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Search for non-resonant Higgs boson pair production in the $2b + 2\ell + E_{\mathrm{T}}^{\mathrm{miss}}$ final state in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

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Abstract: A search for non-resonant Higgs boson pair (HH) production is presented, in which one of the Higgs bosons decays to a b-quark pair ($b\bar{b}$) and the other decays to WW^*, ZZ^*, or $\tau^+\tau^-$, with in each case a final state with $\ell^+\ell^-+$ neutrinos ($\ell = e, \mu$). The analysis targets separately the gluon-gluon fusion and vector boson fusion production modes. Data recorded by the ATLAS detector in proton-proton collisions at a centre-of-mass energy of 13 TeV at the Large Hadron Collider, corresponding to an integrated luminosity of 140 fb^{-1}, are used in this analysis. Events are selected to have exactly two b-tagged jets and two leptons with opposite electric charge and missing transverse momentum in the final state. These events are classified using multivariate analysis algorithms to separate the HH events from other Standard Model processes. No evidence of the signal is found. The observed (expected) upper limit on the cross-section for non-resonant Higgs boson pair production is determined to be 9.7 (16.2) times the Standard Model prediction at 95% confidence level. The Higgs boson self-interaction coupling parameter κ_λ and the quadrilinear coupling parameter κ_{2V} are each separately constrained by this analysis to be within the ranges $[-6.2, 13.3]$ and $[-0.17, 2.4]$, respectively, at 95% confidence level, when all other parameters are fixed.

Keywords: Hadron-Hadron Scattering, Higgs Physics, Proton-Proton Scattering

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1 Introduction

The Standard Model (SM) of particle physics employs the Higgs mechanism [1–6] to formulate a theoretical model in which the weak gauge bosons (W, Z) and the fermions acquire mass. Following the discovery of the Higgs boson, referred to as H, by the ATLAS and CMS collaborations [7, 8] at the Large Hadron Collider (LHC) in 2012, one of the remaining open questions is about the structure of the Higgs potential which is still largely unconstrained. The rate of the double Higgs production (HH) process is sensitive to the trilinear Higgs self-interaction coupling λ_3, i.e. the coupling describing a vertex with three Higgs bosons interacting with one another. It is common practice to define a Higgs boson trilinear coupling modifier as the actual trilinear coupling value divided by its SM expectation value: $\kappa_\lambda \equiv \lambda_3/\lambda_3^{SM}$.

The dominant HH production process at the LHC is through gluon-gluon fusion (ggF), which involves either a top-quark box-loop (also referred to as a *box-diagram*) or decay of an off-shell Higgs boson (also referred to as a *triangle-diagram*) at lowest order; the Feynman diagrams are shown in figures 1(a) and 1(b) respectively. The *box-diagram* and *triangle-diagram* interfere destructively, leading to a small cross-section for the $gg \to HH$ processes, $\sigma_{\text{ggF}} = 31.1^{+6.7\%}_{-23.2\%}$ fb, calculated at the next-to-next-to-leading order (NNLO) and including finite top-quark mass effects for a Higgs boson mass of $m_H = 125\,\text{GeV}$ [9–16].

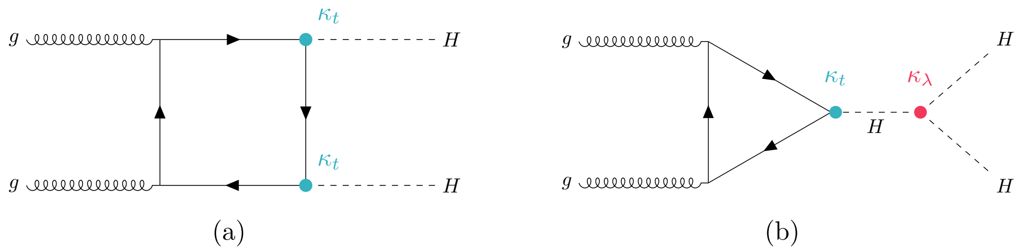

Figure 1. The leading order (LO) Feynman diagrams for the gluon-gluon fusion process of Higgs boson pair production at the LHC, where κ_λ denotes the Higgs boson trilinear coupling modifier $\kappa_\lambda \equiv \lambda_3/\lambda_3^{SM}$ and κ_t the coupling modifier relative to the top-quark-Higgs-boson coupling.

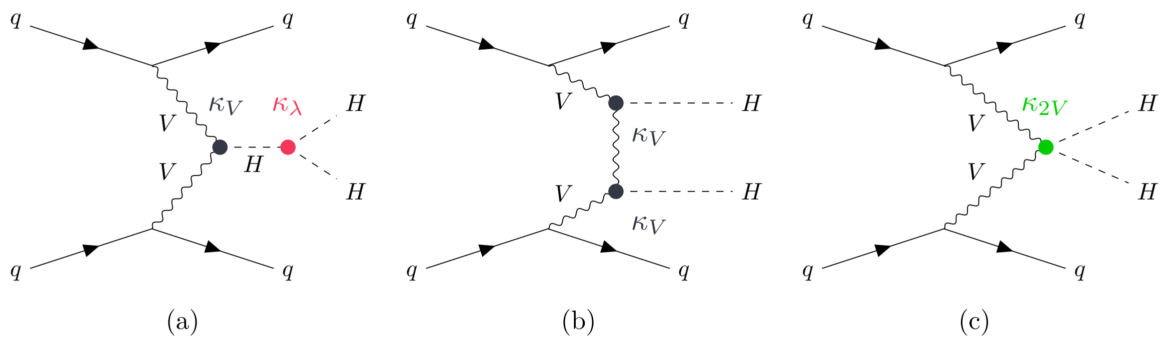

Figure 2. The LO Feynman diagrams for the vector-boson-fusion process of Higgs boson pair production, where κ_λ, κ_V, and κ_{2V} are the coupling modifiers related to the HHH, HVV, and $HHVV$ vertices.

The vector-boson-fusion (VBF) process is the sub-leading Higgs boson pair production mode, with a cross-section of $\sigma_{\text{VBF}} = 1.726 \pm 2.1\%$ fb calculated at next-to-next-to-next-to-leading order (N^{3}LO) QCD for a Higgs boson mass of $m_H = 125$ GeV [17]. The production of HH via fusion of vector bosons (V) is not only sensitive to κ_λ but also depends on the coupling modifier of the Higgs boson to vector bosons (κ_V) and on another coupling modifier related to the quartic vertex involving two vector bosons and two Higgs bosons (κ_{2V}). The corresponding diagrams are shown in figure 2.

In the presence of physics beyond the Standard Model (BSM), the HH production cross-section can be altered by modifying the value of the self-coupling λ_3, leading to values for κ_λ different from the SM prediction as discussed in refs. [18, 19]. Similarly, modifications of the coupling to vector bosons can alter κ_{2V}. Probing the Higgs boson self-coupling can therefore provide additional information about the validity of the SM.

Searches for SM HH production through the decay channels $HH \to bb\gamma\gamma$ [20], $HH \to 4b$ [21] and $HH \to bb\tau\tau$ [22] were performed using the full Run 2 dataset collected by the ATLAS experiment at $\sqrt{s} = 13$ TeV. The results from these three channels have been combined [23] to improve the search sensitivity. The observed (expected in the absence of HH production) combined upper limit on the production rate of SM Higgs boson pairs, at the 95% confidence level (CL), was found to be 2.4 (2.9) times the SM prediction. The value of κ_λ was constrained to be within the observed (expected) range $[-0.6, 6.6]$ ($[-2.1, 7.8]$) at 95% CL and the value for κ_{2V} was constrained to be within the observed (expected) range $[0.1, 2.0]$

([0.0, 2.1]) at 95% CL [23]. With searches for HH production trough the decay channels $HH \to 4b$ [24, 25], $HH \to bb\tau\tau$ [26], $HH \to WW^*/\tau\tau + WW^*/\tau\tau$ [27], $HH \to bb\gamma\gamma$ [28] and $HH \to 4\ell + bb$ [29], similar results have also been obtained by the CMS experiment; according to those results, the observed (expected) 95% upper limit on the production rate of SM Higgs boson pairs is 3.4 (2.5) times the SM prediction, κ_λ is constrained to be within the observed range of $[-1.2, 6.5]$ at 95% CL [30] and κ_{2V} is constrained to be within the observed range of $[-0.67, 1.4]$ at 95% CL [30].

