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Search for Beyond the Standard Model physics with anomaly detection in multilepton final states in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

The ATLAS Collaboration

A model-agnostic search for Beyond the Standard Model physics is presented, targeting final states with at least four light leptons (electrons or muons). The search regions are separated by event topology and unsupervised machine learning is used to identify anomalous events in the full 140 fb^{-1} of proton–proton collision data collected with the ATLAS detector during Run 2. No significant excess above the Standard Model background expectation is observed. Model-agnostic limits are presented in each topology, along with limits on several benchmark models including vector-like leptons, wino-like charginos and neutralinos, or smuons. Limits are set on the flavourful vector-like lepton model for the first time.

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Contents

1 Introduction

Throughout the data taking years of 2015–2018, the ATLAS detector at the LHC has collected proton–proton collisions amassing 140 fb^{-1} of data. The Standard Model (SM) of particle physics has been able to describe collider physics phenomena to outstanding precision. Its last missing component, the Higgs boson, was discovered in 2012 by the ATLAS and CMS Collaborations [1, 2]. However, the SM remains an incomplete theory, as it does not provide answers to open questions such as the hierarchy of masses of elementary fermions, the origin of neutrino masses, the hierarchy and fine-tuning problems, the observed baryon asymmetry in the universe, and the nature of dark matter and dark energy. Many beyond-the-SM (BSM) theories have been proposed to address these and other shortcomings of the SM; however there are no clear indications of which BSM theory (if any) would provide a more accurate description of nature. Consequently the ATLAS experiment continues a broad BSM search program. The traditional route for searching for BSM physics is to design an analysis targeting a specific model that results in detectable signatures at the LHC. However, without a preferred BSM physics model or scale, model-dependent searches will miss signatures of some possible BSM scenarios. This analysis looks to solve this problem in collision events with multiple leptons, by casting a wide net to simultaneously cover a range of possible final states.

High lepton multiplicities are particularly interesting as they provide a comparatively low-SM-background channel to search for potential BSM physics. ATLAS has previously performed searches with minimal model dependence in the multilepton final states [3, 4]. The search presented here is focused on light leptons (electrons, e, or muons, μ). Tau leptons are allowed inclusively but not explicitly selected. As a result, leptons refer to light leptons unless otherwise stated. This paper explores the potential for BSM

physics discovery in a model-agnostic way in final states with 4ℓ or $\geq 5\ell$, while demonstrating sensitivity to specific benchmark models.

In high energy physics, anomaly detection (AD) is used as a technique to boost the sensitivity to BSM physics in a model-agnostic way. Both the ATLAS and CMS experiments have published searches involving AD techniques, ranging from weakly supervised searches [5, 6], semi-supervised searches [7, 8] and fully unsupervised searches [9, 10]. The majority of AD searches are performed in jet-focused final states. In this work, the first ever AD search is performed in multilepton final states. This analysis focuses on the branch of AD named outlier detection, where the type of anomalous events targeted are out-of-distribution data (excesses in tails) as opposed to over-densities such as bumps. Using generative models to explicitly calculate the probability density of events originating from SM processes, the sensitivity to rare excesses (SM or BSM) is boosted in a model-agnostic (denoted model-independent in the remainder) way. Due to the complex, high-dimensional input feature space used, interesting anomaly-enriched regions are constructed from the probability density that could have previously been overlooked.

In order to assess the sensitivity of this search to BSM physics, a range of benchmark BSM scenarios are simulated. This not only demonstrates the generality of model-independent searches but allows comparison to the sensitivity of dedicated searches. The benchmark models tested target the production of high-mass exotic particles that decay to final states with a high lepton multiplicity. The reporting of model-independent limits allows future reinterpretations, and can be used as a benchmark to assess the viability of new BSM models in multilepton final states.

The benchmark models used for model-dependent interpretation in this paper include the production of vector-like leptons (VLLs) or of supersymmetric particles and are described in the following. Vector-like leptons are hypothetical spin-1/2 particles that are part of one of the simplest viable extensions to the SM at the electroweak scale [11–16]. This analysis considers two simple minimal cases of VLLs as defined in Refs. [17, 18], namely an "SU(2) Singlet VLL" and an "SU(2) Doublet VLL" model, with mixings to the SM electron or muon. VLLs are predominantly produced in pairs via the electroweak interaction. In the SU(2) Doublet VLL scenario, the charged VLL decay modes are to an electron or muon, and a Z or SM Higgs boson. In contrast, the neutral VLL decay mode is to an electron or muon and a W boson with 100% branching ratio. In the SU(2) Singlet VLL scenario, only the charged VLL is present and its decay modes are to a neutrino and a W boson, an electron or muon and a Z boson, or an electron or muon and a SM Higgs boson, with branching ratios asymptotically reaching 50%, 25%, and 25%, respectively. The corresponding Feynman diagrams can be found in Ref. [19]. VLL models are also considered with the inclusion of a new complex leptophilic scalar S_{ji} which can decay through fermion mixing to leptons of generation i and j, opening new decay modes of the VLLs, ψ_i, to this scalar, $\psi_i^- \to S_{ji}^* \ell_j^-$ or $\psi_i^0 \to S_{ji}^* \nu_j$, and their conjugates [20]. Once the VLL decay to the S_{ji} scalar is open, the corresponding branching ratio is nearly 100%. The decay mode $S_{ji}^* \to \ell_j^+ \ell_i^-$ with $i = 1, 2$ and $j = 1, 2, 3$, and its conjugate, are considered, with equal branching ratios to the three j lepton flavours for a given i lepton flavour. This can result in final states with large lepton multiplicities (up to six leptons), and allow for lepton flavour violating decays. Figure 1 shows representative Feynman diagrams for this model, referred to as 'flavourful VLL'. Finally, simplified R-parity violating (RPV) SUSY signals are considered, where the lightest SUSY particle is a bino-like neutralino ($\tilde{\chi}_1^0$), and decays as: $\tilde{\chi}_1^0 \to \ell_k^\pm \ell_{i/j}^\mp \nu_{j/i}$. Every pair production event of wino-like charginos and neutralinos $\tilde{\chi}_1^\pm \tilde{\chi}_1^\mp \to \tilde{\chi}_1^0 W^\pm \tilde{\chi}_1^0 W^\mp$ and $\tilde{\chi}_1^\pm \tilde{\chi}_2^0 \to \tilde{\chi}_1^0 W^\pm \tilde{\chi}_1^0 Z/h$ results in at least four lepton final states. In this paper, only light leptons are considered and thus the $\lambda_{ijk} = \lambda_{12k}$ (with $k = 1, 2$) coupling scenario is used as benchmark model. The corresponding Feynman diagrams can be found in Ref. [21]. A variation on the RPV SUSY model is also considered, where smuons are pair produced and decay to a bino-like neutralino, which in turn decays via the RPV coupling λ'_{i33} (with $i = 2, 3$). This allows the

bino-like neutralino to decay to a lepton and third-generation quarks. This model can result in final states with high lepton multiplicity and high b-jet multiplicity. The corresponding Feynman diagrams can be found in Ref. [22].

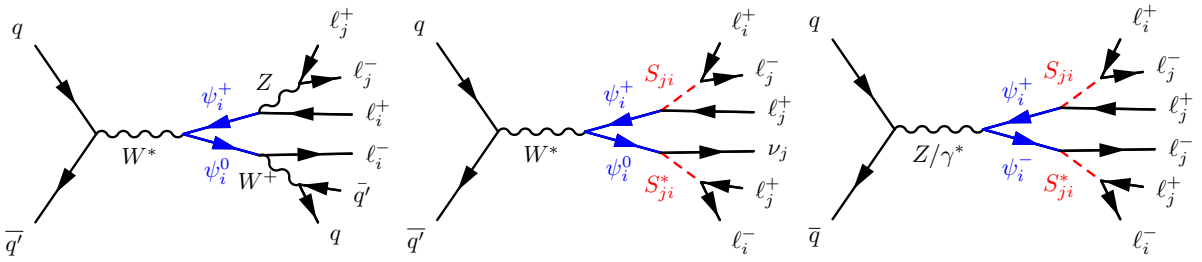


Figure 1: Example Feynman diagram for the pair production of VLL, denoted by ψ_i, in the flavourful model, with the VLLs produced via a (a, b) W^* boson and (c) a Z boson, with the decay of the VLLs into SM leptons and (a) two SM vector bosons, and (b, c) two scalars S_{ji}. Considering the decays of (a) $W^+ \to q\bar{q}'$ and $Z \to \ell_j^+\ell_j^-$, and (b, c) $S_{ji}^{(*)} \to \ell_j^{-(+)}\ell_i^{+(-)}$, these processes result in multilepton final states. The subscripts i and j refer to the lepton generation, with allowed values $i = 1, 2$ and $j = 1, 2, 3$.

Two separate searches are performed and referred to as 'model-independent' and 'model-dependent'. Both searches analyse the same pre-selected events but categorise them differently according to the multiplicity and flavour of various objects and the AD score. The model-independent search assumes BSM signals populating one signal region at a time, whereas the model-dependent search is designed to assess the sensitivity to specific BSM models by fitting the AD score in all regions in a simultaneous fit.

2 ATLAS detector

The ATLAS detector [23] at the LHC covers nearly the entire solid angle around the collision point.[1] It consists of an inner tracking detector surrounded by a thin superconducting solenoid, electromagnetic and hadronic calorimeters, and a muon spectrometer incorporating three large superconducting air-core toroidal magnets.

The inner-detector system (ID) is immersed in a 2 T axial magnetic field and provides charged-particle tracking in the range of $|\eta| < 2.5$. The high-granularity silicon pixel detector covers the vertex region and typically provides four measurements per track, the first hit generally being in the insertable B-layer (IBL) installed before Run 2 [24, 25]. It is followed by the SemiConductor Tracker (SCT), which usually provides eight measurements per track. These silicon detectors are complemented by the transition radiation tracker (TRT), which enables radially extended track reconstruction up to $|\eta| = 2.0$. The TRT also provides electron identification information based on the fraction of hits (typically 30 in total) above a higher energy-deposit threshold corresponding to transition radiation.

[1] 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, ϕ) are used in the transverse plane, ϕ being the azimuthal angle around the z-axis. The pseudorapidity is defined in terms of the polar angle θ 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. Angular distance is measured in units of $\Delta R \equiv \sqrt{(\Delta y)^2 + (\Delta\phi)^2}$.

The calorimeter system covers the pseudorapidity range $|\eta| < 4.9$. Within the region $|\eta| < 3.2$, electromagnetic calorimetry is provided by barrel and endcap high-granularity lead/liquid-argon (LAr) calorimeters, with an additional thin LAr presampler covering $|\eta| < 1.8$ to correct for energy loss in material upstream of the calorimeters. Hadronic calorimetry is provided by the steel/scintillator-tile calorimeter, segmented into three barrel structures within $|\eta| < 1.7$, and two copper/LAr hadronic endcap calorimeters. The solid angle coverage is completed with forward copper/LAr and tungsten/LAr calorimeter modules optimised for electromagnetic and hadronic energy measurements, respectively.

The muon spectrometer (MS) comprises separate trigger and high-precision tracking chambers measuring the deflection of muons in a magnetic field generated by the superconducting air-core toroidal magnets. The field integral of the toroids ranges between 2.0 and 6.0 T m across most of the detector. Three layers of precision chambers, each consisting of layers of monitored drift tubes, cover the region $|\eta| < 2.7$, complemented by cathode-strip chambers in the forward region, where the background is highest. The muon trigger system covers the range $|\eta| < 2.4$ with resistive-plate chambers in the barrel, and thin-gap chambers in the endcap regions.

The luminosity is measured mainly by the LUCID–2 [26] detector that records Cherenkov light produced in the quartz windows of photomultipliers located close to the beampipe.

Events were selected by the first-level trigger system implemented in custom hardware, followed by selections made by algorithms implemented in software in the high-level trigger [27]. The first-level trigger accepted events from the 40 MHz bunch crossings at a rate close to 100 kHz, which the high-level trigger further reduced to record complete events to disk at about 1.25 kHz.

A software suite [28] 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 simulated event samples

This analysis uses data from pp collisions at $\sqrt{s} = 13$ TeV collected by the ATLAS experiment from 2015 to 2018. After the application of data-quality requirements [29] to ensure that all parts of the detector are operational during data-taking, the data sample corresponds to an integrated luminosity of 140 fb^{-1}. The number of additional pp interactions per bunch crossing (pile-up) in this sample ranges from about 8 to 70, with an average of 34. The trigger requirements are discussed in Section 5.

