu}$	= 2
$n_{ m jets}$	[4, 7]
$n_{b-\mathrm{jets}}$	≥ 3
$\Delta\phi_{ m min}^{4j}$	> 0.4
$p_{\mathrm{T}}^{\mathrm{miss}-\mu}$ [GeV]	> 200
$p_{\mathrm{T}}^{\mathrm{miss}-\mu}/\sqrt{H_{\mathrm{T}}} \ [\sqrt{\mathrm{GeV}}]$	> 7
$m_{\mathrm{T,min}}^{b-\mu}[\mathrm{GeV}]$	> 80
$p_{\mathrm{T}}^{\mathrm{miss}}$ [GeV]	< 75
$ m_{\mu\mu} - m_Z $ [GeV]	< 15

 $(m_{T,\min}^{b-\mu})$ . An event-based proxy of the muon-corrected missing transverse momentum significance is used  $(p_T^{\text{miss}-\mu}/\sqrt{H_T})$ , with the same lower bound of 7. Events are required to have an unmodified  $p_T^{\text{miss}}$  below 75 GeV to reduce top quark backgrounds. High purity in Z + jets is ensured by requiring that the muons are consistent with a Z boson decay, with an  $m_{\mu\mu}$  invariant mass within 15 GeV of  $m_Z$ . This CR has relatively limited yields but the predicted Z + jets background was found to reproduce the SR kinematics and  $m_{hh}$  distribution well, avoiding the need to mirror the NN requirement by developing analogous NN input features based on  $p_T^{\text{miss}-\mu}$ . The resulting Z + jets purity in CRZ is  $\sim 80\%$ , with a sub-leading contribution from  $t\bar{t}+Z$ . A summary of the CRZ definition is given in Table 5.

To estimate the  $t\bar{t}$  + light and  $t\bar{t}$  +  $\geq 1b$  backgrounds, control regions (summarised in Table 6) are defined to fulfil the preselection requirements and have a NN score in the 0.35 to 0.85 range to reduce signal contamination whilst remaining kinematically similar to the search regions. The  $t\bar{t}$  +  $\geq 1b$  component is targeted by the CR4b region, requiring exactly four b-tagged jets, which increases its fractional yield to  $\sim 45\%$ . To target the  $t\bar{t}$  + light background, a control region requiring exactly three b-tagged jets is defined. To further increase its purity, an  $80 \, \text{GeV} < m_{T,\text{min}}^b < 200 \, \text{GeV}$  requirement is made, ensuring the  $m_{T,\text{min}}^b$  value is compatible with the  $m_t$  endpoint. The resulting CR3b-low region, is  $\sim 57\%$  pure in  $t\bar{t}$  + light, with secondary contributions from other top quark background processes. Its complement, with  $m_{T,\text{min}}^b$  above 200 GeV and exactly three b-tagged jets forms the control region CR3b-high. This is used to check the modelling of background components contributing beyond  $m_{T,\text{min}}^b = m_t$ , and has larger contributions from Z + jets ( $\sim 25\%$ ), single top quark processes ( $\sim 20\%$ ) and  $t\bar{t}$  +  $\geq 1b$  events ( $\sim 16\%$ ).

To validate that the normalisation factors derived from the control regions lead to a good agreement between data and the background prediction in a signal-depleted region, a validation region (VR) is defined. This is made kinematically similar to the search regions using the adjacent 0.85 to 0.95 NN score region and the same preselection requirements, as shown in Table 6.

# 7 Systematic uncertainties

Experimental uncertainties in luminosity, pile-up reweighting, jet energy scale and resolution, JVT efficiency,  $p_{\rm T}^{\rm miss}$  soft term scale and resolution, and b-jet tagging efficiency are considered. The  $p_{\rm T}^{\rm miss}$  soft term uncertainty is estimated following the procedure described in Ref. [101]. Uncertainties in the jet energy

Table 6: Selections for all single top and  $t\bar{t}$  CRs, and the VR.