This paper focuses on a data analysis using $2b + 2\ell + E_{\mathrm{T}}^{\mathrm{miss}}$ ($\ell = e, \mu$) final states arising from different HH decay channels,

$$HH \to b\bar{b} + WW^*/ZZ^*/\tau^+\tau^- \to b\bar{b} + \ell^+\ell^- + \text{neutrinos},$$

with one of the Higgs bosons decaying to a b-quark pair ($b\bar{b}$) and the other decaying to a boson (WW^*, ZZ^*) or a $\tau^+\tau^-$ pair, which further decays to $\ell^+\ell^-$ + neutrinos. The leptons can be of different flavour. The experimental signature is characterised by two b-tagged jets with the invariant mass m_{bb} close to m_H, two leptons with opposite charges, and large missing transverse energy $E_{\mathrm{T}}^{\mathrm{miss}}$ due to neutrinos escaping detection. The decay channel with a Higgs boson decaying to two Z bosons and the subsequent final state with two leptons and two quark-initiated jets from the ZZ system, $bbZZ \to bb2\ell 2q$, is also considered. Although this final state does not have $E_{\mathrm{T}}^{\mathrm{miss}}$ due to the presence of neutrinos, it can have $E_{\mathrm{T}}^{\mathrm{miss}}$ due to detector and reconstruction inefficiencies. Dominant background arises from top-quark processes ($t\bar{t}$, Wt and $t\bar{t}V$ with $V = W, Z$), and production of a Z boson associated with heavy-flavour jets (Z+HF). The search uses the full Run 2 dataset collected with the ATLAS experiment in proton-proton (pp) collisions at 13 TeV, corresponding to a total integrated luminosity of 140 fb^{-1}.

A search for HH production in the $2b + 2\ell + E_{\mathrm{T}}^{\mathrm{miss}}$ final state considering only $HH \to bbWW^*$ using the full Run 2 dataset has already been performed [31]; the work presented in this paper significantly improves the analysis techniques by optimizing a deep neural network (DNN) to better classify the $2b+2\ell+E_{\mathrm{T}}^{\mathrm{miss}}$ events into HH signal or background and considers additional decay channels, leading to a factor of two better sensitivity. Furthermore, studies of HH production through the VBF process are included for the first time in the $2b + 2\ell + E_{\mathrm{T}}^{\mathrm{miss}}$ final state. In addition, the compatibility of the data with non-SM values of the κ_λ and κ_{2V} parameters is constrained in this paper.

2 ATLAS detector

The ATLAS detector [32] 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 hadron calorimeters, and a muon spectrometer incorporating three large superconducting air-core toroidal magnets.

[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. Cylindrical 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 $\eta = -\ln\tan(\theta/2)$. Angular distance is measured in units of $\Delta R \equiv \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$.

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The inner-detector system (ID) is immersed in a 2 T axial magnetic field and provides charged-particle tracking in the range $|\eta| < 2.5$. The high-granularity silicon pixel detector covers the vertex region and typically provides four measurements per track, the first hit normally being in the insertable B-layer (IBL) installed before Run 2 [33, 34]. It is followed by the silicon microstrip 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.

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. Hadron calorimetry is provided by the steel/scintillator-tile calorimeter, segmented into three barrel structures within $|\eta| < 1.7$, and two copper/LAr hadron 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.

Interesting events are 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 [35]. The first-level trigger accepts events from the 40 MHz bunch crossings at a rate below 100 kHz, which the high-level trigger further reduces in order to record events to disk at about 1 kHz.

An extensive software suite [36] 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 samples

The analysis is based on the full Run 2 dataset collected in pp collisions at the LHC with a centre-of-mass energy of $\sqrt{s} = 13$ TeV and a 25 ns bunch crossing interval. The data used in this analysis are required to have been recorded while all relevant components of the ATLAS detector were in their nominal operating conditions [37]. The integrated luminosity of the dataset collected over the full Run 2 data-taking period and suitable for physics analysis corresponds to 140 fb^{-1} [38]. The candidate events with oppositely charged leptons are

Process	ME Generator	ME PDF	PS/UE model	UE Tune
SM HH (ggF)	Powheg Box v2	PDF4LHC15nlo	Pythia 8.244	A14
SM HH (VBF)	MadGraph5_aMC@NLO 2.7.3	NNPDF3.0nlo	Pythia 8.244	A14
$t\bar{t}$	Powheg Box v2	NNPDF3.0nlo	Pythia 8.230	A14
Single-top	Powheg Box v2	NNPDF3.0nlo	Pythia 8.230	A14
$t\bar{t} + W/Z$	MadGraph5_aMC@NLO 2.3.3	NNPDF3.0nlo	Pythia 8.210	A14
W/Z + jets	Sherpa 2.2.1	NNPDF3.0nnlo	Sherpa 2.2.1	Sherpa default
WW, WZ, ZZ	Sherpa 2.2.1/Sherpa 2.2.2	NNPDF3.0nnlo	Sherpa 2.2.1/Sherpa 2.2.2	Sherpa default
ggF, H	Powheg Box v2	NNPDF3.0nlo	Pythia 8.212	AZNLO
VBF, H	Powheg Box v2	NNPDF3.0nlo	Pythia 8.230	AZNLO
WH, ZH	Powheg Box v2	NNPDF3.0nlo	Pythia 8.230/Pythia 8.186	AZNLO
$t\bar{t}H$	Powheg Box v2	NNPDF3.0nlo	Pythia 8.230	A14

Table 1. Summary of nominal SM background processes considered in the analysis along with a description of the event generators used for matrix element (ME) generation, the set of parton distribution functions (PDF), the hadronisation, parton shower (PS) and underlying event (UE) model, and the underlying event tune.

selected based on a combination of single-lepton and di-lepton triggers.[2] The use of a given trigger depends on the flavour and the transverse momenta (p_{T}) of the two leptons in the event, and on the data-taking period. Single-lepton triggers have p_{T} thresholds between 21 GeV and 28 GeV. Di-lepton triggers are only considered if no single-lepton trigger criteria are met and have p_{T} thresholds as low as 13(9) GeV for the leading (sub-leading) lepton.

Monte Carlo (MC) simulation [39] is generally used to model the HH signal and SM background processes. The generation of the physics processes of interest, including the underlying event and immediate decays, are carried out by dedicated event generators. The generated events are then passed through a simulation of the ATLAS detector based on Geant4 [40]. Some background MC event samples, including Z+jets with $10\,\mathrm{GeV} < m_{\ell\ell} < 40\,\mathrm{GeV}$ and the $t\bar{t}$ and Wt alternative samples used for estimating systematic uncertainties, are simulated through the ATLAS fast simulation framework, Atlfast-II (AF2) [39] instead. Additionally, the effect of multiple interactions in the same and neighbouring bunch crossings (pile-up) is modelled by overlaying the simulated hard-scattering event with inelastic pp events generated with Pythia 8.186 [41] using the NNPDF2.3lo set of parton distribution functions (PDF) [42] and the A3 set of tuned parameters [43]. A summary of the event samples used for the simulation of the signal and background processes is shown in table 1.

SM HH signal events produced via the ggF production mechanism are generated with Powheg Box v2 at next-to-leading order (NLO) interfaced with Pythia 8.244 [44] using the PDF4LHC15nlo [45] PDF set and the A14 tune [46]. For parton shower variations, Herwig 7.1.5 [47] is used instead. Samples for non-SM ggF production, i.e. with $\kappa_\lambda \neq 1$ are obtained from simulated samples at different values of these coupling modifiers and combined using morphing techniques [48] with detailed validation studies of this procedure available in ref. [49]. The SM VBF HH signal samples are generated with MadGraph5_aMC@NLO 2.7.3 [50] using the NNPDF3.0nlo [51] PDF set and

[2] Distinct sets of single-lepton triggers are used for electrons and muons. Di-lepton triggers require either two electrons, two muons, or one electron and one muon.

the A14 tune [46] interfaced to Pythia 8.244 [44] with Herwig 7.2.1 [47] used for parton shower variations. As is the case in ref. [23], signal templates with coupling modifiers ($\kappa_\lambda \neq 1, \kappa_{2V} \neq 1$) are obtained by linear combination of six samples with different values for the κ_λ and κ_{2V} parameters [52]. Therefore five more independent samples with $(0,0)$, $(1,0.5)$, $(1,3)$, $(2,1)$ and $(10,1)$ are generated as well with MadGraph interfaced to Pythia8. To vary only κ_{2V}, three independent samples are enough: two more independent samples with $\kappa_{2V} = 1.5$ and $\kappa_{2V} = 2$ are generated in the same manner. The decays of bottom and charm hadrons of all SM HH signal events were performed by EvtGen 1.6.0 [53].