Monte Carlo (MC) simulation samples are produced for the different signal and background processes. Processes contributing to the background with at least one non-prompt lepton or one electron from conversion in the 4ℓ final state are mainly $t\bar{t}$, Z + jets, $t\bar{t}W$ and $W^{\pm}Z$. The main background contributions with prompt leptons are from the $t\bar{t}Z/\gamma^*(Z/\gamma^* \to \ell^+\ell^-)$, ZZ, and $t\bar{t}H$ processes. In the $\geq 5\ell$ final state, $t\bar{t}Z/\gamma^*(Z/\gamma^* \to \ell^+\ell^-)$ and ZZ processes contribute to the background with at least one non-prompt lepton or electron from photon conversion.

All samples showered with Pythia use the A14 set of tuned parameters [30] (referred to as 'tune'), whereas those showered with Herwig use the H7-UE tune [31]. In all samples simulated with Sherpa [32], the matrix elements (MEs) are calculated with the Comix [33] and OpenLoops [34–36] libraries. They are matched with the Sherpa parton shower (PS) [37] using the MEPS@NLO prescription [38–41] with the set of tuned parameters developed by the Sherpa authors. Pile-up is modelled using events from minimum-bias interactions generated with Pythia 8.186 [42] with the A3 tune [43], and overlaid onto the

simulated hard-scatter events according to the luminosity profile of the recorded data [44]. All samples include leading-logarithm photon emission, either modelled by the PS generator or by PHOTOS [45]. The generated events are processed through either a full simulation of the ATLAS detector geometry and response using GEANT4 [46], or a faster simulation where the full GEANT4 simulation of the calorimeter response is replaced by a detailed parameterisation of the shower shapes (ATLAS Fast Simulation) [47]. Both types of simulated events are processed through the same reconstruction software used for the pp collision data. Corrections are applied to the simulated events so that the particle candidates' selection efficiencies, energy scales and energy resolutions match those determined from data control samples.

Background events from $t\bar{t}Z/\gamma^*$ production were simulated using the MADGRAPH5_AMC@NLO 2.8.1 [48] generator at next-to-leading-order (NLO) in α_s with the NNPDF3.0NLO [49] PDF set. The functional form of the renormalisation and factorisation scales (μ_r, μ_f) was set to the default scale $0.5 \times \sum_i \sqrt{m_i^2 + p_{T,i}^2}$, where the sum runs over all the particles generated from the ME calculation. The invariant mass of the lepton pair, $m(\ell\ell)$, in the $t\bar{t}Z/\gamma^*(Z/\gamma^* \to \ell^+\ell^-)$ sample is set to be greater than 1 GeV. Top quarks were decayed at leading-order (LO) using MADSPIN [50, 51] to preserve all spin correlations. Showering and hadronisation were performed using PYTHIA 8.244 [52] with the A14 tune, and the NNPDF2.3LO [53] PDF set with $\alpha_s = 0.130$. The decays of bottom and charm hadrons were performed by EVTGEN 1.7.0 [54].

Diboson (VV) background processes are simulated with SHERPA 2.2.2 [55] and include $W^{\pm}Z$, ZZ, and W^+W^- processes. The ME is calculated with NLO accuracy in QCD for up to one additional parton and at LO accuracy for up to three additional partons. The NNPDF3.0NNLO set of PDFs is used. The simulation includes off-shell effects and Higgs boson contributions, where appropriate. The invariant mass of any pair of SFOS leptons is required to be $m(\ell\ell) > 4$ GeV. Samples for the loop-induced processes $gg \to VV$ are simulated using LO-accurate MEs for up to one additional parton emission. The triboson (VVV) background processes are also simulated with SHERPA 2.2.2 and using the NNPDF3.0NNLO set of PDFs, with the ME calculated with NLO accuracy in QCD for the inclusive process and LO accuracy for up to two additional partons.

Samples for $t\bar{t}H$, and single top production are simulated using the NLO generator POWHEG BOX v2 [56–62] and interfaced with PYTHIA 8 for the PS and fragmentation. These samples used the NNPDF3.0NLO PDF set. The decays of bottom and charm hadrons are performed by EVTGEN 1.6.0. The production of a top quark in association with a W boson (tW) is modelled using the five-flavour scheme. The diagram removal scheme [63] is used to remove interference and overlap with $t\bar{t}$ production. Single-top s- and t-channel production is modelled using the five- and four-flavour schemes, respectively.

The production of $t\bar{t}$ events is modelled using the POWHEG BOX v2 generator at NLO with the NNPDF3.0NLO PDF set. The events are interfaced to PYTHIA 8.230 to model the PS, hadronisation, and underlying event, using the NNPDF2.3LO set of PDFs. The decays of bottom and charm hadrons are performed by EVTGEN 1.6.0. The $t\bar{t}$ process is modelled with the h_{damp} parameter [2] set to $1.5\,m_t$ [64]. The $t\bar{t}$ sample is normalised to the cross-section prediction at next-to-next-to-leading-order (NNLO) in QCD including the resummation of next-to-next-to-leading logarithmic (NNLL) soft-gluon terms calculated using TOP++ 2.0 [65–71]. This cross-section is $\sigma(t\bar{t})_{\text{NNLO+NNLL}} = 832 \pm 51$ pb.

The $Z/\gamma^* \to \ell\ell$ process (with $\ell = e, \mu, \tau$) is simulated with SHERPA 2.2.11 using the NNPDF3.0NNLO PDF set. Processes with up to two coloured partons are modelled at NLO in the strong coupling, while

[2] The h_{damp} parameter is a resummation damping factor and one of the parameters that controls the matching of POWHEG MEs to the PS, thus effectively regulating the high-p_T radiation against which the hard-process system recoils.

processes with up to five additional partons are modelled at LO accuracy. The Z+jets sample is normalised to the theoretical cross-section calculated at NLO accuracy in QCD [72].

The $t\bar{t}W$ background sample is simulated using MadGraph5_aMC@NLO 2.6.7 with NLO multileg merging using the FxFx algorithm [73], where the MEs are calculated for up to one additional partons at NLO in QCD, and up to two partons at LO in QCD. The events are interfaced with Pythia 8.244. The NNPDF3.0nlo and NNPDF2.3lo PDF sets are used for the ME and PS, respectively. The merging scale parameter is used in the matching of a ME with the PS and is set to 30 GeV. In addition to this $t\bar{t}W$ prediction at NLO in QCD, higher-order corrections related to electroweak (EW) contributions are also included. First, event-by-event correction factors are applied that provide virtual NLO EW corrections of the order $\alpha^2\alpha_s^2$ derived using the formalism described in Ref. [74] along with LO corrections of order α^3. Second, real emission contributions from the sub-leading EW corrections at order $\alpha^3\alpha_s$ [75] are simulated with MadGraph5_aMC@NLO 2.6.7 produced at LO in QCD and included as a separate sample.

A dedicated $t\bar{t}$ sample with rare $t \to Wb\gamma^*(\to \ell^+\ell^-)$ radiative decays, $t\bar{t} \to W^+bW^-\bar{b}\ell^+\ell^-$, is simulated using a ME calculated at LO in QCD and requiring $m(\ell\ell) > 1$ GeV. In this sample the photon can be radiated from the top quark, the W boson, or the b-quark. Both the $t\bar{t}Z/\gamma^*(Z/\gamma^* \to \ell^+\ell^-)$ and $t\bar{t} \to W^+bW^-\bar{b}\ell^+\ell^-$ samples are combined and together form the '$t\bar{t}Z/\gamma^*$' sample. The contribution from internal photon conversions ($\gamma^* \to \ell^+\ell^-$) with $m(\ell\ell) < 1$ GeV is modelled by QED multi-photon radiation via the PS in an inclusive $t\bar{t}$ sample. The contribution from muons from internal conversions for $m(\ell\ell) < 1$ GeV is negligible in this analysis. Dedicated Z+jets samples are generated with Powheg Box and interfaced with Pythia 8 for the PS and fragmentation. These samples are used to model the data in a control region enriched in material and internal conversion electrons, as explained in Section 5.

The production of $t\bar{t}t\bar{t}$ events was modelled using the MadGraph5_aMC@NLO v2.6.2 generator that provides MEs at NLO in QCD with the NNPDF3.1nlo [76] PDF set. The functional form of the renormalisation and factorisation scales are set to $\mu_r = \mu_f = m_T/4$, where m_T is defined as the scalar sum of the transverse masses $\sqrt{m^2 + p_T^2}$ of the particles generated from the ME calculation. The events are interfaced with Pythia 8.230 for the PS and hadronisation, using the NNPDF2.3lo PDF set. The production of $t\bar{t}t\bar{t}$ events is normalised to a cross section of 12 fb computed at NLO in QCD including EW corrections [75].

Other minor background contributions are included in the analysis: tZq, tWZ, W + jets and VH processes are normalised to their NLO cross-section, whereas $t\bar{t}t$, $t\bar{t}W^+W^-$, $t\bar{t}ZZ$, $t\bar{t}HH$, and $t\bar{t}WH$ are normalised to their LO cross-section.

Signal samples for VLL$_e$ and VLL$_\mu$ from $SU(2)$ singlet (VLL$_e^S$, VLL$_\mu^S$) and doublet (VLL$_e^D$, VLL$_\mu^D$) models, as well as the flavourful VLL$_e$ and VLL$_\mu$ processes, are simulated using MadGraph5_aMC@NLO 2.9.5 at NLO in QCD with the NNPDF3.0nlo PDF set and Pythia 8.245, and processed through the ATLAS Fast Simulation. The NLO cross-section obtained from MadGraph is used for the normalisation of the signals. The RPV SUSY wino-like chargino and neutralino signal processes are simulated using MadGraph5_aMC@NLO 2.2.2 + Pythia 8.230 at LO in QCD with up to two extra partons. Jet–parton matching followed the CKKW-L prescription [77], with a matching scale set to one quarter of the mass of the pair-produced SUSY particles. The RPV SUSY smuon signal samples were generated with MadGraph5_aMC@NLO 2.9.3 with up to two extra jets at LO in QCD and Pythia 8.245. The matching scale is set at 1/4 of the mass of the SUSY particle being produced. Cross-sections for the RPV SUSY signals were calculated to NLO in the strong coupling constant, adding the resummation of soft gluon emission at next-to-leading-logarithm accuracy [78–85].

4 Event reconstruction

Candidate events are required to have at least one pp interaction vertex. Interaction vertices are reconstructed from at least two tracks with transverse momentum p_{T} larger than 500 MeV that are consistent with originating from the beam collision region in the x–y plane. In events with multiple vertices, the primary vertex is defined as the one with the highest scalar sum of the squared transverse momenta of the associated tracks [86].

Electron candidates are reconstructed from energy clusters in the electromagnetic calorimeter matched to a track in the ID [87]. They are required to satisfy $p_{\mathrm{T}} > 10$ GeV and $|\eta| < 2.47$, excluding the transition region between the endcap and barrel calorimeters ($1.37 < |\eta| < 1.52$). The 'Loose' electron identification working point (WP) is used, based on a likelihood discriminant employing calorimeter, tracking and combined information that provide separation between electrons and jets.

The reconstruction of muon candidates is based on tracking information from the MS and the ID, as well as energy deposits in the calorimeter system [88]. Muons are required to satisfy $p_{\mathrm{T}} > 10$ GeV and $|\eta| < 2.5$. The 'Loose' muon identification WP is used.

Electron (muon) candidates are matched to the primary vertex by requiring that the significance of their transverse impact parameter, d_0 (defined as the distance of closest approach of the track to the beamline in the x–y plane) satisfies $|d_0|/\sigma_{d_0} < 5$ (3), where σ_{d_0} is the measured uncertainty in d_0, and by requiring that their longitudinal impact parameter, z_0 (defined as the distance in z between the primary vertex and the point on the track used to evaluate d_0) satisfies $|z_0 \sin\theta| < 0.5$ mm.

Light lepton candidates are also required to be isolated in the tracker and in the calorimeter to further suppress leptons from heavy-flavour (HF) hadron decays, misidentified jets, or photon conversions (collectively referred to as 'non-prompt leptons'). Electrons with an incorrect charge assignment (referred to as 'QMisID') are further suppressed with a boosted decision tree (BDT) discriminant in 4ℓ events with total lepton electric charge $Q = \pm 2$ and same-sign electric charge dilepton (2ℓSS) μe events. Electrons are further separated into three classes, 'material conversion', 'internal conversion', and 'non-conversion', following the same procedure as described in Ref. [19]. Electrons are required to pass the 'non-conversion' class in all regions except in the control region enriched in material and internal conversion electrons, as explained in Section 5.