Variable	Region requirement			
	CR3b-low CR3b-high CR4b			VR
Preselection	pass			pass
NN score	[0.35, 0.85)			[0.85, 0.95)
$n_{b-\mathrm{jets}}$	= 3	= 3	= 4	≥ 3
$m_{\mathrm{T,min}}^{b}$ [GeV]	[80, 200)	≥ 200	≥ 80	≥ 80

scale and resolution and *b*-jet tagging efficiency are estimated at a per-jet level from calibrations and comparisons between different event simulation models [90, 93, 96]. The uncertainty in the JVT efficiency is estimated following the technique in Ref. [94]. Uncertainties related to lepton reconstruction and identification are found to be negligible.

Systematic uncertainties associated with the MC generator choice, parton shower, and the modelling of initial and final state radiation are considered for the  $t\bar{t}$  and single top backgrounds. The generator (parton shower) uncertainty is evaluated by comparing the nominal Powheg +Pythia 8 set-up against an alternative sample generated with MadGraph5\_AMC@NLO +Pythia 8 (Powheg +Herwig 7). The uncertainty due to initial-state radiation is estimated by simultaneously varying the  $h_{\rm damp}$  parameter and the  $\mu_{\rm r}$  and  $\mu_{\rm f}$  scales, and choosing the Var3c up/down variants of the A14 tune as described in Ref. [112]. The final-state radiation uncertainty is evaluated by varying the renormalisation scale up or down by a factor of two. The uncertainty associated with modelling the interference between  $t\bar{t}$  and single top processes is evaluated by comparing the nominal diagram removal [113] set-up to an alternative sample with diagram subtraction [113, 114].

Uncertainties related to missing higher-order corrections are assessed by variations of the choice of renormalisation and factorisation scales for the W+ jets and Z+ jets backgrounds, evaluated as the envelope of a set of seven variations [115]. Uncertainties in the resummation and matching were also assessed and found to be negligible. A conservative 50% uncertainty is used for the  $t\bar{t}+\geq 1c$  and single top backgrounds to account for the uncertainty in their cross-sections in the signal phase space [39], which has negligible impact on the results. For the minor  $t\bar{t}+X$  and diboson backgrounds, a 20% uncertainty is used to account for modelling uncertainties in these processes [116]. For the dark Higgs signal model, uncertainties in the renormalisation and factorisation scale choices are evaluated following the same procedure as used for SM backgrounds. The uncertainty in the luminosity is also included and has a negligible impact.

# 8 Statistical interpretation

The statistical interpretation of the search results is performed via simultaneous likelihood fits to the observed data, using the HistFitter framework [117]. The likelihood consists of a product of Poisson probability density functions describing the observed and expected numbers of events in the relevant regions. The systematic uncertainties in the backgrounds and signal processes are included as Gaussian distributed nuisance parameters in the likelihood expression. For the background processes scaled by normalisation factors ( $t\bar{t}$  + light,  $t\bar{t}$  +  $\geq$  1b, Z + jets), these appear as freely floating parameters multiplying the expected MC yields. MC statistical uncertainties are included as nuisance parameters in the likelihood with Poisson distributions.

A background-only fit is first performed to validate the SM background estimate. For this fit, only the four control region yields are included, and it is assumed that no signal is present. The fit constrains the values of the background normalisation factors, and the results of the fit are applied to the validation region to assess the post-fit agreement between the observed VR data and background prediction.

To test the SM-only hypothesis and place limits on the possible number of BSM signal events entering each DR at 95% confidence level (CL) without making explicit assumptions about the signal  $m_{hh}$  shape, fits are performed. One fit is performed for each DR in turn, simultaneously fitting the four control regions and the DR. A dummy signal is included in each DR, whose signal strength is the parameter of interest for the fit. It is assumed the signal contributions to the control regions are negligible.

To place limits on the dark Higgs models at 95% CL using the  $CL_s$  method [118], the four control regions and the binned SR are fitted simultaneously. The parameter of interest in the fit is the signal strength  $\mu_{\text{sig}}$ , which multiplies the signal yield nominally predicted by the model.