SM background processes are generally estimated using simulation, although the cross-sections of the dominant background components, $t\bar{t}$, Wt and Z+jets, are constrained using control regions (CRs) to better predict their contribution in the signal regions (SRs). The estimate is therefore said to be *semi-data-driven* with the normalization being constrained from data and the shape being taken from simulation. For processes not constrained from dedicated CRs, both the shape and the overall normalization are taken from simulation. In addition, the fake-lepton background is estimated in a data-driven way.

SM top-quark production ($t\bar{t}$) and the production of top-quarks in association with W bosons (Wt) contribute as a significant background contamination in the $2b + 2\ell + E_{\mathrm{T}}^{\mathrm{miss}}$ final state. At NLO, non-trivial interference arises between these two processes that may be enhanced in phase-space regions with high fractions of Wt events [54]. The two most commonly used schemes to remove the overlap between these two processes are the diagram removal (DR) and diagram subtraction (DS) schemes [55]. The former is used in the present analysis to remove the overlapping events while the latter is used to evaluate the systematic uncertainty in corresponding background event yields.

The decays of bottom and charm hadrons of all SM background events not simulated with Sherpa were performed by EvtGen 1.6.0 [53].

Production of $t\bar{t}$ events is modelled using the Powheg Box v2 [56–59] generator at NLO with the NNPDF3.0nlo [51] PDF set and the h_{damp} parameter[3] set to 1.5 times the top-quark mass [60]. The events are interfaced to Pythia 8.230 [44] to model the parton shower, hadronisation, and underlying event, with parameters set according to the A14 tune [46] and using the NNPDF2.3lo set of PDFs [42]. In order to reduce mis-modelling, events are reweighted [61] to match the predictions at NNLO QCD and NLO EW based on the true p_{T}-value of the top-quark (i.e. not the anti-top-quark) provided by the MC event samples.

Production of Wt events is modelled by the Powheg Box v2 [57–59, 62] generator at NLO in QCD using the five-flavour scheme and the NNPDF3.0nlo set of PDFs [51]. The events are interfaced to Pythia 8.230 [44] using the A14 tune [46] and the NNPDF2.3lo set of PDFs [42].

The V+jets samples ($V = W$ or Z) are simulated with Sherpa 2.2.1 [63] interfaced with NNPDF3.0nlo [42] for both the matrix element (ME) calculation and the parton shower (PS) tuning. The merging of different parton multiplicities is achieved through a matching scheme based on the CKKW-L [64, 65] merging technique using a scale parameter of $Q_{cut} = 20\,\mathrm{GeV}$.

[3]The h_{damp} parameter is a re-summation damping factor and one of the parameters that controls the matching of Powheg matrix elements to the parton shower and thus effectively regulates the high-p_{T} radiation against which the $t\bar{t}$ system recoils.

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The modelling of higher jet multiplicities relies on the parton shower algorithm. The parton shower and underlying event models used are the ones provided internally by SHERPA. The SHERPA 2.2.1 generator adopts a full 5-flavour scheme, with massless b- and c-quarks in the matrix elements, while massive quarks can be produced in the parton shower. The V+jets samples are split according to the p_{T} of the vector boson and the scalar sum of jet transverse momenta, H_{T}, of the event, introducing a cut at generation level and producing samples for different slices in $\max(H_{\mathrm{T}}, p_{\mathrm{T}}^{V})$ where p_{T}^{V} is defined as the transverse momentum of the true lepton pair from the decay of the V boson. The samples are also generated by applying different filters to select the flavour composition of the jets produced in association with the V boson.

Di-boson processes with four charged leptons, three charged leptons and one neutrino, or two charged leptons and two neutrinos are simulated with the SHERPA 2.2.2 event generator [63], and di-boson processes with leptons and jets are simulated with SHERPA 2.2.1 [63]. The matrix elements contain all diagrams with four electroweak vertices. They are calculated for up to one parton at NLO and up to three partons at LO using Comix [66] and OpenLoops [67] and merged with the SHERPA parton shower according to the ME+PS@NLO prescription [68]. The NNPDF3.0nnlo PDF set is used in conjunction with dedicated parton shower tuning developed by the SHERPA authors. The event generator cross-sections are used in this case (already at NLO).

Finally, single Higgs boson samples from all the main production modes ggF, VBF, Higgs-strahlung (WH, ZH) and associated production with a pair of top-quarks ($t\bar{t}H$) are considered. For all Higgs boson samples the normalization accounts for the decay branching ratio calculated with HDECAY [69–71] and PROPHECY4F [72–74]. Higgs boson production via gluon-gluon fusion is simulated at NNLO accuracy in QCD using POWHEG BOX v2 [57–59, 75, 76]. The simulation achieves NNLO accuracy for arbitrary inclusive $gg \to H$ observables by reweighting the Higgs boson rapidity spectrum in HJ-MINLO [77–79] to that of HNNLO [80]. The NNPDF3.0NLO [51] PDF set and the AZNLO tune [81] of PYTHIA 8.212 [44] are used. The gluon-gluon fusion prediction from the MC event samples is normalised to the N^{3}LO cross-section in QCD plus electroweak (EW) corrections at NLO [82–92]. Higgs boson production via vector-boson fusion is simulated with POWHEG BOX v2 [57–59, 93] and interfaced with PYTHIA 8.230 [44] for parton shower and non-perturbative effects, with parameters set according to the AZNLO tune [81]. The POWHEG BOX prediction is accurate to NLO and uses the NNPDF3.0NLO [51] PDF set. It is normalised to an approximate-NNLO QCD cross-section with NLO EW corrections [94–96]. Higgs boson production in association with a vector boson is simulated using POWHEG BOX v2 [57–59, 93] and interfaced with PYTHIA 8.230 [44] for parton shower and non-perturbative effects. The POWHEG BOX prediction is accurate to NLO for VH boson plus one-jet production. The loop-induced $gg \to ZH$ process is generated separately at leading order. The NNPDF3.0NLO [51] PDF set and the AZNLO tune [81] of PYTHIA 8.186 [44] are used. The MC prediction is normalised to cross-sections calculated at NNLO in QCD with NLO EW corrections for $q\bar{q}/qg \to VH$ and at NLO and next-to-leading-logarithm accuracy in QCD for $gg \to ZH$ [97–103]. The production of ttH events is modelled using the POWHEG BOX v2 [56–59, 104] generator at NLO with the NNPDF3.0NLO [51] PDF set. The events are interfaced to PYTHIA 8.230 [44] using the A14 tune [46] and the NNPDF2.3LO [51] PDF set.

4 Object definition and event selection

Proton-proton interaction vertices are reconstructed in events with at least two tracks, each with $p_{\mathrm{T}} > 0.5\,\mathrm{GeV}$. The primary hard-scatter vertex for each event is defined as the one with the highest value of the sum of squared track transverse momenta [105].

Electron candidates are reconstructed from energy deposits measured in the electromagnetic calorimeter which are matched to ID tracks [106]. They are required to satisfy $|\eta| < 2.47$, excluding the calorimeter transition region $1.37 < |\eta| < 1.52$, and have a transverse momentum $p_{\mathrm{T}} > 10\,\mathrm{GeV}$. Electron candidates are required to satisfy a "medium" identification criterion based on the use of shower shape, track-cluster matching and TRT parameters in a likelihood-based algorithm [106]. Additionally, a "loose" isolation requirement [106] is applied to electron candidates to ensure that they are well separated from other objects in the event. This requirement is based on the momentum of nearby tracks and calorimeter energy deposits within a cone around the electron candidate.

Muon candidates are reconstructed from high-quality tracks found in the MS [107]. A matching of these tracks to ID tracks is required in the region $|\eta| < 2.5$. Muon candidates are required to have $|\eta| < 2.7$ and $p_{\mathrm{T}} > 9\,\mathrm{GeV}$, and to satisfy a "medium" identification criterion [108]. Additionally, a "loose" isolation requirement [108] is imposed on muon candidates to ensure that they are well separated from other objects in the event. This requirement is based on investigating the nearby activities within a cone around the muon candidate.