For the control regions enriched in non-prompt leptons from the decay of hadrons that contain bottom- or charm-quarks (referred to as 'HF non-prompt leptons') as described in Section 7, leptons are required to fail a selection based on a WP of a BDT discriminant (referred to as the non-prompt-lepton BDT [89]). The BDT uses isolation and lifetime information about a track-jet that matches the selected electron or muon to discriminate between prompt and non-prompt leptons.

The constituents for jet reconstruction are identified by combining measurements from both the ID and the calorimeter using a particle flow (PFlow) algorithm [90]. Jet candidates are reconstructed from these PFlow objects using the anti-k_{T} algorithm [91, 92] with a radius parameter of $R = 0.4$. They are calibrated based on jet energy scale (JES) and resolution (JER), as derived from 13 TeV data and simulation [93], such that in simulation they have on average the same energy and momentum as matched particle level jets. Only jet candidates with $p_{\mathrm{T}} > 25$ GeV and within $|\eta| < 2.5$ are selected. To reduce the effect of pile-up, each jet with $p_{\mathrm{T}} < 60$ GeV and $|\eta| < 2.4$ is required to have an origin compatible with the primary vertex, as defined by the jet vertex tagger (JVT) [94] criteria. A set of quality criteria is also applied to reject events containing at least one jet arising from non-collision sources or detector noise [95].

Jets containing b-hadrons are identified (b-tagged) via an algorithm [96] that uses a deep-learning neural network based on the distinctive features of b-hadron decays, primarily the impact parameters of tracks and the displaced vertices reconstructed in the ID. Additional input to this network is provided by discriminating variables constructed by a recurrent neural network, which exploits the spatial and kinematic correlations between tracks originating from the same b-hadron. A multivariate b-tagging discriminant value is calculated for each jet. In this search, a jet is considered b-tagged if it passes the WP corresponding to 77% average expected efficiency [3] to tag a b-quark jet in all regions except for the fake light-flavour electron control region where the 85% b-tagging efficiency WP is used. The corresponding light-jet[4] rejection factor [5] is about 40 to 192, and the charm-jet (c-jet) rejection factor is about 3 to 6. The b-tagging distribution obtained by ordering from higher to lower b-jet efficiency the resulting five exclusive bins from the four WPs corresponding to 85%, 77%, 70%, or 60% average expected efficiency to tag a b-quark jet, is referred to as pseudo-continuous b-tagging score. Each jet is assigned a pseudo-continuous b-tagging score that defines if a jet passes a given operating point but fails the adjacent tighter one. The sum of the pseudo-continuous b-tagging scores of all jets in the event is used as input to the AD discriminant described in Section 5. Correction factors derived from dedicated calibration samples enriched in b-jets, c-tagged jets, or light-tagged jets, are applied to the simulated event samples [97–99].

To uniquely identify objects, a sequential 'overlap removal' procedure is performed. If two electrons are separated by $\Delta R < 0.1$, only the one with the higher p_{T} is kept. If an electron and a muon overlap within $\Delta R < 0.1$, the muon is removed if it is reconstructed only from an ID track and calorimeter energy deposits consistent with a minimum-ionising particle (i.e. if it is 'calo-tagged'), otherwise the electron is removed. If an electron and a selected jet are found within $\Delta R < 0.2$, the jet is removed. For each electron in the event a p_{T}-dependent variable-size cone of maximum size $\Delta R = 0.4$ is defined. If a selected jet, surviving all previous overlap criteria, is found in this cone, the lepton is rejected. The same procedure is also applied between jets and muons, with the exception that, if a muon and a jet overlap with $\Delta R < 0.2$, the jet is removed, unless the number of tracks in the jet is more than two.

The missing transverse momentum $\vec{p}_{\mathrm{T}}^{\,\mathrm{miss}}$ (with magnitude $E_{\mathrm{T}}^{\mathrm{miss}}$) is defined as the negative vector sum of the p_{T} of all selected and calibrated objects in the event that satisfy the overlap removal procedure, and an additional term to account for the momenta of soft particles that are not associated with any of the selected objects [100]. This soft term is calculated from inner-detector tracks matched to the primary vertex, which makes it more resilient to contamination from pile-up interactions.

5 Search region definition

Candidate events are selected with a different trigger strategy depending on the lepton multiplicity of the event: single-lepton triggers are used to select events in 2ℓSS and 3ℓ regions, and dilepton triggers are used in 4ℓ and $\geq 5\ell$ regions, requiring the electrons or muons to satisfy identification criteria similar to those used in the offline reconstruction and isolation requirements [101, 102]. Single-electron triggers require a minimum p_{T} threshold of 24 (26) GeV in the 2015 (2016, 2017 and 2018) data-taking period(s), while single-muon triggers have a lowest p_{T} threshold of 20 (26) GeV in 2015 (2016–2018). The dielectron triggers require two electrons with minimum p_{T} thresholds ranging from 12 GeV in 2015 to 24 GeV in 2017–2018, whereas the dimuon triggers use asymmetric p_{T} thresholds for leading (subleading) muons:

[3] Efficiencies for tagging b-jets are determined for jets with $p_{\mathrm{T}} > 20$ GeV and $|\eta| < 2.5$ in simulated $t\bar{t}$ events.
[4] 'Light jet' refers to a jet originating from the hadronisation of a light quark (u, d, s) or a gluon.
[5] The rejection factor is defined as the reciprocal of the efficiency.

18 (8) GeV in 2015 and 22 (8) GeV in 2016–2018. Finally, an electron+muon trigger requires events to have an electron candidate with a 17 GeV threshold and a muon candidate with a 14 GeV threshold for all periods. In the offline selection, leptons are required to match, with $\Delta R < 0.15$, the corresponding leptons reconstructed by the trigger and to have a p_{T} exceeding the trigger p_{T} threshold by at least 1 GeV.

Events containing at least four light leptons are selected and further divided into three orthogonal final states:

- 4ℓ $Q = 0$: four light leptons with a total charge of zero,
- 4ℓ $Q = \pm 2$: four light leptons with a total charge of ± 2, and
- $\geq 5\ell$: five or more light leptons.

The total number of observed events in 4ℓ $Q = 0$, 4ℓ $Q = \pm 2$, and $\geq 5\ell$ are 4097, 77, and 21, respectively.

Two searches are defined: one following a model-independent strategy consisting of 'discovery regions', and the other designed to be sensitive to the benchmark models described in Section 1, consisting of 'benchmark regions'. The different event splitting in each of these regions is described below. However the events in the sum of all discovery regions are the same as the events in the sum of all benchmark regions. Regions are defined through a trade-off between various considerations. First, the sensitivity to specific multilepton final states, covering possible combinations of number of leptons, lepton flavour, number of b-jets, number of same-flavour opposite-sign (SFOS) lepton pairs, and those consistent with a Z boson decay. Second, the granularity of the region splitting is limited by the available MC background simulated events to ensure a reliable background estimation in all regions. Third, the reduction of the look-elsewhere effect in the model-independent search is achieved with a smaller region multiplicity than in the model-dependent search.

In the 4ℓ $Q = 0$ channel, discovery regions are defined by the number of SFOS lepton pairs, and by the number of SFOS lepton pairs with an invariant mass within 10 GeV of the nominal Z boson mass, referred to as a Z boson candidate, allowing the separation of on-shell Z boson processes from off-shell and photon backgrounds. The benchmark regions have the same categorisation of events as the discovery regions, with further splitting based on the b-tagged jet multiplicity (zero or ≥ 1 b-jets) and the number of electrons and muons that are not part of a Z boson candidate ($N_e > N_\mu$, $N_e = N_\mu$ and $N_\mu > N_e$). The b-jet-based classification improves the discrimination against top-quark processes. The main background contributions originate from ZZ and $t\bar{t}Z/\gamma^*$ processes.

In the 4ℓ $Q = \pm 2$ channel, where the main background processes contain at least one non-prompt lepton, the discovery region is not split. The benchmark regions are split into events with zero or ≥ 1 b-jets, and these categories are further divided into three sub-regions based on N_e and N_μ as done in the $Q = 0$ channel. The Z boson candidates are defined as in the 4ℓ $Q = 0$ channel but without requiring the leptons to have opposite charge.

In the $\geq 5\ell$ channel, the discovery regions are defined by the number of Z boson candidates: 5ℓ 0Z and 5ℓ $\geq$1Z. To define the benchmark regions, events are further split by the presence of b-jets (0 or ≥ 1 b-jets) and by lepton flavour when there are no b-tagged jets, due to the limited number of data events in b-tagged regions. The main background processes are VVV, $t\bar{t}H$, and events with at least one non-prompt lepton.

Five control regions (CRs) orthogonal to the discovery/benchmark regions and among each other are defined to fit the normalisation of the leading backgrounds. A region enriched in $W^{\pm}Z$ and $t\bar{t}Z$ is defined ('WZ/ttZ') by selecting events with three leptons, from which one SFOS lepton pair is required to be compatible with a Z boson, $|m^{\mathrm{SFOS}}_{\ell^+\ell^-} - m_Z| < 10$ GeV. Events in the WZ/ttZ CR are also required to have at

least one jet and zero b-jets satisfying the 77% WP. A region enriched in photon conversions ('Conversions') from $Z \to \mu\mu\gamma^{(*)}(\to ee)$ is defined by requiring three leptons (two muons and one electron), from which the electron must fulfil the material conversion or internal conversion candidate requirements. Events in the Conversion CR are also required to have no SFOS lepton pairs compatible with a Z boson, the three lepton invariant mass fulfilling $|m_{3\ell} - m_Z| < 10$ GeV, and zero b-jets satisfying the 77% WP. For the two CRs enriched in HF non-prompt leptons, events with two same-sign leptons are selected, requiring the leading lepton to additionally pass the non-prompt-lepton BDT WP, and the same-sign lepton pair to be μe with the electron being the sub-leading lepton and passing the QMisID BDT requirement (CR enriched in non-prompt electrons from HF hadron decays, 'HFe') or $\mu\mu$ (CR enriched in non-prompt muons from HF hadron decays, 'HFμ'). Additionally, at least two jets and exactly one b-jet satisfying the 77% WP are required. Finally, a CR enriched in non-prompt electrons from LF hadron decays ('LFe') consists of events with 3ℓ, from which two same-flavour muons with an invariant mass consistent with that of a Z boson plus one additional electron are required. In addition, the $E_{\mathrm{T}}^{\mathrm{miss}}$ has to be lower than 20 GeV to reduce the $W^{\pm}Z$ background contamination and zero b-jets satisfying the 85% WP are required. The contamination in the control regions from the non-excluded signal benchmark models described in Section 1 is negligible.

6 Anomaly detection

An event-level AD technique is used based on normalising flows to enhance the sensitivity to BSM physics in a model-independent way. The AD technique is designed to be sensitive to out-of-distribution data (outlier detection), and it is thus sensitive to BSM physics populating low probability regions of phase space. Anomalies are defined with respect to a reference distribution, for which the simulated SM background is used.

To build an anomaly score that is sensitive to rare (kinematically extreme) events, the normalising flows are used to directly evaluate the probability density of the MC background. Normalising flows are an unsupervised machine learning model typically used to model complex distributions, allowing efficient and exact density estimation [103]. To do so, flows employ a series of invertible bijective functions to transform from a closed-form latent distribution to a target distribution, allowing the explicit calculation of the probability density. In this work, a Real-valued Non-Volume Preserving flow (RealNVP) is used with the standard choice of a Normal distribution in the latent space [104]. In order to use the normalising flows in the context of AD, the flow is trained on the background MC prediction only, using the background probability density $p(x)$, where x is the set of input variables, as the target distribution within the search regions. Once learned, the evaluated probability is then transformed to give the anomaly score according to:

$$s(x) = \frac{\log p(x) - \log p_{\max}}{\log p_{\min} - \log p_{\max}}, \tag{1}$$

where $p_{\min}$ and $p_{\max}$ are the minimum and maximum probability densities, respectively, evaluated from the MC background dataset. The transformation is chosen such that the log probability is scaled to be within the range [0,1] with anomalous events at higher score values.