#### 9 Results

The background normalisation factors obtained in the background-only fit are:  $\mu_{Z+jets} = 1.24 \pm 0.14$ ,  $\mu_{t\bar{t}} + \geq 1b = 1.2 \pm 0.6$  and  $\mu_{t\bar{t}+light} = 0.91 \pm 0.14$ . The agreement between the observed data and the SM background prediction after the background-only fit is shown in Figure 3. The  $m_{hh}$  distribution in the VR after the background-only fit is shown in Figure 4, demonstrating no mismodelling trend and a small upward fluctuation (< 1.7 $\sigma$ ). The distribution of the NN score after the background-only fit is shown in Figure 5(a), for the range of score values used in the analysis regions. A good agreement between the SM background prediction and data is observed throughout the range. The  $m_{hh}$  distribution in the binned signal region after the background-only fit is shown in Figure 5(b). The overlaid benchmark signal points highlight the good discrimination power of the NN and  $m_{hh}$  distributions. There are no significant excesses or deficits in the data compared with the SM prediction. Additionally, the distribution has a similar shape to that seen in the VR in Figure 4, demonstrating that the NN score is not highly correlated with  $m_{hh}$ , in line with the NN design.

To place limits on the possible number of BSM events of a similar topology entering each DR, more model-agnostic fits are performed, as described in Section 8. The post-fit agreement between the observed data and the expected SM background yields follows from the fitted  $m_{hh}$  distribution, and is shown in Figure 6, with the derived upper limits detailed in Table 7.

In the absence of evidence for a signal, exclusion limits are set on the dark Higgs model in the plane of the masses of the dark Higgs boson (s) and Z' mediator. The impacts of each category of uncertainties in the SR yields in the exclusion fits are assessed in Table 8 for a representative signal point with  $m_{Z'} = 1400 \,\text{GeV}$  and  $m_s = 385 \,\text{GeV}$ . Consistent with the limited yields in the SR, the results are statistically limited, with the statistical uncertainty of the data dominating. The larger systematic uncertainty components are those from the modelling of the predicted backgrounds, such as the normalisation of the freely floating components and the theoretical modelling and cross-section uncertainties of the other sub-leading components. Smaller contributions come from the limited size of the Monte-Carlo simulations and experimental uncertainties pertaining to the jet and b-jet calibration and identification.

The observed and expected exclusion limits are calculated from the binned signal region, and shown in Figure 7. The observed limits follow the expectation closely, and are constrained by the large acceptance changes at the  $Z' \to \chi \chi$  threshold of  $m_{Z'} \sim 400 \,\text{GeV}$  and the s-decay thresholds at  $m_s \sim 250 \,\text{GeV}$  and

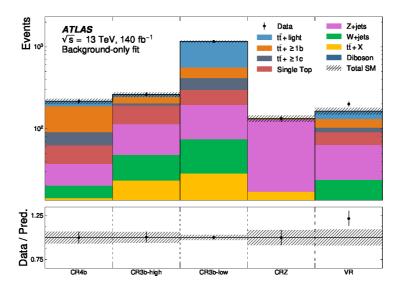


Figure 3: Observed data and expected background yields in each control and validation region after the backgroundonly fit. The hashed band shows the total systematic and MC statistical uncertainty. In the lower panel the ratio of data and background yields is shown.

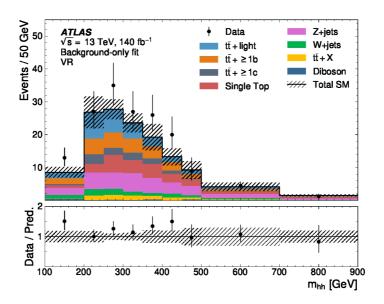


Figure 4: The observed data and expected background  $m_{hh}$  distribution in the VR, after the background-only fit. The hashed bands show the total systematic and MC statistical uncertainty. The lower panel shows the ratio of data and predicted background yields.