Jets are reconstructed using the anti-k_t algorithm [109, 110] with a radius parameter of $R = 0.4$. It is applied to $|\eta| < 4.5$ noise-suppressed positive-energy topological energy clusters [111, 112] and charged particle tracks processed using a particle-flow algorithm [113]. Pile-up is taken into account in the formation of topological energy clusters [114]. Jet candidates are required to have $p_{\mathrm{T}} > 20\,\mathrm{GeV}$ and those with $|\eta| < 2.5$ are considered to select the candidate jets for the reconstruction of the hadronic decay of the Higgs to b-tagged jets while jets with $|\eta| > 2.5$ are considered "forward" jets. To reject jet candidates originating from pile-up interactions, they must satisfy a tight pile-up suppression requirement based on a multivariate method [115]. The method removes jets that appear to be inconsistent with the primary vertex and have $p_{\mathrm{T}} < 60\,\mathrm{GeV}$ [105]. In the end, a neural network-based b-tagging algorithm [116] is used to identify jets containing b-hadrons (b-tagged jets) at a 77% efficiency working point in simulated $t\bar{t}$ events. The rejection rate for this working point is $\sim$6 for jets originating from c-quarks and $\sim$200 for jets originating from light quarks [116].

The missing transverse momentum, $\boldsymbol{p}_{\mathrm{T}}^{\mathrm{miss}}$, the magnitude of which is denoted as $E_{\mathrm{T}}^{\mathrm{miss}}$, quantifies the amount of energy and momentum carried by invisible particles that do not interact with the detector. It is determined as the magnitude of the negative vectorial sum of the transverse momenta of the selected and calibrated physics objects, including jets, electrons, and muons, and inner detector tracks from the hard-scatter collision vertex not associated with any physics object [117].

Different reconstructed objects can share the same detector signature, leading to ambiguities in the identification of these objects. To resolve these ambiguities, as in [22], an overlap removal procedure is performed sequentially, such that only objects that survive the previous step are considered in the following steps. The steps are as follows: if any electrons

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ggF and VBF event selection cut	$bbWW$		$bb\tau\tau$		$bbZZ(\to 2\ell 2\nu)$		$bbZZ(\to 2\ell 2q)$	
	ggF	VBF	ggF	VBF	ggF	VBF	ggF	VBF
Initial number of events ($\mathcal{L} \times \sigma \times \mathcal{B}$)	70	3.9	39	2.2	3.8	0.21	18	1.0
$N_{\text{leptons}} = 2$, opposite sign, pass trigger requirement	22	0.99	8.3	0.35	1.3	0.057	3.6	0.17
$N_{b\text{-jets}} = 2$	9.8	0.39	3.7	0.14	0.57	0.022	1.6	0.067

Table 2. Cutflow for event selection using SM $gg/qq \to HH$ signal samples in various decay channels. For both ggF and VBF signal samples, the SM HH cross-section, σ, and branching ratio, $\mathcal{B}$, are assumed when computing event yields for a luminosity of $\mathcal{L} = 140\,\text{fb}^{-1}$. Efficiencies are different for $bbZZ(\to 2\ell 2\nu)$ compared to $bbZZ(\to 2\ell 2q)$ since the initial number of events considers $Z \to \tau\tau$ while the former does not.

share a track, only the highest p_{T} electron is kept. If a hadronically decaying τ-lepton candidate is within[4] $\Delta R_y = 0.2$ of any electron or muon, it is removed. If an electron and a muon share a track, the muon is kept only if it is associated with a signature in the muon spectrometer. Any jet within $\Delta R_y = 0.2$ of an electron and subsequent any electron within $\Delta R_y = 0.4$ of any jet is removed. Any jet within $\Delta R_y = 0.2$ of a muon, or having an inner detector track ghost-matched [118] to a muon within $\Delta R_y = 0.2$ of the jet, is removed if it has fewer then three associated tracks. Any muon within $\Delta R_y = 0.4$ of a jet is removed as well as any jet within $\Delta R_y = 0.2$ of a hadronically decaying τ-lepton candidate.

The analysis selects candidate events that contain exactly two opposite-charge light leptons, either electrons or muons, and exactly two b-tagged jets. While the signal processes contain sources of $E_{\text{T}}^{\text{miss}}$, an explicit selection on $E_{\text{T}}^{\text{miss}}$ is not performed, to ensure high training statistics available for the MVA discriminants. To suppress the contribution of misidentified jets, the analysis excludes events that contain jets satisfying one of the bad jet criteria [115]. The yields of the ggF and VBF signal samples at different preselection steps are summarized in table 2; about an order of magnitude of reduction in the event yields is observed from this initial selection.

The events that satisfy the preselection criteria are further divided into two categories: the signal region (SR) and dedicated background control regions (CRs) for Z plus heavy flavour jets (Z+HF), $t\bar{t}$ and Wt, as depicted in figure 3. The greyed out region is not considered since it does not add significantly to the sensitivity. The CRs are used to constrain the background normalization in the SRs. The SR and CRs are separated based on the invariant mass of the two leptons, with a lower threshold set at 15 GeV and an upper threshold set at 75 GeV for same flavour (SF) leptons and 110 GeV for different flavour (DF) leptons, as illustrated in figure 3(a) and figure 3(b). The mass of the di-lepton system is required to be $m_{\ell\ell} > 110$ GeV for the CRs enriched in events coming from top-quark processes. This region is further split into dedicated $t\bar{t}$- and Wt-enriched control regions by requiring[5] $m_{b\ell}$ [54] to be below or above 250 GeV, respectively. The Z+HF CR is required to have two SF leptons in the events, and to satisfy the di-lepton invariant mass requirement, 75 GeV $< m_{\ell\ell} <$ 110 GeV, excluding events where the invariant mass of the two b-tagged jets satisfies 40 GeV $< m_{bb} <$ 210 GeV.

[4]This is the angular distance ΔR considering the rapidity y instead of the pseudorapidity η and is defined as $\Delta R_y \equiv \sqrt{(\Delta y)^2 + (\Delta\phi)^2}$.
[5]See Table 4 for its definition.

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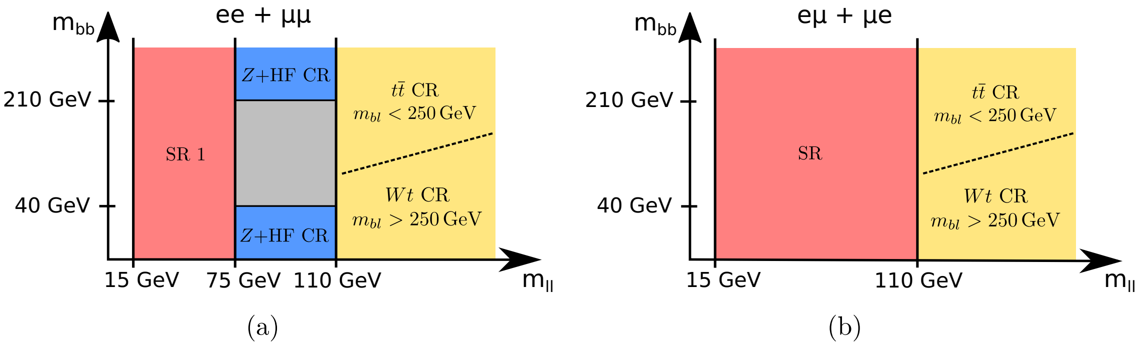

Figure 3. Definition of signal and control regions for same lepton flavour (a) and different lepton flavour (b) events, where either the electron ($e\mu$) is leading in p_{T} or the muon (μe). The greyed-out region is excluded as it makes a negligible contribution to the final results. The $m_{b\ell}$ discriminant variable [54] is used to further separate the top CR into separate $t\bar{t}$ and Wt control regions.

A VBF selection is applied to further categorize the events into two orthogonal ggF/VBF enriched regions by reverting (for ggF-like regions) or applying (for VBF-like regions) the VBF selection. The VBF selection requires the presence of at least two forward jets: these jets must have $p_{\mathrm{T}} > 30\,\mathrm{GeV}$, at least one pair of these extra jets must have a minimum pseudorapidity separation larger than 4.0, and at least one pair of these jets must have a mass larger than 600 GeV. The jets pairs considered are not required to be the same for the pseudorapidity separation and mass requirements; in less than $\sim$1% of the MC events, different pairs of jets are chosen. The VBF selection has a relative selection efficiency of $\sim$60% on VBF signal events. Table 3 shows the yields for SM background processes and non-resonant SM ggF and VBF signals in the SRs and CRs with their statistical uncertainty taken either directly from MC or from the statistics of the template, derived as described in section 6, in case for the fake-lepton background. For two minor backgrounds negative yields are observed due to NLO MC statistical fluctuations; the total is always positive. The SRs are then used to extract the final results, with the backgrounds constrained by the CRs, as described later. To enhance the sensitivity to the signal process and maximize the rejection of the expected SM backgrounds, a multivariate approach is used to select signal events, as described in the next section.