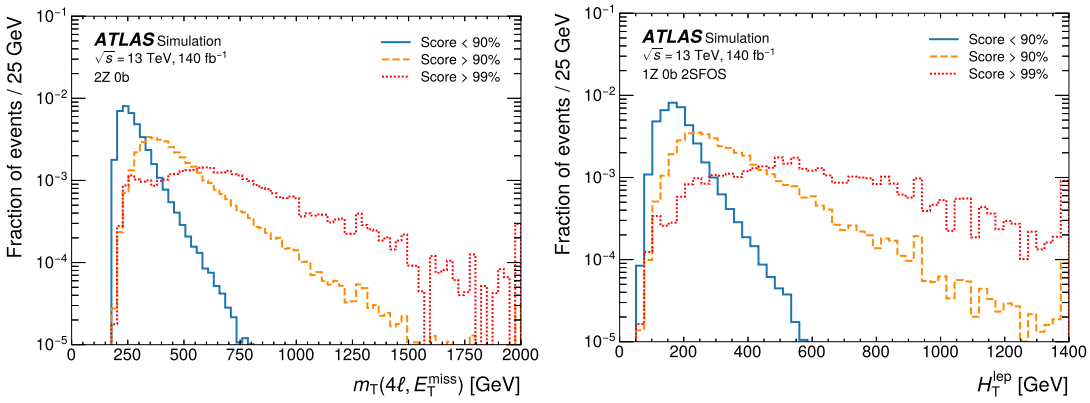
The choice of input variables used to calculate the background density is crucial for defining the space of BSM models that the AD is sensitive to. Physically motivated high-level variables are chosen which can provide sensitivity to a wide range of BSM models while also aiding in the characterisation of any excess that may be found. Table 1 shows the training variables used in each search region. The pairing of leptons with the closest invariant mass to that of the Z boson is denoted by the label Z ("lepton pair

closest to Z boson"), and the remaining pair of leptons amongst the four leptons in the event ("lepton pair second-closest to Z boson") is denoted by the label $\ell\ell$. In the $\geq 5\ell$ region, a reduced number of input variables are used due to the relatively small sample size of the simulated events and the training is performed only on events with at least one Z boson candidate. No AD is applied to $\geq 5\ell$ 0Z region, where event counting is used instead.

Table 1: A summary of the input variables used for training the normalising flows for AD in the 4ℓ $Q = 0$, 4ℓ $Q = \pm 2$, and $\geq 5\ell$ regions. Each variable is scaled to mean zero and unit variance before being used as training data. The "lepton pair closest to Z boson" is given by the SFOS lepton pair with invariant mass closest to 91.2 GeV, with the remaining pair of leptons amongst the four leptons in the event referred to as the "lepton pair second-closest to Z boson".

Training variable	Description
	Input to 4ℓ $Q = 0$, 4ℓ $Q = \pm 2$, and $\geq 5\ell$ 1Z
$H_{\mathrm{T}}^{\mathrm{lep}}$	Sum of transverse momenta of leptons
$H_{\mathrm{T}}^{\mathrm{jets}}$	Sum of transverse momenta of jets
$E_{\mathrm{T}}^{\mathrm{miss}}$	Missing transverse energy
N_{jets}	Number of jets
$p_{\mathrm{T}}(Z)$	Transverse momentum of lepton pair closest to Z boson
	Input to 4ℓ $Q = 0$ and 4ℓ $Q = \pm 2$
$p_{\mathrm{T}}(\ell\ell)$	Transverse momentum of lepton pair second-closest to Z boson
$m(Z)$	Invariant mass of lepton pair closest to Z boson
$m(\ell\ell)$	Invariant mass of lepton pair second-closest to Z boson
$m^{\mathrm{high}}(3\ell)$	Largest invariant mass of lepton pair closest to Z boson and another lepton
$m^{\mathrm{low}}(3\ell)$	Smallest invariant mass of lepton pair closest to Z boson and another lepton
$m(4\ell)$	Invariant mass of four-lepton system
$m_{\mathrm{T}}(4\ell, E_{\mathrm{T}}^{\mathrm{miss}})$	Transverse mass of four leptons and $E_{\mathrm{T}}^{\mathrm{miss}}$
$m_{\mathrm{T}}(Z, E_{\mathrm{T}}^{\mathrm{miss}})$	Transverse mass of lepton pair closest to Z boson and $E_{\mathrm{T}}^{\mathrm{miss}}$
$m_{\mathrm{T}}(\ell\ell, E_{\mathrm{T}}^{\mathrm{miss}})$	Transverse mass of lepton pair second-closest to Z boson and $E_{\mathrm{T}}^{\mathrm{miss}}$
$\sum_{i=1}^{\mathrm{jets}} \mathrm{pcb}_i$	Sum of pseudo-continuous b-tagging score

The same AD training is used for the model-dependent and independent analyses. Normalising flows are trained in each of the discovery regions. In the 4ℓ regions the flows are trained in two sub-regions, after splitting events according to the presence or absence of b-jets. The anomaly score distributions are then merged into one distribution for the model-independent analysis, while they are used separately for the model-dependent analysis. The `PyTorch` library was used to train the normalising flows used in this work, and the `normflows` package used to define the architecture of the flows [105, 106]. The flows are made up of eight affine coupling layers, each containing two hidden layers of fully connected neural networks (FCN), each with 64 nodes. Each FCN uses the `Tanh` activation function, and the parameters of the flows are initialised to zero. The Adam optimiser [107] is used within back-propagation, along with a small weight decay of 10^{-4} (an L2 regularisation on the model weights). Trainings are performed with a fixed learning rate of 10^{-4} or 10^{-5} depending on the available statistics in the region used, and with a fixed batch size of 512. The flows are trained using weighted MC events, with overall weights calculated through the combination of weights and scale factors as described in Section 4. Events with negative weights are rare and removed from the training to improve stability.



(a) (b)

Figure 2: Comparison of background shapes for (a) $m_{\mathrm{T}}(4\ell, E_{\mathrm{T}}^{\mathrm{miss}})$ in the 2Z 0b region and (b) $H_{\mathrm{T}}^{\mathrm{lep}}$ in the 1Z 0b 2SFOS region, considering various requirements on the anomaly score corresponding to the specified background rejection cuts. The last bin contains the overflow.

Once the final anomaly score distributions are obtained, two different strategies are used to bin the distribution. For the model-independent search, background rejection points of 90%, 99% and 99.9% are used to define overlapping discovery signal bins. Each discovery signal bin is required to have at least 0.1 expected background events and less than 20% MC statistical uncertainty, or otherwise the bin is dropped. Discovery regions where the 90% bin is dropped use a 50% background rejection point, as long as the above criteria on background events and statistical uncertainty are fulfilled; otherwise, no AD is used in the corresponding region. The remaining low-anomaly score distribution is used as a region for measuring background normalisation effects. For the model-dependent search, the most sensitive bin is defined by tightening the selection on the anomaly score until both threshold criteria on the 0.1 background and 20% MC statistical uncertainty are satisfied. From there, successive bins are defined such that the background yield increases in each bin by a factor of four until the entire distribution is binned. This results in distributions with higher granularity at high-anomaly score, and conversely low granularity at low-anomaly score.

In order to quantify which input features the AD technique is most sensitive to, the distortion of the kinematic variables is quantified after applying a series of cuts to the anomaly score. For this purpose, the Energy Distance [108] is calculated between each input variable after separating by low- and high-anomaly score. Figure 2 shows two example input variable distributions and the distortions after applying the specified background rejection cut to the anomaly score. The most impactful input variables are typically $m_{\mathrm{T}}(4\ell, E_{\mathrm{T}}^{\mathrm{miss}})$, $m(\ell\ell)$, $p_{\mathrm{T}}(Z)$, $m(4\ell)$, and $H_{\mathrm{T}}^{\mathrm{lep}}$.

Two distinct fit setups, as defined in Section 9, are used to perform the model-independent and model-dependent searches, as illustrated schematically in Figure 3. Both searches share the same five control regions ('HFe', 'HFμ', 'LFe','Conversions','WZ/ttZ'; coloured in light blue in Figure 3). The model-independent search includes ten additional low-anomaly score discovery regions ('Discovery regions'; coloured in darker blue in Figure 3 (left)). These correspond to the pre-selected events categorised following the discovery region definitions in Section 5, not passing the discovery signal bin anomaly score cuts (denoted as "<90%" or "<50%"). The low-anomaly score discovery regions 4ℓ $Q = 0$ 1Z 2SFOS and 4ℓ $Q = 0$ 2Z are further split in events with zero or at least one b-jet. Each layer in Figure 3 (left)

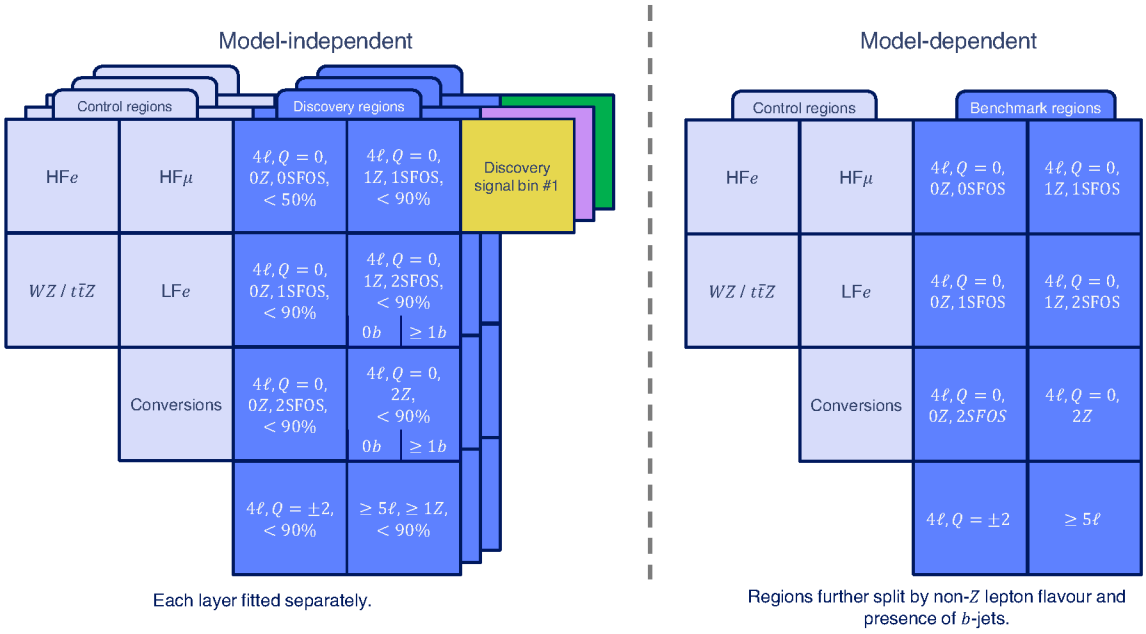


Figure 3: Illustrative sketch of the control regions and (left) discovery or (right) benchmark regions in the (left) model-independent or (right) model-dependent search. For the model-independent scenario, the discovery regions correspond to low-anomaly score regions fitted together with a high-anomaly score discovery signal bin at a time, illustrated with different layers. The <90% (<50%) label corresponds to the requirement on the anomaly score to be below the 90% (50)% background rejection point. For the model-dependent scenario, all benchmark regions are used simultaneously in a single profile likelihood fit to data, illustrated with one single layer.

represents the model-independent fit performed with the five control regions, the ten low-anomaly score discovery regions, and one discovery signal bin at a time. The discovery signal bin (the stack of differently coloured boxes in Figure 3 (left)) is defined by the discovery region selection and the cut at the optimised background rejection value ">99.9/99/90/50%". In total there are 16 discovery signal bins corresponding to 16 different fits. Fitting each discovery signal bin allows to probe BSM physics in different multilepton final states. The model-dependent search includes the same pre-selected events as the model-independent search but additionally splitting them according to the flavour of the non-Z leptons and the presence of 0 or ≥ 1 b-jets ('Benchmark regions'; coloured in darker blue in Figure 3 (right)). A single fit per benchmark signal hypothesis is performed with the five control regions and 32 benchmark regions (and thus only one layer is displayed in Figure 3 (right)), fitting the anomaly score distribution in all regions except in the $\geq 5\ell$ 0Z regions, where the total event yield is used instead.

7 Background estimation

All background processes are estimated by using the simulation samples described in Section 3. Before the simultaneous fit to data, the event kinematics of the simulated $t\bar{t}$ and VV backgrounds require dedicated corrections derived from data control samples to better describe the data. During the simultaneous fit to data discussed in Section 9, the yields of ZZ with additional light-flavour jets with zero, one or two on-shell Z boson candidates (ZZ_{0Z} + LF, ZZ_{1Z} + LF, ZZ_{2Z} + LF), ZZ with additional heavy-flavour

jets (ZZ + HF), $W^{\pm}Z$ with additional light- and heavy-flavour jets ($W^{\pm}Z$ + LF, $W^{\pm}Z$ + HF), $t\bar{t}Z$, and non-prompt-lepton backgrounds, are adjusted via normalisation factors included in the likelihood fit, as described in Section 9.