400 GeV. At high  $m_{Z'}$ , the falling cross-section leads to a wider variation in the expected limits, and small fluctuations in the data result in slightly stronger or weaker exclusions than the median expectation accordingly. A comparison of the observed contours with limits placed from other ATLAS dark Higgs boson searches [41–43] is shown in Figure 8, highlighting the complementary sensitivities that different dark Higgs boson signatures have to different areas of mass parameter space. The di-Higgs decay of the dark Higgs boson is sensitive to  $m_s > 250$  GeV and the high Higgs boson branching ratio to bb provides unique sensitivity in this region, where other dibosonic final states lose sensitivity from their decreased

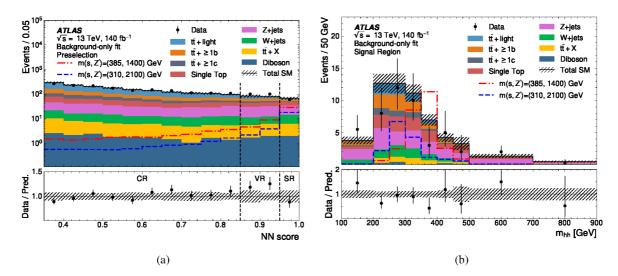


Figure 5: The observed data and expected background (a) NN score distribution after the preselection requirements and (b)  $m_{hh}$  distribution in the SR, after the background-only fit. The hashed bands show the total systematic and MC statistical uncertainty. Benchmark signal distributions are overlaid as dashed lines. The lower panel shows the ratio of data and predicted background yields.

Table 7: Upper limits on the expected (observed) number of BSM events  $S_{\rm exp}^{95}$  ( $S_{\rm obs}^{95}$ ) at 95% confidence level, the  $\pm 1\sigma$  variations on the expected upper limit, and the observed limit on the effective visible BSM cross-section ( $\langle \epsilon \sigma_{\rm obs}^{95} \rangle$ ), for each of DRa-DRg. The discovery  $p_0$ -value is also shown, capped at 0.5 if the data yield is smaller than the SM prediction.

Region	$m_{hh}[\text{GeV}]$	Data	Fitted background	$S_{ m exp}^{95}$	$S_{ m obs}^{95}$	$\langle \epsilon \sigma_{ m obs}^{95} \rangle$ [fb]	p <sub>0</sub> -value
DRa	[100, 250)	19	$20.1 \pm 4.9$	$11.1^{+5.1}_{-3.3}$	10	0.072	0.50
DRb	[200, 300)	20	$24.1 \pm 2.7$	$12.1^{+5.5}_{-3.6}$	8.8	0.063	0.50
DRc	[250, 350)	22	$23.4 \pm 4.7$	$11.9^{+5.5}_{-3.6}$	11	0.076	0.50
DRd	[300, 400)	13	$17.6 \pm 1.9$	$10.2^{+4.9}_{-3.1}$	6.9	0.049	0.50
DRe	[350, 450)	8	$10.9 \pm 1.4$	$8.2^{+4.1}_{-2.5}$	5.9	0.042	0.50
DRf	[400, 900)	16	$14.8 \pm 2.7$	$10.0^{+4.7}_{-3.0}$	11	0.079	0.40
DRg	[500, 900)	9	$7.4 \pm 2.3$	$7.2^{+3.6}_{-2.3}$	8.7	0.062	0.33

branching fraction and the increasing collimation of the decay products. Also shown in Figure 8 is the predicted DM relic density as calculated by MadDM [120]. At  $m_s \simeq 2m_\chi = 400$  GeV, DM annihilation via a dark Higgs boson is enhanced, strongly depleting the surviving relic abundance of DM. For this benchmark with  $m_\chi = 200$  GeV, the  $s \to \chi \chi$  decay dominates above this  $m_s$  value; however these results have generic sensitivity to  $m_s > 400$  GeV, e.g. in scenarios with larger  $m_\chi$ .