5 Multivariate analyses

Events that pass the selections described in the previous section are then passed through a MVA to separate rare signal events from the large amount of background events. A DNN and a Boosted Decision Tree (BDT) are used to classify events into the ggF and VBF categories, respectively. The outputs of the MVA models are used as discriminants in the statistical analysis discussed in section 8.

In the ggF category, the Keras library [119] with Tensorflow as the backend [120] is used to design a DNN classifier with a multi-output architecture to optimise the separation between the ggF HH signal, background from $t\bar{t}$ and Wt and all other background processes simultaneously. In a first stage, 50% of the simulated events are used to optimize the set of

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Process	ggF-SR	VBF-SR	$t\bar{t}$-CR	Wt-CR	Z+HF-CR
			SM background		
$t\bar{t}$	561220 ± 150	52670 ± 50	436840 ± 130	2270 ± 10	34700 ± 40
$t\bar{t}+V$	1121 ± 4	194.7 ± 1.9	1133 ± 5	97.0 ± 1.1	440.1 ± 1.9
Single top (Wt)	16260 ± 50	1165 ± 12	14100 ± 40	2901 ± 20	1237 ± 13
Single top (s/t-channel)	12.7 ± 0.8	2.48 ± 0.35	1.21 ± 0.28	0.35 ± 0.14	0.25 ± 0.11
$Z \to \ell\ell$ (HF)	16090 ± 180	1178 ± 34	3610 ± 70	525 ± 11	43390 ± 260
$Z \to \ell\ell$ (LF)	2720 ± 170	260 ± 40	600 ± 90	55 ± 8	5470 ± 190
$Z \to \tau\tau$ (HF)	2200 ± 40	154 ± 13	3 ± 7	1.9 ± 0.5	4 ± 6
$Z \to \tau\tau$ (LF)	370 ± 50	24 ± 4	-1.3 ± 1.5	0.11 ± 0.06	0.8 ± 0.5
W+jets	0.7 ± 0.5	0.09 ± 0.08	-0.2 ± 0.4	—	—
Diboson	288 ± 4	32.6 ± 0.8	159.0 ± 2.8	39.0 ± 0.9	226.8 ± 3.3
Single Higgs	601.0 ± 1.1	105.1 ± 0.4	336.5 ± 0.5	22.06 ± 0.12	48.28 ± 0.29
Fakes	18510 ± 170	2390 ± 60	10020 ± 140	529 ± 35	1360 ± 50
Total SM bkg.	619390 ± 350	58170 ± 100	466810 ± 230	6440 ± 40	86890 ± 330
			HH signal, ggF		
ggF $HH \to bbWW$	8.318 ± 0.016	0.857 ± 0.005	0.00113 ± 0.00019	0.00033 ± 0.00010	0.0014 ± 0.0002
ggF $HH \to bb\tau\tau$	3.138 ± 0.009	0.3284 ± 0.0029	0.00332 ± 0.00029	0.00068 ± 0.00015	0.0047 ± 0.0004
ggF $HH \to bbZZ$	0.633 ± 0.005	0.0873 ± 0.0018	0.00083 ± 0.00018	0.00020 ± 0.00009	0.0442 ± 0.0013
$\sum$ ggF HH	12.088 ± 0.019	1.272 ± 0.006	0.0053 ± 0.0004	0.00121 ± 0.00020	0.0504 ± 0.0014
			HH signal, VBF		
VBF $HH \to bbWW$	0.1518 ± 0.0014	0.2138 ± 0.0017	0.00013 ± 0.00004	—	0.00009 ± 0.00004
VBF $HH \to bb\tau\tau$	0.0537 ± 0.0006	0.0769 ± 0.0007	0.000086 ± 0.000022	0.000048 ± 0.000018	0.00024 ± 0.00004
VBF $HH \to bbZZ$	0.0097 ± 0.0004	0.0184 ± 0.0006	0.000040 ± 0.000024	0.0000029 ± 0.0000016	0.00236 ± 0.00023
$\sum$ VBF HH	0.2152 ± 0.0016	0.3091 ± 0.0019	0.00026 ± 0.00005	0.000051 ± 0.000018	0.00269 ± 0.00024
			HH signal, ggF+VBF		
$\sum$ ggF+VBF HH	12.303 ± 0.019	1.582 ± 0.006	0.0055 ± 0.0004	0.00126 ± 0.00020	0.0531 ± 0.0014

Table 3. Pre-fit yields for SM background processes and non-resonant SM ggF and VBF signals in the SRs and CRs. The event yields in the row "Fakes" come from the data-driven fake-lepton background estimate described in section 6. The event yields for Z+jets processes are split into ones with heavy-flavour (HF) and light-flavour (LF) jets as defined in section 6. A dash represents no contribution of the respective MC event sample in the respective region. Uncertainties are from MC statistics and template statistics only.

input variables and the hyperparameters of the DNN in a five-fold cross-validation with a train/test split fraction of 80%/20%. The final set of input variables is selected based on the permutation feature importance [121] to keep only the most important ones; this strategy allows the analysis to not compromise the performance but reduces the complexity of the model and therefore its goodness given the finite training statistics. These input variables are listed in table 4, with $E_{\mathrm{T}}^{\mathrm{miss}}$ significance being ranked as the ninth and $E_{\mathrm{T}}^{\mathrm{miss}}$ being ranked as the twelfth most important input variables with respect to the overall sensitivity. The data are well described by MC for these variables. The hyperparameters of the DNN are optimized through an automatic process using the Optuna [122] package, with the figure of merit being the 95% CL upper limit on the signal strength, i.e. the ratio of the measured HH production cross section to its SM prediction, without considering systematic uncertainties, using the CL_s prescription [123]. The final DNN model includes nine fully connected (FC) layers, each with 512 nodes, and is trained at a learning rate of 0.00011, with ReLU activations [124]

Input feature	Description
same flavour	unity if final state leptons are ee or $\mu\mu$, zero otherwise
p_{T}^{ℓ}, p_{T}^{b}	transverse momenta of the leptons, b-tagged jets
$m_{\ell\ell}$, $p_{\mathrm{T}}^{\ell\ell}$	invariant mass and the transverse momentum of the di-lepton system
m_{bb}, p_{T}^{bb}	invariant mass and the transverse momentum of the b-tagged jet pair system
m_{T2}^{bb}	stransverse mass of the two b-tagged jets [125, 126]
$\Delta R_{\ell\ell}$, ΔR_{bb}	ΔR between the two leptons and two b-tagged jets
$m_{b\ell}$	$\min\{\max(m_{b_0\ell_0}, m_{b_1\ell_1}), \max(m_{b_0\ell_1}, m_{b_1\ell_0})\}$ [54]
$\min\Delta R_{b\ell}$	minimum ΔR of all b-tagged jet and lepton combinations
$m_{bb\ell\ell}$	invariant mass of the $bb\ell\ell$ system
$E_{\mathrm{T}}^{\mathrm{miss}}$, $E_{\mathrm{T}}^{\mathrm{miss}}$-sig	missing transverse energy and its significance [127]
$m_{\mathrm{T}}(\ell_0, E_{\mathrm{T}}^{\mathrm{miss}})$	transverse mass of the p_{T}-leading lepton with respect to $E_{\mathrm{T}}^{\mathrm{miss}}$
$\min m_{\mathrm{T},\ell}$	minimum value of $m_{\mathrm{T}}(\ell_0, E_{\mathrm{T}}^{\mathrm{miss}})$ and $m_{\mathrm{T}}(\ell_1, E_{\mathrm{T}}^{\mathrm{miss}})$
$H_{\mathrm{T2}}^{\mathrm{R}}$	measure for boostedness[6] of the two Higgs bosons

Table 4. Input features used for the DNN in the ggF category. Indices 0 and 1 refer to p_{T}-leading and p_{T}-sub-leading objects respectively.

used for the FC layers and softmax activations used for the output layer. It is trained with a two-fold cross-validation strategy with a train/test split fraction of 50%/50%. A dropout rate of 0.3 is applied to the FC layers to prevent over-fitting; as a result the loss curve reaches a plateau for both training and test datasets at the end of the training. The score of the signal output node is binned so that the statistical uncertainty of the backgrounds is less than 30% and ~ 1 HH signal event from the combined ggF and VBF production modes is expected in each bin. The seven bins with the highest DNN output score are further considered for the statistical analysis, leading to a maximum of $\mathcal{O}(10^2)$ background events being present in a bin to be considered as part of the final signal region.