The main background contributions with prompt leptons in the regions with $\geq 4\ell$ originate from ZZ, $t\bar{t}Z/\gamma^*$, and VVV production. Smaller contributions originate from the following rare processes: $t\bar{t}H$, $t\bar{t}t\bar{t}$, tZq, tW, tWZ, $t\bar{t}WW$, and $t\bar{t}t$ production.

A data-driven correction to the VV jet multiplicity spectrum is derived from a $W^{\pm}Z$ region enriched in $W^{\pm}Z$ + LF jets, following the procedure described in Ref. [19]. The WZ/ttZ CR is used in the likelihood fit to improve the prediction of the background contribution from the $W^{\pm}Z$ + LF jets, $W^{\pm}Z$ + HF jets, and $t\bar{t}Z/\gamma^*$ processes. The number of b-jets provides good discrimination in the WZ/ttZ CR between the $W^{\pm}Z$ and $t\bar{t}Z/\gamma^*$ processes and is the variable used in this region in the fit. The low-anomaly-score regions, as defined in Section 6, are enriched in ZZ background and provide constraints on the ZZ background process, where different normalisation factors are assigned to the contributions from ZZ + LF jets (ZZ_{0Z} + LF, ZZ_{1Z} + LF, ZZ_{2Z} + LF), and ZZ + HF jets. The splitting of the low-anomaly score discovery regions 4ℓ $Q = 0$ 1Z 2SFOS and 4ℓ $Q = 0$ 2Z based on the b-jet multiplicity allows further discrimination between ZZ + LF jets against $t\bar{t}Z$ and ZZ + HF jets. The modelling of the dominant background processes was validated using events with low-anomaly scores. Figure 4 shows the modelling of some of the input variables to the AD training in regions enriched in ZZ and $t\bar{t}Z/\gamma^*$ processes.

Non-prompt leptons originate from material conversions, LF and HF hadron decays, or the improper reconstruction of other particles, and their relative composition depends on the lepton quality requirements and event categories. These backgrounds are estimated from simulation, with the normalisation determined by the likelihood fit. The main contribution to the non-prompt-lepton background is from $t\bar{t}$ production, with smaller contributions from V+jets, single-top-quark, $t\bar{t}W$, and $W^{\pm}Z$ processes. A correction based on theoretical predictions at NNLO QCD and NLO EW [109] is applied to the $t\bar{t}$ process to improve the distributions of the p_{T} and of the invariant mass of the $t\bar{t}$ system ($m(t\bar{t})$) at parton level. The non-prompt leptons in the simulated samples are labelled according to whether they originate from HF or LF hadron decays, or from a material conversion candidate. The HF category includes leptons from both bottom and charm decays. In the discovery/benchmark regions there are additional contributions from backgrounds with more than one non-prompt lepton (referred to as "multifakes"). The non-prompt lepton composition in multifakes varies depending on the region, and the presence of each non-prompt lepton type is corrected with the corresponding normalisation factor.

Normalisation factors for four non-prompt-lepton background contributions (HF non-prompt electron, HF non-prompt muon, LF non-prompt electron, and electron from internal or material conversion) are estimated from the likelihood fit to data. The measured values of the six prompt-lepton and four non-prompt-lepton background normalisation factors in the fit to data for the background-only hypothesis using the CRs and the low-anomaly score discovery regions are:

$\lambda_{W^{\pm}Z\,+\,\mathrm{LF}} = 0.98 \pm 0.09$, $\lambda_{W^{\pm}Z\,+\,\mathrm{HF}} = 1.15 \pm 0.31$, $\lambda_{ZZ_{0Z}\,+\,\mathrm{LF}} = 0.87 \pm 0.07$, $\lambda_{ZZ_{1Z}\,+\,\mathrm{LF}} = 1.01 \pm 0.04$, $\lambda_{ZZ_{2Z}\,+\,\mathrm{LF}} = 1.04 \pm 0.04$, $\lambda_{t\bar{t}Z} = 1.31 \pm 0.11$, $\lambda_e^{\mathrm{heavy}} = 0.95 \pm 0.06$, $\lambda_\mu^{\mathrm{heavy}} = 0.95 \pm 0.04$, $\lambda_e^{\mathrm{light}} = 0.66 \pm 0.09$, and $\lambda_e^{\mathrm{conv}} = 1.03 \pm 0.09$.

Kinematic variables were constructed in the fake-enriched CRs in order to validate the modelling of inputs to the AD from fake processes. Figure 5 shows representative variables in the HFe CR, HFμ CR, LFe CR, and the Wγ^*/$t\bar{t}\gamma^*$ validation region, where good background modelling is seen after the fit to data. The

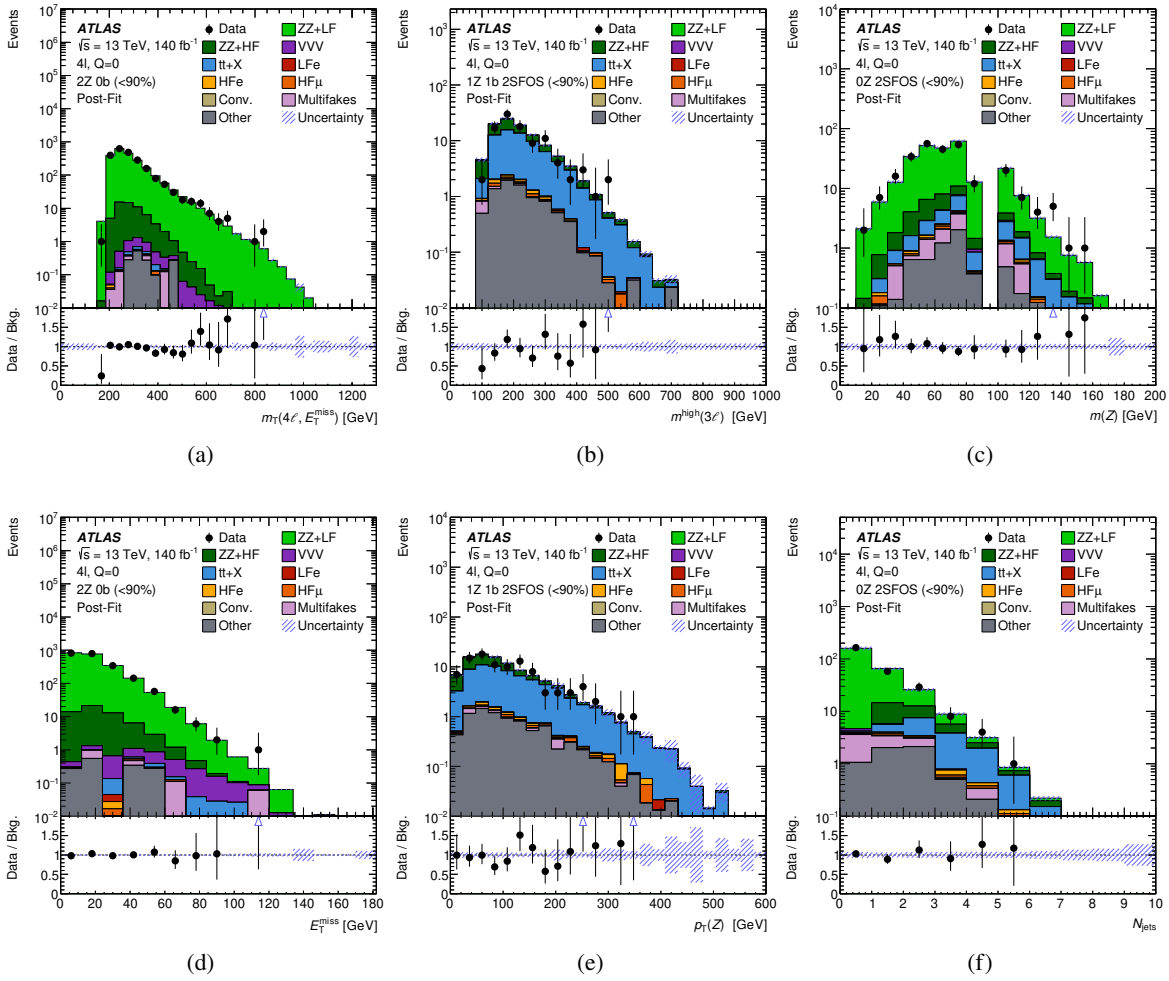


Figure 4: Comparison between data and the background prediction for the (a) $m_{\mathrm{T}}(4\ell, E_{\mathrm{T}}^{\mathrm{miss}})$, (b) $m^{\mathrm{high}}(3\ell)$, (c) $m(Z)$, (d) $E_{\mathrm{T}}^{\mathrm{miss}}$, (e) $p_{\mathrm{T}}(Z)$, and (f) N_{jets} distribution in the (a, d) 2Z 0b, (b, e) 1Z 1b 2SFOS, and (c, f) 0Z 2SFOS region, after requiring the anomaly score to be below the 90% background rejection point. The background contributions after the likelihood fit to data ('post-fit') for the background-only hypothesis are shown as filled histograms. The 'tt+X' background component includes the $t\bar{t}Z$, and $t\bar{t}H$ processes. The 'HF ℓ' ('LF ℓ') background component refers to processes containing one non-prompt light lepton from heavy-flavour (light-flavour) hadron decays. The ratio of the data to the background prediction ('Bkg.') is shown in the lower panel. The 'Other' contribution is dominated by the tWZ production. The size of the combined statistical and systematic uncertainty in the background prediction is indicated by the blue hatched band. The upward-pointing blue arrows indicate points for which the data-to-background ('Data/Bkg.') ratio exceeds the vertical range of the figure. The last bin contains the overflow.

latter validation region is defined as the WZ/ttZ CR with the exception that a Z boson candidate veto is applied. It is used to validate the modelling of the electron conversion background.

Backgrounds with leptons with the charge incorrectly assigned affect primarily the $2\ell SS$ and 4ℓ $Q = \pm 2$ channels and predominantly arise from $t\bar{t}$ production, where one electron undergoes a hard bremsstrahlung and an asymmetric conversion ($e^{\pm} \rightarrow e^{\pm}\gamma^{*} \rightarrow e^{\pm}e^{+}e^{-}$) or a mismeasured track curvature. The muon charge misassignment rate is negligible in the p_{T} range relevant to this analysis. The electron charge misassignment rate is measured in data using samples of $Z \rightarrow e^{+}e^{-}$ events reconstructed as same-charge

pairs and as opposite-charge pairs, with the background subtracted via a sideband method [87]. The charge misassignment rate is parameterised as a function of electron p_{T} and $|\eta|$. It varies from about 10^{-4} for low-p_{T} electrons ($17 \leq p_{\mathrm{T}} \leq 50$ GeV) that satisfy $|\eta| \leq 1.37$, to about 3×10^{-2} for high-p_{T} electrons ($p_{\mathrm{T}} \geq 200$ GeV) in the region $2 \leq |\eta| \leq 2.47$. To estimate the electron QMisID background in each of the corresponding event categories, the measured charge misassignment rate is then applied to data events satisfying the requirements of the $2\ell SS$ and 4ℓ $Q = \pm 2$ channels, except that the total lepton charge is required to be zero.

8 Systematic uncertainties

The search sensitivity is limited by the number of data events rather than by the systematic uncertainties in the background estimate. The uncertainty in the measurement of the combined 2015–2018 integrated luminosity is 0.83% [110], obtained using the LUCID-2 detector [26] for the primary measurements, complemented by the ones using the inner detector and calorimeters.

Uncertainties associated with the lepton selection arise from the trigger, reconstruction, identification and isolation efficiencies, and the lepton momentum scale and resolution [87, 111, 112].

Uncertainties associated with the jet selection arise from the JES, the JVT requirement and the JER [93, 94]. The JES and its uncertainties are derived by combining information from test-beam data, collision data and simulation [93]. The JES (JER) have 30 (13) components included in the fit. The uncertainties in the JES, JER and JVT increase at lower jet p_{T}. The efficiency of the flavour-tagging algorithm is measured for each jet flavour using control samples in data and in simulation. From these measurements, correction factors are derived to correct the tagging rates in the simulation [97–99]. Experimental uncertainties in these correction factors are taken as uncorrelated between b-jets, c-jets, and light-flavour jets. An additional uncertainty is assigned to account for the extrapolation of the b-tagging efficiency measurement from the p_{T} region used to determine the correction factors to regions with higher transverse momentum. Uncertainties on $E_{\mathrm{T}}^{\mathrm{miss}}$ are estimated by propagating the uncertainties on the energy and momentum scale of each of the objects contributing to its calculation, and on the soft term resolution and scale [100].