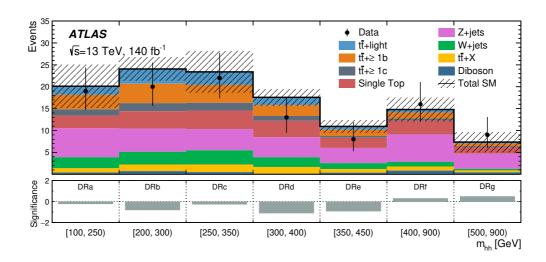


Figure 6: Observed data and fitted background yields in each DR region. The hashed band shows the total systematic and MC statistical uncertainty. In the lower panel the statistical significance (measured using Eq. 1 of Ref. [119]) of fluctuations between the data and SM expectation is shown.

Table 8: Summary of the relative impact of each category of uncertainty in the SR yield, in a signal plus background fit to a  $m_{Z'} = 1400 \,\text{GeV}$ ,  $m_s = 385 \,\text{GeV}$  signal simulation.

Source of uncertainty	Percentage of total uncertainty [%]
Signal modelling	<1
<i>b</i> -jet identification	5
Jet calibrations	9
Other experimental	2
$t\bar{t}$ modelling & normalisation	11
Z + jets modelling & normalisation	9
Single top modelling & cross-section	18
Other background modelling & cross-section	13
MC statistical uncertainty	17
Overall systematic error	33
Data statistical	95
Total uncertainty	100

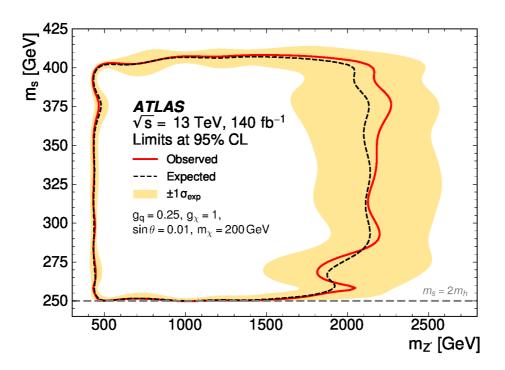


Figure 7: Observed and expected exclusion limits in the  $(m_{Z'}, m_s)$  plane at 95% CL, with the excluded part inside the closed contour. The  $\pm 1\sigma$  expected exclusion intervals are shown as the filled bands. The horizontal dashed line at  $m_s = 2m_h$  indicates the limit where the  $s \to hh$  decay mode becomes kinematically accessible.

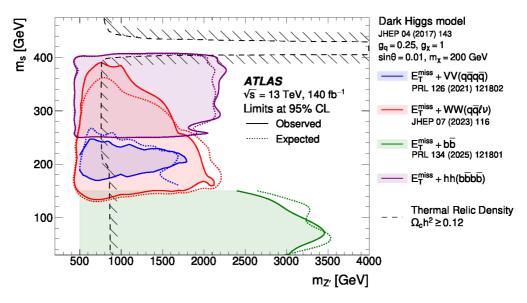


Figure 8: A comparison of this analysis' exclusions with existent ATLAS searches [41–43]. Their observed and expected exclusion limits in the  $(m_{Z'}, m_s)$  plane at 95% CL are shown. The observed relic density is indicated with a dashed line, with the diagonal lines indicating an overabundance of DM.

## 10 Conclusion

A search for dark matter in a final state with significant  $p_{\rm T}^{\rm miss}$  and a resonantly produced pair of Higgs bosons resulting in at least three *b*-tagged jets is performed, using the 140 fb<sup>-1</sup> of Run 2 data recorded by the ATLAS detector at the LHC between 2015 and 2018. The observed data are found to be consistent with Standard Model predictions. Upper limits are placed at 95% confidence level on the effective production cross-section for new particle states with mass greater than 250 GeV decaying into *hh* in association with  $p_{\rm T}^{\rm miss}$ . The result is interpreted using a dark Higgs model, with a dark Higgs boson *s* giving rise to massive dark matter, and a Z' mediator. Upper limits are derived on the hypothesised particle masses for 250 <  $m_s$  < 400 GeV, excluding Z' masses up to 2.3 TeV in a recommended model benchmark. This new signature significantly extends the constraints in this mass region existing from previous dark Higgs analyses by the ATLAS and CMS collaborations in different final states. The results complement other lower-mass dark Higgs boson searches, searches for extended Higgs sectors and collider DM searches more generally.

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