In contrast to the ggF event category, due to limited statistics and a tighter phase space in the VBF category, a DNN approach cannot be fully exploited for such events. Therefore, a BDT classifier is trained using the adaptive boosting (`AdaBoost`) method and the TMVA framework [128] with a cross-validation setup. Input variables are listed in table 5, with $E_{\mathrm{T}}^{\mathrm{miss}}$ significance being ranked as the fourteenth most important input variable with respect to the overall sensitivity. The data are well described by MC for these variables. The training parameters are optimized to have 350 trees with a maximum depth of four and a minimum terminal node size of 2.5%. The signal tree provided to the algorithm consists exclusively of VBF HH events, while the background consists of ggF HH signal events and other SM background events. The ggF HH events are classified as background since maximising the sensitivity to the VBF HH production mode is the goal of this MVA discriminant. A two-fold cross-validation was utilized with a train/test split fraction of 50%/50%. Each BDT was employed for the half of the dataset it had not been trained on, ensuring a reliable evaluation

[6] $H_{\mathrm{T2}}^{\mathrm{R}} = \dfrac{\left|\boldsymbol{E}_{\mathrm{T}}^{\mathrm{miss}} + \boldsymbol{p}_{\mathrm{T}}^{\ell_0} + \boldsymbol{p}_{\mathrm{T}}^{\ell_1}\right| + \left|\boldsymbol{p}_{\mathrm{T}}^{b_0} + \boldsymbol{p}_{\mathrm{T}}^{b_1}\right|}{\left|\boldsymbol{E}_{\mathrm{T}}^{\mathrm{miss}}\right| + \left|\boldsymbol{p}_{\mathrm{T}}^{\ell_0}\right| + \left|\boldsymbol{p}_{\mathrm{T}}^{\ell_1}\right| + \left|\boldsymbol{p}_{\mathrm{T}}^{b_0}\right| + \left|\boldsymbol{p}_{\mathrm{T}}^{b_1}\right|}$.

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Input feature	Description
η_{ℓ_0}, η_{ℓ_1}, ϕ_{ℓ_0}, ϕ_{ℓ_1}, $p_{\mathrm{T}}^{\ell_0}$, $p_{\mathrm{T}}^{\ell_1}$	η, ϕ, p_{T} of the p_{T}-(sub)leading lepton
η_{b_0}, η_{b_1}, ϕ_{b_0}, ϕ_{b_1}, $p_{\mathrm{T}}^{b_0}$, $p_{\mathrm{T}}^{b_1}$	η, ϕ, p_{T} of the p_{T}-(sub)leading b-tagged jet
η_{j_0}, η_{j_1}, ϕ_{j_0}, ϕ_{j_1}, $p_{\mathrm{T}}^{j_0}$, $p_{\mathrm{T}}^{j_1}$	ϕ, η, p_{T} of the p_{T}-(sub)leading non b-tagged jet
$E_{\mathrm{T}}^{\mathrm{miss}}$, $\phi^{E_{\mathrm{T}}^{\mathrm{miss}}}$, $E_{\mathrm{T}}^{\mathrm{miss}}$-sig	missing transverse energy, its ϕ and significance [127]
p_{T}^{bb}, ΔR_{bb}, $\Delta\phi_{bb}$, m_{bb}	p_{T}, ΔR, $\Delta\phi$ and invariant mass of di-b-jet system
$p_{\mathrm{T}}^{\ell\ell}$, $\Delta R_{\ell\ell}$, $\Delta\phi_{\ell\ell}$, $m_{\ell\ell}$, $\phi^{\ell\ell}_{\mathrm{centrality}}$	p_{T}, ΔR, $\Delta\phi$, p_{T} and centrality[7] of di-leptons system
$p_{\mathrm{T}}^{bb\ell\ell}$, $m_{bb\ell\ell}$	p_{T} and invariant mass of the $bb\ell\ell$ system
$p_{\mathrm{T}}^{bb\ell\ell+E_{\mathrm{T}}^{\mathrm{miss}}}$, $m_{bb\ell\ell+E_{\mathrm{T}}^{\mathrm{miss}}}$	p_{T} and invariant mass of $bb\ell\ell$ + $E_{\mathrm{T}}^{\mathrm{miss}}$ system
$m_{\ell\ell+E_{\mathrm{T}}^{\mathrm{miss}}}$	invariant mass of di-lepton + $E_{\mathrm{T}}^{\mathrm{miss}}$ system
$p_{\mathrm{T}}^{E_{\mathrm{T}}^{\mathrm{miss}}+\ell\ell}$, $\Delta\phi_{E_{\mathrm{T}}^{\mathrm{miss}},\ell\ell}$	p_{T} of and $\Delta\phi$ between $E_{\mathrm{T}}^{\mathrm{miss}}$ and di-lepton system
$p_{\mathrm{T}}^{\mathrm{tot}}$	p_{T} of $bb\ell\ell+E_{\mathrm{T}}^{\mathrm{miss}}+$ p_{T}-leading and -sub-leading jet
m_{tot}	invariant mass of $bb\ell\ell+E_{\mathrm{T}}^{\mathrm{miss}}+$ p_{T}-leading and -sub-leading jet
m_t^{KLF}	Kalman fitter top-quark mass [129]
$\min\Delta R_{\ell_0 j}$, $\min\Delta R_{\ell_1 j}$	minimum ΔR between p_{T}-(sub)leading ℓ-j couples
$\sum m_{\ell j}$	sum of the invariant masses of all ℓ+jet combinations
$\max p_{\mathrm{T}}^{jj}$, $\max m_{jj}$	maximum p_{T} and invariant mass of any two non b-tagged jets
$\max\Delta\eta_{jj}$, $\max\Delta\phi_{jj}$	maximum $\Delta\eta$ and $\Delta\phi$ between any two non b-tagged jets
$\min\Delta R_{b\ell}$	minimum ΔR of all b-tagged jet and lepton combinations
$N_{\mathrm{forward\ jets}}$, N_j	number of forward jets, number of non b-tagged jets
m_{T2}^{bb}	stransverse mass of the two b-tagged jets [125, 126]
m_{coll}	collinear mass (reconstruction of $m_{\tau\tau}$) [130]
m_{MMC}	value of the MMC algorithm (reconstruction of $m_{\tau\tau}$) [130]

Table 5. Input features for the BDT algorithm in the VBF category. The usage of j in variable names indicates that only non b-tagged jets being considered. Indices 0 and 1 refer to p_{T}-leading and p_{T}-sub-leading objects respectively.

of performance across the entire dataset. After careful examination, it has been decided to train the BDT on a VBF sample with $\kappa_\lambda = 0$, as it showed the best overall performance across a set of SM and BSM scenarios. The BDT output score is binned into ten bins taking into account their signal over background ratio, with the most sensitive bin being required to have a minimum of $\sim$2 background events. The five bins with the highest BDT output score are further considered for the statistical analysis, leading to a maximum of $\mathcal{O}(10^3)$ background events being present in a bin to be considered as part of the final signal region.

[7]The centrality $\phi^{\ell\ell}_{\mathrm{centrality}}$ indicates the location of the missing transverse energy with respect to the two final state leptons in the ϕ-plane. It is one when the direction of $E_{\mathrm{T}}^{\mathrm{miss}}$ lies directly between the two leptons and $1/\sqrt{2}$ if it is aligned with one of the leptons. It is defined as $\phi^{\ell\ell}_{\mathrm{centrality}} = (1/\sqrt{2})(\phi_A + \phi_B)/(\phi_A^2 + \phi_B^2)^{1/2}$ with $\phi_A = \sin(\phi_{E_{\mathrm{T}}^{\mathrm{miss}}} - \phi_{\ell_0})/\sin(\phi_{\ell_1} - \phi_{\ell_0})$ and $\phi_B = \sin(\phi_{\ell_1} - \phi_{E_{\mathrm{T}}^{\mathrm{miss}}})/\sin(\phi_{\ell_1} - \phi_{\ell_0})$.

6 Background estimation

The dominant background processes expected to contribute to the signal region are top quark pair production ($t\bar{t}$), single top-quark in association with a W boson (Wt), and Z/γ^* production in association with heavy-flavour jets. The contributions of these background processes are constrained in dedicated CRs as defined in section 4.

The simulated Z+jets background events are divided into heavy flavour (HF) and light flavour (LF), based on the generator-level information on the true origin of the jets. If at least one of the two p_{T}-ordered leading jets in the Z+jets sample is matched at generator level with either a b- or c-quark, events are classified as "heavy flavour". All other Z+jets events, i.e. events where at least one of the two p_{T}-leading jets is a light flavour jet, are classified as light flavour. As the cross-section of Z boson production in association with heavy flavour jets is known to be mis-modelled [131, 132], the MC prediction is constrained with data in control regions enriched in the Z+HF processes.