The modelling uncertainties in the main backgrounds are assessed through comparisons with alternative MC samples. Additional uncertainties are evaluated from renormalisation and factorisation scale variations by a factor of 0.5 and 2, relative to the nominal scales, for the $t\bar{t}$, Z + jets, $t\bar{t}W$, $t\bar{t}Z$, and diboson samples. An additional 20% uncertainty is assigned to the $t\bar{t}W$ electroweak contribution [113].

For the $t\bar{t}$ process, four additional uncertainties are considered related to the reweighting method itself, derived by comparing the nominal reweighted SM $t\bar{t}$ sample to a sample obtained through an alternative reweighting, where the renormalisation and the factorisation scales are separately varied by a factor of 0.5 and 2 and the reweighting is applied on the (anti-)top quark p_{T} or on the $m(t\bar{t})$ distribution independently.

All alternative $t\bar{t}$ MC samples are reweighted to the same higher-order predictions as the nominal Powheg +Pythia 8.230 MC sample. In addition to the comparison to the alternative MC sample Powheg Box +Herwig 7.1.3, the nominal predictions are also compared with those obtained from an alternative sample generated as the nominal sample but setting the $p_{\mathrm{T}}^{\mathrm{hard}}$ parameter in Pythia to 1 instead of 0 [114]. This parameter regulates the definition of the vetoed region of the showering to avoid holes or overlaps in the phase space filled by Powheg and Pythia. An uncertainty related to the choice of the h_{damp} parameter is estimated by comparing the predictions of the nominal sample to those obtained with an alternative sample with the h_{damp} parameter increased by a factor of 1.5 compared with its nominal value. Variations

in the initial-state radiation (ISR) are estimated by varying the factorisation and renormalisation scales independently up and down by a factor of two. Similarly, the uncertainty related to final-state radiation (FSR) is assessed by varying the renormalisation scale for final-state PS emissions up and down by a factor of two. Finally, the uncertainty associated with the A14 tune is derived by varying the A14 tune (Var3c), which affects the renormalisation scale variations in the ISR PS. No theory reweighting is applied to this systematic.

For the Z + jets process, the uncertainty related to the upper cut-off of perturbative calculations for PS evolution is known as the re-summation scale. This uncertainty is evaluated at truth level by varying the nominal value of 2 GeV by a factor of 4 up and $1/4$ down. Fiducial cuts are applied at truth level to define a phase space close to that used at reconstruction level in the discovery/benchmark regions where Z + jets is a dominant background. Additionally, the uncertainty related to the choice of the CKKW merging scale, i.e. the scale for calculating the overlap between jets from the ME and the PS, is derived similarly; the nominal value of 20 GeV is varied down to 15 GeV and up to 30 GeV and differences relative to the nominal distribution are evaluated at truth level.

The statistical uncertainty in the fitted parameters for the VV jet-multiplicity correction is propagated as an uncertainty in the diboson background. Finally, additional normalisation uncertainties are included for all processes whose normalisation is not obtained from the fit. In particular, for the $t\bar{t}t\bar{t}$, $t\bar{t}H$, and tZ processes, cross-section uncertainties of 20% [75], 11% [115], and 5% [116] are assigned, respectively, while for $t\bar{t}t$, tWZ, $t\bar{t}WW$, and triboson backgrounds a 50% cross-section uncertainty is assigned as a conservative estimate, since they are small backgrounds and have low impact on the search. Additional modelling uncertainties are considered for $t\bar{t}W$, $t\bar{t}H$, and $t\bar{t}t\bar{t}$ by comparing the nominal MC event generation described in Section 3 to alternative samples: Sherpa 2.2.10 ($t\bar{t}W$ and $t\bar{t}t\bar{t}$) and MadGraph5_aMC@NLO and Pythia 8 ($t\bar{t}H$).

Uncertainties in the modelling of the signal samples are evaluated from independently varying the renormalisation and factorisation scale by a factor of 0.5 and 2, relative to the nominal scales.

A systematic uncertainty of 20% is assigned to the background from electrons with a misidentified charge and accounts for the disagreement observed between the MC simulation for this background and data in the same-sign charge ee inclusive region.

9 Results

A maximum-likelihood fit is performed on all bins in the control regions and discovery/benchmark regions considered in this search as shown in Figure 3 to simultaneously determine the signal and background yields that are most consistent with the data. In the case of the model-independent fit, five cut-based control regions and ten low-anomaly score discovery regions are fitted together with one signal bin at a time (16 discovery signal bins corresponding to 16 different fits). The total event yields are used in all regions, except for the WZ/ttZ CR where the $N_{b-\text{jets}}$ distribution is used. In the case of the model-dependent fit, the same five cut-based control regions are fitted together with 32 benchmark regions. In each benchmark region, the anomaly score distribution is fitted to data with the exception of the $\geq 5\ell$ 0Z benchmark regions, where the total event yield is fitted.

The likelihood function $\mathcal{L}(\mu, \vec{\lambda}, \vec{\theta})$ is constructed as a product of Poisson probability terms over all bins considered in the search, and depends on: the signal-strength parameter, μ, a multiplicative factor applied to the predicted yield for the probed signal (model-dependent, as detailed in Section 9.2) or a dummy

signal (model-independent, as detailed in Section 9.1); $\vec{\lambda}$, the normalisation factors for several backgrounds; $\vec{\theta}$, a set of nuisance parameters (NPs), encoding systematic uncertainties in the signal and background expectations [117]. Both μ and $\vec{\lambda}$ are treated as free parameters in the likelihood fit. The NPs $\vec{\theta}$ allow variations of the expectations for signal and background according to the systematic uncertainties, subject to Gaussian or Poisson constraints in the likelihood fit. Statistical uncertainties in each bin due to the limited size of the simulated samples are taken into account by dedicated parameters using the Beeston–Barlow 'lite' technique [118].

The test statistic q_μ is defined as the profile likelihood ratio: $q_\mu = -2\ln(\mathcal{L}(\mu, \hat{\hat{\lambda}}_\mu, \hat{\hat{\theta}}_\mu)/\mathcal{L}(\hat{\mu}, \hat{\hat{\lambda}}_{\hat{\mu}}, \hat{\hat{\theta}}_{\hat{\mu}}))$, where $\hat{\mu}$, $\hat{\hat{\lambda}}_{\hat{\mu}}$, and $\hat{\hat{\theta}}_{\hat{\mu}}$ are the values of the parameters that maximise the likelihood function, and $\hat{\hat{\lambda}}_\mu$ and $\hat{\hat{\theta}}_\mu$ are the values of the parameters that maximise the likelihood function for a given value of μ. The test statistic q_μ is evaluated with the RooFit package [119]. A related statistic is used to determine the probability that the observed data are incompatible with the background-only hypothesis by setting $\mu = 0$ in the profile likelihood ratio (q_0). The p-value (referred to as p_0) representing the probability of the data being compatible with the background-only hypothesis is estimated by integrating the distribution of q_0 from background-only pseudo-experiments above the observed value of q_0. Upper limits on the signal production cross-section, calculated for either a dummy signal in the model-independent scenario or for each of the signal scenarios considered in the model-dependent scenario, are derived by using q_μ in the $\mathrm{CL_s}$ method [120, 121]. For a given signal scenario, values of the production cross-section (parameterised by μ) yielding $\mathrm{CL_s} < 0.05$ are excluded at $\geq 95\%$ CL, where $\mathrm{CL_s}$ is computed using pseudo-experiments for the model-independent scenario and the flavourful VLL model-dependent search, and the asymptotic approximation [122] for the other model-dependent signal benchmarks.

9.1 Model-independent results

Figure 6 shows the data and background prediction for the adjacent anomaly score distributions including all signal bins used. No significant deviations from the SM expectations are observed in any of the signal bins considered, with the largest excess seen in the $Q = \pm 2$ and $0Z$ 2SFOS ($> 99.9\%$) regions corresponding to 2σ local significance each. The global significance is 0.90σ and takes into account the look-elsewhere effect.

To calculate an excluded visible cross section, a dummy signal is injected into each signal bin, with a free-floating normalisation parameter (signal strength), denoted μ. The signal bin is then used along with the control regions and low-anomaly score discovery regions in a profile-likelihood fit, and a 95% confidence limit is found. The excluded visible cross section, σ_{vis}, is then given by:

$$\sigma_{vis} = \mu \frac{N_{sig}}{\mathcal{L}} \tag{2}$$

where N_{sig} is the number of injected dummy signal events and $\mathcal{L}$ is the integrated luminosity.

Figure 7 shows the expected excluded visible cross section, along with the observed excluded cross section for each model-independent signal bin. The expected significances in each of the model-independent fits to some benchmark signal models (single and doublet VLL_e and VLL_μ, flavourful VLL_e and VLL_μ, wino-like chargino and neutralino, and smuon) can be seen in Figure 8. The discovery regions with the largest sensitivity to the benchmark models are 4ℓ $Q = 0$ $0Z$ 2SFOS ($> 99.9\%$) and $\geq 5\ell$ $0Z$ for flavourful VLL_e and wino-like chargino and neutralino, 4ℓ $Q = 0$ ($> 99\%$) for $\mathrm{VLL}_\mu^{\mathrm{D}}$, and $\geq 5\ell$ $0Z$ for smuon.

The search is dominated by statistical uncertainties due to the requirement of a large lepton multiplicity: the expected limits obtained with full systematic uncertainties worsen at most 12% relative to the limits including only statistical uncertainties.

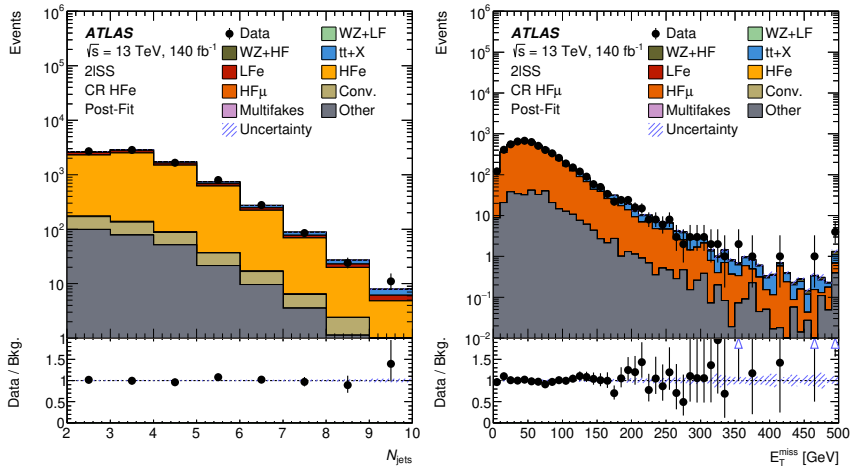
9.2 Model-dependent results

Comparisons between data and the background prediction for the anomaly score distributions used in a selection of benchmark regions are shown in Figure 9. Representative benchmark signal models are overlaid in the regions where they are expected to be dominant. No significant deviations from the SM expectations are observed in any of the benchmark regions considered. The smallest p-value for the newly probed flavourful VLL is 0.26 for a VLL_μ of mass 800 GeV and a scalar mass of 350 GeV, which corresponds to a local significance of 0.63 σ.

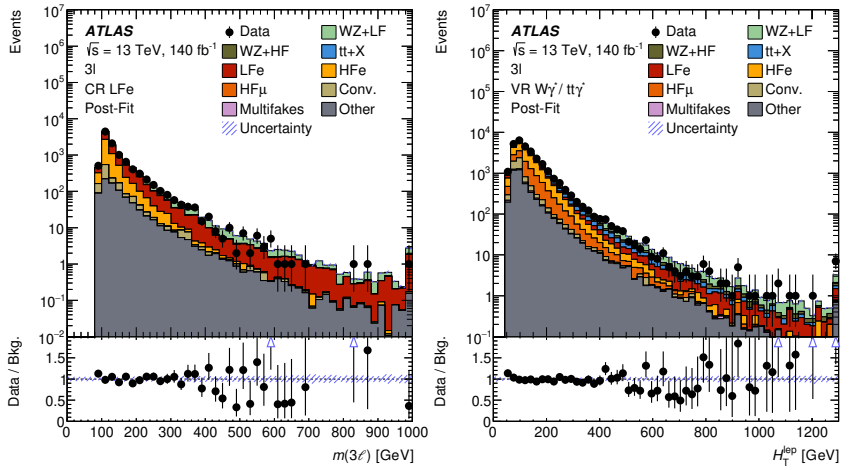
Limits at 95% CL on the cross-section of relevant benchmark signal models as a function of particle masses are set. Figures 10(a)- 10(d) show the limits on the cross-section for the models: VLL_e^{D}, $\text{VLL}_\mu^{\text{D}}$, VLL_e^{S}, and $\text{VLL}_\mu^{\text{S}}$. Limits from the dedicated ATLAS search [19] are overlaid, considering only the 4ℓ channel. The VLL_e^{S} is observed (expected) to be excluded at 95% CL for masses up to 290 (290) GeV while the VLL_e^{D} is observed (expected) to be excluded at 95% CL for masses up to 925 (880) GeV. The $\text{VLL}_\mu^{\text{S}}$ is observed (expected) to be excluded at 95% CL for masses up to 320 (320) GeV while the $\text{VLL}_\mu^{\text{D}}$ is observed (expected) to be excluded at 95% CL for masses up to 850 (925) GeV. These limits are more stringent than those from the dedicated analysis considering only the 4ℓ channel where a simple counting analysis is performed.