The contribution from events containing photons or jets that are mis-identified as leptons as well as leptons from the hadronic decays of heavy flavour quarks is collectively referred as "fake-lepton" background. It is estimated using a data-driven method.

Firstly, the corresponding CR is defined to have the same selections as the SR, except reverting the opposite-sign (OS) requirement of the di-lepton system in the SR definition to have only same-sign (SS) lepton pairs. The contribution of fake-lepton events in the SS region is then estimated by subtracting the predicted contribution from prompt leptons of SM backgrounds from the observed number of the SS di-lepton events in the data. Next, transfer factors binned as a function of sub-leading lepton p_{T} are calculated as the ratio of the number of OS fake-lepton events to the number of SS fake-lepton events,

$$f_{\mathrm{SS}\to\mathrm{OS}} = \frac{N^{\mathrm{fake}}_{\mathrm{MC,OS}}}{N^{\mathrm{fake}}_{\mathrm{MC,SS}}},$$

as estimated from the background MC events; they range from 1.2 to 1.9. In the end, the number of fake-lepton events in the SRs is extrapolated by applying the transfer factors to the number of fake-lepton events estimated in the SS region:

$$N^{\mathrm{fake}}_{\mathrm{OS}} = f_{\mathrm{SS}\to\mathrm{OS}} \times \left(N_{\mathrm{data,SS}} - N^{\mathrm{prompt}}_{\mathrm{MC,SS}}\right).$$

7 Systematic uncertainties

The results account for several sources of systematic uncertainty on the signal and background processes, which are classified as either experimental (detector- or luminosity-related) or theoretical modelling uncertainties. Statistical uncertainties of the simulated event samples are also taken into account. The total pre-fit event yields, with their uncertainties, and the background composition in the different signal and control regions, are shown in figure 4.

The uncertainties due to experimental sources are primarily due to the mismeasurement of reconstructed object momentum and to the finite level of precision when determining reconstruction efficiencies. They include uncertainties on the jet energy scale [114] and jet energy resolution [133]. Additional uncertainties for b-tagged jets arise from the precision

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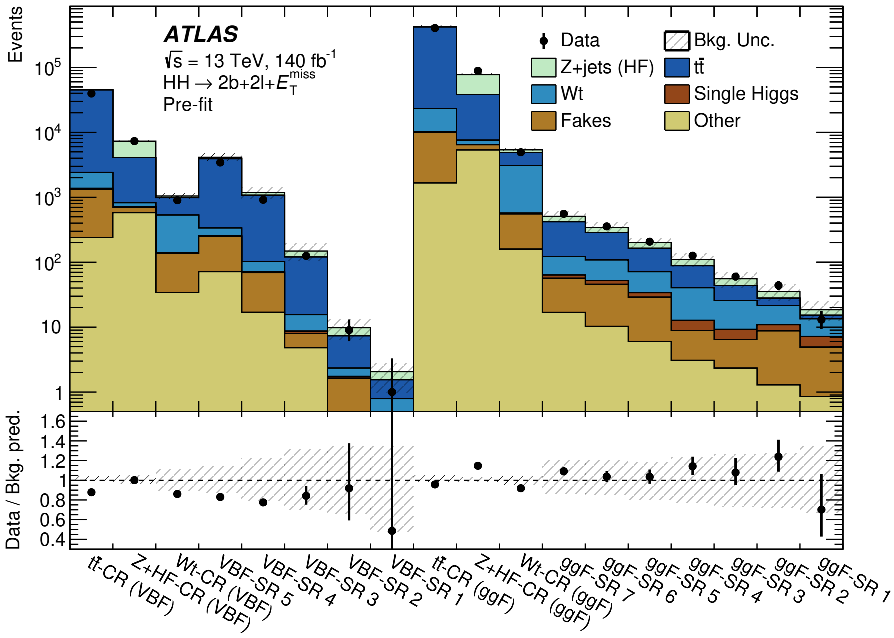

Figure 4. Pre-fit yields of the $t\bar{t}$, Z+HF and Wt CRs, both for the ggF and VBF event selection, as well as the highest-score bins, numbered from high (VBF-SR 1 and ggF-SR 1) to low score (VBF-SR 5 and ggF-SR 7), of the BDT and DNN output distribution in the VBF and ggF event categories, respectively, as used in the final result. The shaded bands include both statistical and systematic uncertainties.

of the b-tagging efficiency and from the rates at which charm- and light-flavoured jets are selected as b-tagged jets [116]. Lepton-related uncertainties arise on the electron [134] and muon [111] reconstructed energy (momentum) measurements, as well as on the precision of their reconstruction and identification efficiencies. The E_T^{miss} scale and resolution [117] uncertainties, as well as uncertainties from the mis-modelling of pile-up, trigger efficiency and luminosity, are also taken into account. The uncertainty in the combined 2015–2018 integrated luminosity is 0.83% [38], obtained using the LUCID-2 detector [135] for the primary luminosity measurements, complemented by measurements using the inner detector and calorimeters.

The normalization corrections on the dominant background processes, namely $t\bar{t}$, Wt and $Z+$jets, are determined using data in the control regions during the statistical analysis. The experimental uncertainties and the systematic uncertainties from the modelling of these processes are taken into account and constrained during the fitting process. For the $t\bar{t}$ and Wt processes, the QCD uncertainty is estimated by comparing events with different renormalization scale (μ_R) and factorization scale (μ_F) settings, where the largest deviation is chosen as the systematic uncertainty. The uncertainties arising from the modelling of initial- and final-state radiation in the generators used to simulate the $t\bar{t}$ (Wt) background processes are evaluated using the method described in ref. [136]. The effects of uncertainties due to the choice of PDF and the value of α_S are evaluated by varying the PDF as well as the value for α_S and taking the maximum variation into account as uncertainty. The ME and PS uncertainties are estimated by comparing events from the nominal simulation samples with events from samples using alternative ME generators and PS generators, taking their difference as the respective uncertainty and then symmetrising it. The uncertainty arising from the interference between the NLO predictions for $t\bar{t}$ and Wt processes is estimated by taking the difference between the predicted yields obtained with the DR and DS schemes [136]. The $Z+$jets modelling uncertainties are estimated using the nominal Sherpa 2.2.1 samples by considering different merging and re-summation scales [137, 138]. The uncertainties due to PDF variations and changes in μ_R and μ_F are calculated using the same procedures as for the $t\bar{t}$ and Wt backgrounds.

Systematic uncertainties in the signal acceptance obtained by varying μ_R and μ_F, as well as PDF-induced uncertainties, are taken into account as recommended [15] and evaluated using the same procedure as for the top-quark background processes. The uncertainty due to the parton shower modelling is computed by comparing Herwig 7 with Pythia 8. The uncertainty in the HH production cross-section, evaluated to be $\pm 3\%$ for PDF+α_S and $^{+6\%}_{-23\%}$ for the combined scale and top-quark mass scheme for ggF, and $\pm 2.1\%$ for PDF+α_S and $^{+0.03\%}_{-0.04\%}$ for the scale for VBF, is included as an uncertainty in $\sigma^{SM}_{gg/qq\to HH/HHjj}$ when computing the upper limits on the signal strength.