Figures 10(e) and 10(f) show the first ever limits on the flavourful VLL_e or VLL_μ mass and the scalar S. The flavourful VLL_e is observed (expected) to be excluded at 95% CL for masses up to 1300 (1340) GeV while the flavourful VLL_μ is observed (expected) to be excluded at 95% CL for masses up to 1280 (1375) GeV, for all allowed scalar S masses except for the lowest and highest values, where the exclusion can be up to about 50 GeV weaker.

Figure 11 shows the limits on the supersymmetric models considered, wino-like chargino and neutralino, and smuon. Wino-like charginos are observed (expected) to be excluded at 95% CL for masses up to 1600 (1600) GeV. Smuon masses up to 495 (530) GeV are observed (expected) to be excluded at 95% CL. Whereas the limits from the dedicated wino-like chargino and neutralino analysis are more stringent than the current analysis, for the smuon model this result is more sensitive for $\Delta m(\tilde{\mu}_{\text{L,R}}, \tilde{\chi}_1^0)$ larger than 140 GeV compared to the existing expected limits.



(a) (b)



(c) (d)

Figure 5: Comparison between data and the background prediction for the (a) N_{jets}, (b) $E_{\text{T}}^{\text{miss}}$, (c) $m(3\ell)$, and (d) $H_{\text{T}}^{\text{lep}}$ distribution in the (a) HFe CR, (b) HFμ CR, (c) LFe CR, and (d) the Wγ^*/$t\bar{t}\gamma^*$ validation region. The background contributions after the likelihood fit to data ('post-fit') for the background-only hypothesis are shown as filled histograms. The ratio of the data to the background prediction ('Bkg.') is shown in the lower panel. The 'tt+X' background component includes the $t\bar{t}W$, $t\bar{t}Z$, and $t\bar{t}H$ processes. The 'Other' contribution in the $2\ell SS$ regions is dominated by the $t\bar{t}$ and $t\bar{t}W$ production, and in the 3ℓ regions is dominated by the ZZ + LF production. The size of the combined statistical and systematic uncertainty in the background prediction is indicated by the blue hatched band. The upward-pointing blue arrows indicate points for which the data-to-background ('Data/Bkg.') ratio exceeds the vertical range of the figure. The last bin contains the overflow.

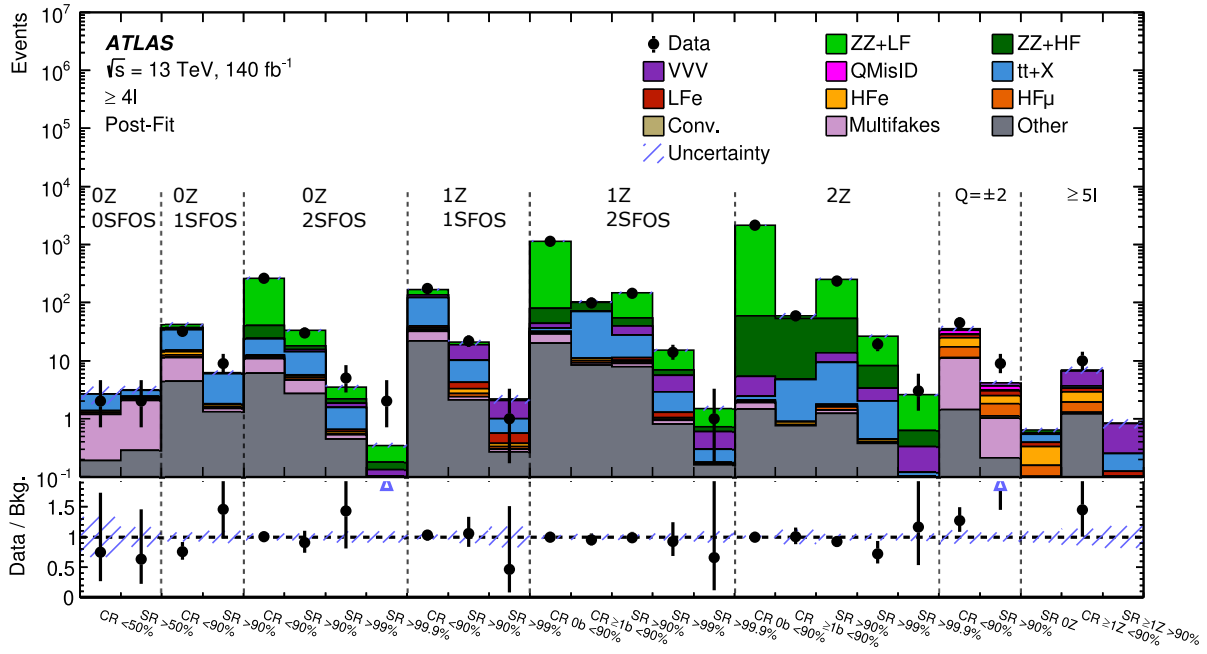


Figure 6: Comparison between data and the background prediction for the discovery regions included in the model-independent fit, after a background-only fit to data in the five cut-based control regions and ten low-anomaly score discovery regions ('post-fit'). All signal bins are shown ('SR') together with the low-anomaly score discovery regions ('CR'). The various requirements on the anomaly score corresponding to the specified background rejection cuts (99.9/99/90/50%) are shown for all the applicable SRs and CRs. The lower panels show the ratio of data to the background estimate ('Bkg'). The 'tt+X' background component includes the $t\bar{t}Z$ (4ℓ only) and $t\bar{t}H$ processes. The 'Other' contribution is dominated by the VH process. The size of the combined statistical and systematic uncertainty in the background prediction is indicated by the blue hatched band. The upward-pointing blue arrows indicate points for which the data-to-background ('Data/Bkg.') ratio exceeds the vertical range of the figure.

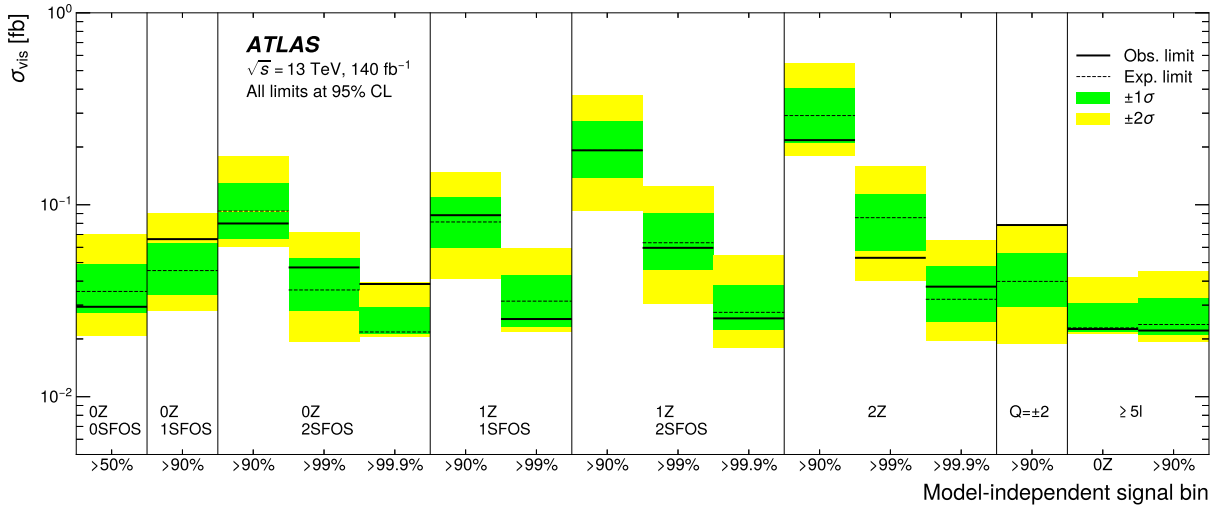


Figure 7: Observed and expected excluded visible cross section limits, σ_{vis} for the model-independent regions. The various requirements on the anomaly score corresponding to the specified background rejection cuts (99.9/99/90/50%) are shown for all the applicable regions.

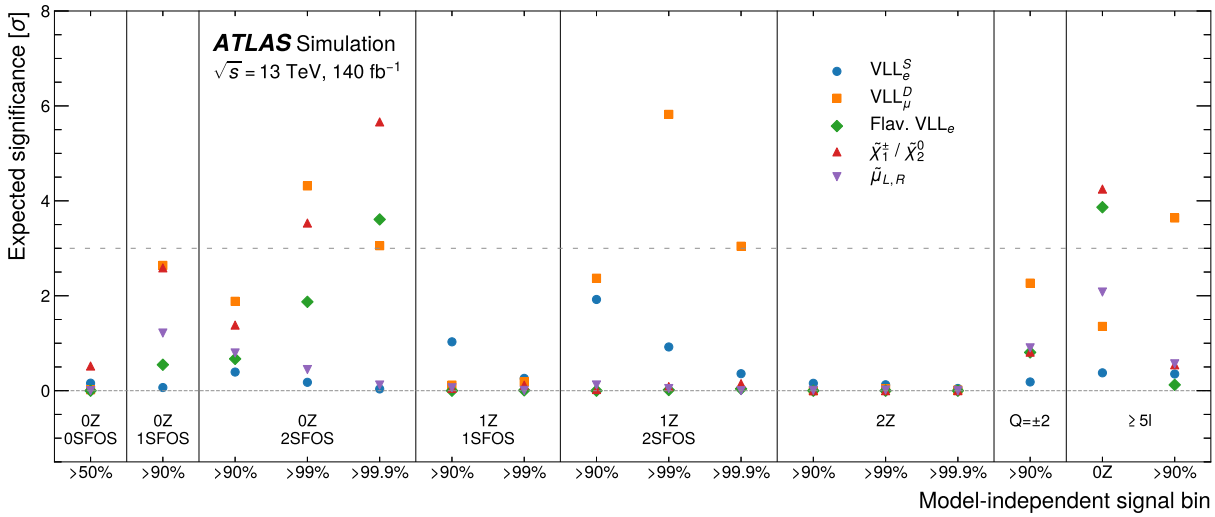


Figure 8: Expected significance in the model-independent regions to the benchmark signal models: $\mathrm{VLL}_e^{\mathrm{S}}$ with a mass of 200 GeV, $\mathrm{VLL}_\mu^{\mathrm{D}}$ with a mass of 600 GeV, flavourful VLL_e with a mass of 1200 GeV and a scalar S mass of 550 GeV, wino-like chargino with a mass of 1300 GeV and a neutralino mass of 800 GeV, and smuon with a mass of 350 GeV and a neutralino mass of 250 GeV. The various requirements on the anomaly score corresponding to the specified background rejection cuts (99.9/99/90/50%) are shown for all the applicable regions.

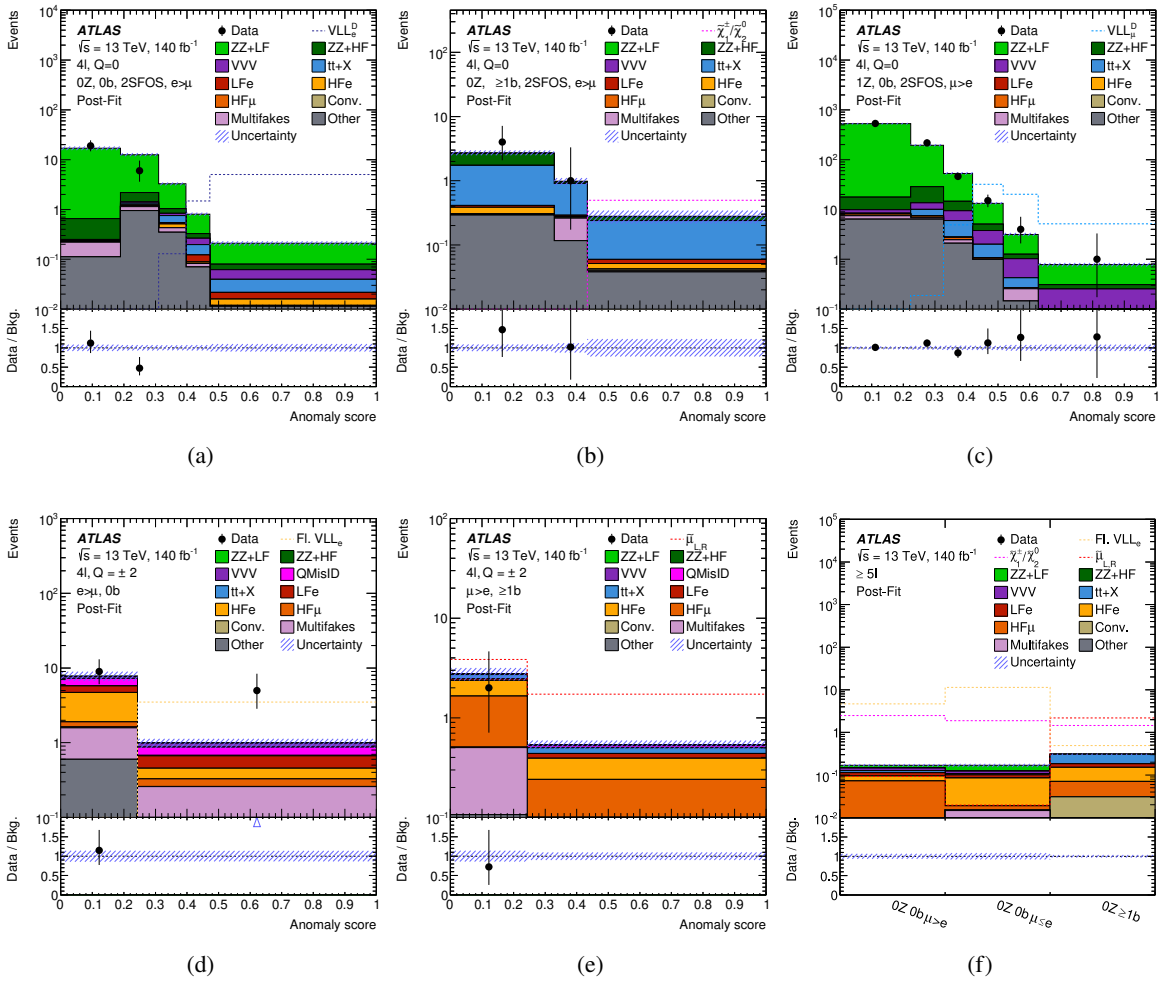


Figure 9: Comparison between data and the background estimate for the anomaly score distribution used in different benchmark regions, after a background-only fit to data ('post-fit'): (a) 4ℓ $Q = 0$ 0Z 0b 2SFOS $e > \mu$, (b) 4ℓ $Q = 0$ 0Z ≥1b 2SFOS $e > \mu$, (c) 4ℓ $Q = 0$ 1Z 0b 2SFOS $\mu > e$, (d) 4ℓ $Q = \pm 2$ 0b $e > \mu$, (e) 4ℓ $Q = \pm 2$ ≥1b $\mu > e$, and (f) the three $\geq 5\ell$ regions: 0Z 0b $\mu > e$, 0Z 0b $e \geq \mu$, and 0Z ≥1b, defined without AD. Distributions for one flavourful VLL_e signal point for a VLL mass of 1 TeV and scalar of 550 GeV, a wino-like chargino and neutralino signal point of mass 1.3 TeV, and a smuon signal point of mass 350 GeV and neutralino mass of 250 GeV are overlaid for comparison. The lower panels show the ratio of data to the background estimate ('Bkg.'). The 'tt+X' background component includes the $t\bar{t}Z$ (4ℓ only) and $t\bar{t}H$ processes. The 'Other' contribution is dominated by the VH process. The size of the combined statistical and systematic uncertainty in the signal-plus-background prediction is indicated by the blue hatched band. The upward-pointing blue arrow indicates a point for which the data-to-background ('Data/Bkg.') ratio exceeds the vertical range of the figure.

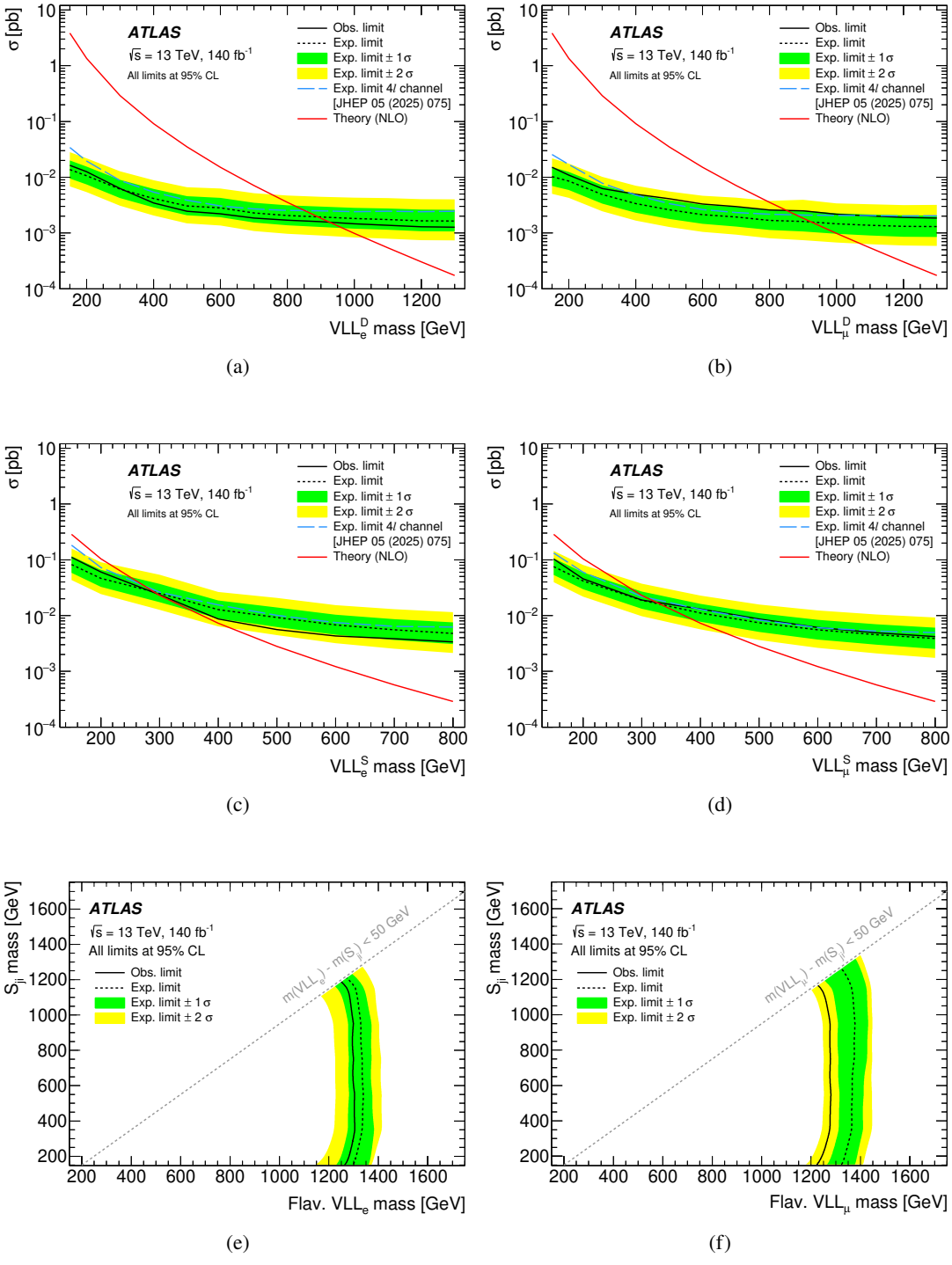
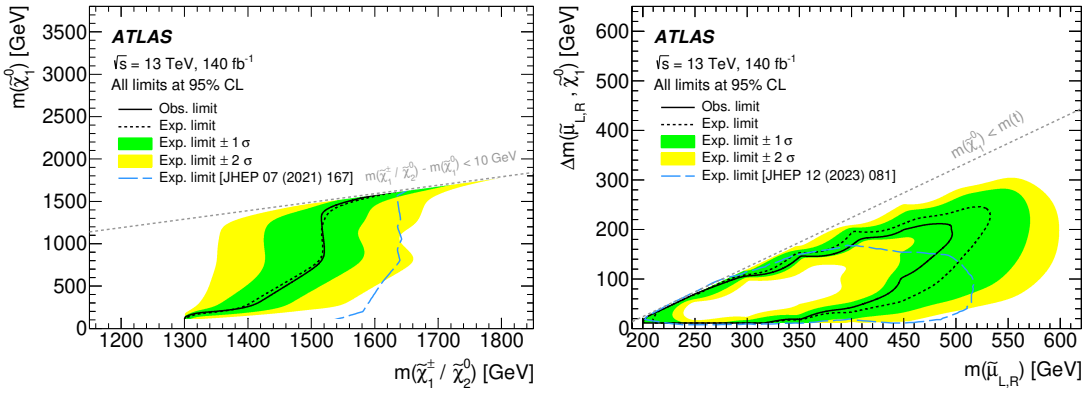


Figure 10: Combined observed and expected limits at 95% CL on the cross-section (σ) as a function of the VLL mass for the (a) VLL_e^{D}, (b) $\text{VLL}_\mu^{\text{D}}$, (c) VLL_e^{S}, (d) $\text{VLL}_\mu^{\text{S}}$ models, and on the plane of the S_{ji} mass versus the VLL mass for the (e) flavourful VLL_e, and (f) flavourful VLL_μ models. The expected limits from the dedicated ATLAS search [19], considering only the 4ℓ channel, are overlaid in dashed grey lines in (a-d). The inner and outer bands around the expected limit are the $\pm 1\sigma$ and $\pm 2\sigma$ variations including all uncertainties, respectively.



(a) (b)

Figure 11: Combined observed and expected limits at 95% CL for the (a) wino-like chargino and neutralino, and (b) smuon models, as a function of the masses of $\tilde{\chi}_1^{\pm}/\tilde{\chi}_2^0$ and $\tilde{\chi}_1^0$, and $\tilde{\mu}_{\mathrm{L,R}}$ and $\Delta m(\tilde{\mu}_{\mathrm{L,R}}, \tilde{\chi}_1^0)$, respectively. The expected limits from the dedicated ATLAS searches [21, 22] are overlaid in dashed grey lines. The inner and outer bands around the expected limit are the $\pm 1\sigma$ and $\pm 2\sigma$ variations including all uncertainties, respectively.

10 Conclusions

A model-independent search for BSM physics with anomaly detection techniques is presented. The search is based on a data sample of proton–proton collisions recorded at $\sqrt{s}$ = 13 TeV by the ATLAS detector during Run 2 of the LHC, corresponding to an integrated luminosity of 140 fb^{-1}. The search is performed in final states with ≥ 4 light leptons (e, μ). The use of anomaly detection optimises the sensitivity of the signal regions to Beyond the Standard Model physics without assuming a specific model. A model-dependent analysis is also performed to demonstrate the sensitivity of the anomaly detection technique with respect to a selection of benchmark models. The dominant backgrounds originate from ZZ, $t\bar{t}Z/\gamma^*$, and VVV production, as well as SM processes with fake leptons, and are estimated from Monte-Carlo simulation and normalised to data in a simultaneous fit. The data are found to be consistent with the Standard Model predictions and exclusion limits are set on the visible cross section for each model-independent signal region. Additionally, exclusion limits on the mass of vector-like leptons, wino-like charginos and neutralinos, and smuons are set in the model-dependent analysis using the same anomaly detection discriminant as with the model-independent search, with a different event categorisation. The expected exclusion limits are generally competitive to the ones from dedicated searches, in some cases improving the sensitivity in corners of the available phase space. Exclusion limits are set on the flavourful VLL mass for the first time, excluding flavourful VLL$_e$ (VLL$_\mu$) masses up to 1300 (1280) GeV.

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