8 Statistical treatment and results

8.1 Statistical procedure

The statistical procedure used to interpret the data is described in ref. [139]. The likelihood function is constructed from the product of Poisson probabilities:

$$L(\mathrm{data}|\mu, \boldsymbol{\theta}) = \prod_{i=1}^{N} \mathrm{Poisson}(\mathrm{data}_i|\mu \cdot s_i(\boldsymbol{\theta}) + \mu_b b_i(\boldsymbol{\theta})) \times \mathrm{G}(\tilde{\boldsymbol{\theta}}|\boldsymbol{\theta})$$

where s_i and b_i are the signal and background contributions in the i-th bin of the fitted variable distribution; μ is the signal strength, μ_b is the normalization factor for the respective background, and $\boldsymbol{\theta}$ denotes the nuisance parameters, which account for the uncertainties of the measurements; $\mathrm{G}(\tilde{\boldsymbol{\theta}}|\boldsymbol{\theta})$ is the Gaussian scaling function of the nuisance parameters constructed as deviations from the nominal model of the systematic uncertainties, where $\tilde{\boldsymbol{\theta}}$ provides a maximum likelihood estimate for $\boldsymbol{\theta}$. The parameter of interest in the statistical analysis is the global signal strength factor $\mu = \sigma/\sigma^{\mathrm{SM}}$, which acts on the total number of events predicted by the signal model. This factor is defined such that $\mu = 0$ corresponds to the background-only hypothesis and $\mu > 0$ corresponds to a HH signal in addition to the background. Hypothesised values of μ are tested based on the profile likelihood ratio [140], which compares data with background-only (b) and signal+background ($s+b$) models using the following test statistic:

$$q_\mu = \begin{cases} -2\ln\frac{L(\mathrm{data}|\mu,\hat{\hat{\boldsymbol{\theta}}}_\mu)}{L(\mathrm{data}|0,\hat{\hat{\boldsymbol{\theta}}}_0)} & \hat{\mu} < 0 \\ -2\ln\frac{L(\mathrm{data}|\mu,\hat{\hat{\boldsymbol{\theta}}}_\mu)}{L(\mathrm{data}|\hat{\mu},\hat{\boldsymbol{\theta}})} & 0 \le \hat{\mu} \le \mu \\ 0 & \hat{\mu} > \mu \end{cases}$$

where $\hat{\mu}$ and $\hat{\boldsymbol{\theta}}$ are the values for μ and $\boldsymbol{\theta}$ when maximizing L with all parameters floating (referred to as the unconditional maximum-likelihood (ML) estimators). The $\hat{\hat{\theta}}_\mu$ is the conditional ML estimator of θ for a fixed value of μ. This test statistic extracts the information on the signal strength from a full likelihood fit to the data. The likelihood function includes all the parameters that describe the systematic uncertainties and their correlations. The constraints on the coupling modifiers are obtained by using the respective modifier (κ_λ or κ_{2V}) in place of the signal strength as the parameter of interest in the profile likelihood ratio.

Exclusion limits at 95% CL are based on the CL$_s$ prescription [123], and they are set on the HH production cross-section times branching fraction divided by the corresponding SM prediction. The statistical analysis uses the distributions of the MVA output score in both the ggF and VBF SRs as final discriminant. The background CRs are used to constrain the overall normalization for the $t\bar{t}$, Wt and Z+HF backgrounds in the SR. Other background normalizations and shapes are fixed with prior uncertainties included in the fit.

8.2 Limits on HH production

All regions used for this search are displayed in figure 5 after a fit with the signal strength fixed to the upper limit, while pre-fit distributions are shown in figure 4. A downward fluctuation of the data in the last bin of both the NN and BDT distributions is observed. A negative signal strength has been extracted from the fit: $\mu_{HH} = -8.5^{+7.7}_{-8.4}$. Using the approach described in section 8.1, the upper limits on the signal strength parameter for Higgs boson pair production with consideration of both the ggF and VBF signals are determined. Figure 6 summarizes the ggF, VBF and combined results with the impact of all systematic uncertainties being shown. The observed combined upper limit at 95% CL on the signal strength is $\mu_{HH} = 9.7$. In the CRs, the normalization and modelling of the backgrounds play a prominent role, and they dominate the sources of uncertainty. In the SRs, the systematic uncertainties mostly arise from background modelling, experimental sources and the signal normalization. In the most sensitive bins, i.e. ggF-SR 1 to ggF-SR 3 and VBF-SR 1 and VBF-SR 2, the statistical uncertainty becomes dominant due to the limited number of expected events.

8.3 Constraints on Higgs coupling parameters

This analysis is extended by performing likelihood scans on the κ_λ and κ_{2V} parameters. The single Higgs boson background has a small dependence upon κ_λ through loop effects, which is neglected. Coupling modifiers other than the one tested in the respective scan are set to their SM value. Hence, the κ_t, κ_V and κ_{2V} coupling modifiers are set to $\kappa_t = \kappa_V = \kappa_{2V} = 1$ for the κ_λ-scan. Both the ggF and VBF HH signal regions are used in the analysis, and the result is shown in figure 7(a). The observed result constrains κ_λ to be within the range $[-6.2, 13.3]$ at 95% CL which is slightly better than the expected range of $[-8.1, 15.5]$ at 95% CL due to the observed downward fluctuation of the data.

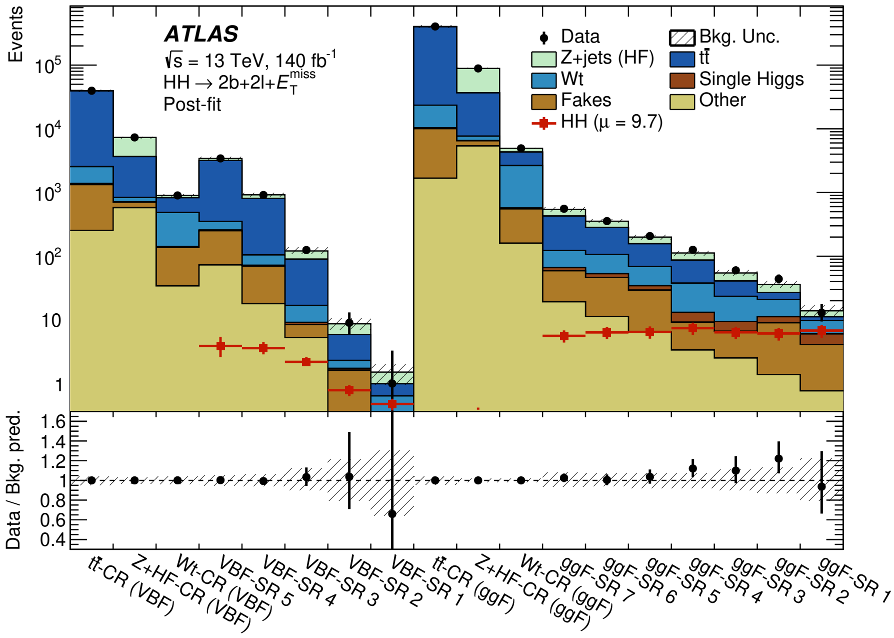

Figure 5. Post-fit yields from the signal+background fit of the $t\bar{t}$, Z+HF and Wt CRs, both for the ggF and VBF event selections, as well as the highest-score bins, numbered from high (VBF-SR 1 and ggF-SR 1) to low score (VBF-SR 5 and ggF-SR 7), of the BDT and DNN output distribution in the VBF and ggF event categories respectively as used in the final result. The fit is a conditional fit with the signal strength fixed to the observed upper limit of $\mu_{HH} = 9.7$. The shaded bands include both statistical and systematic uncertainties.

A scan over the κ_{2V} parameter is also conducted. Again, all other couplings are set to their respective SM values. Although only the VBF production mode of Higgs boson pairs is sensitive to the κ_{2V} coupling modifier, both the ggF and VBF SRs are included in the scan, allowing the analysis to achieve a slight enhancement of sensitivity from the presence of VBF HH events within the ggF SR. A likelihood scan is performed to set constraints on the κ_{2V} parameter; this is shown in figure 7(b). Values for κ_{2V} are constrained to be within the range of $[-0.17, 2.4]$ at 95% CL which is slightly better than the expected range of $[-0.51, 2.7]$ at 95% CL due to the observed downward fluctuation of the data.

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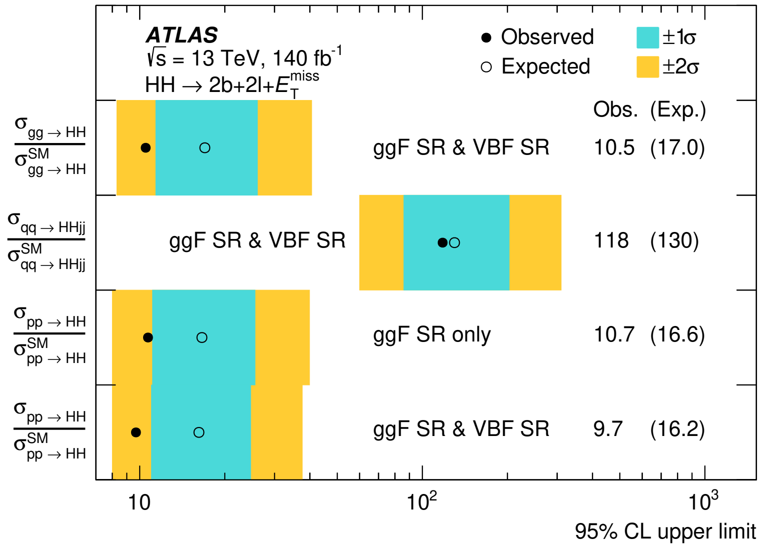
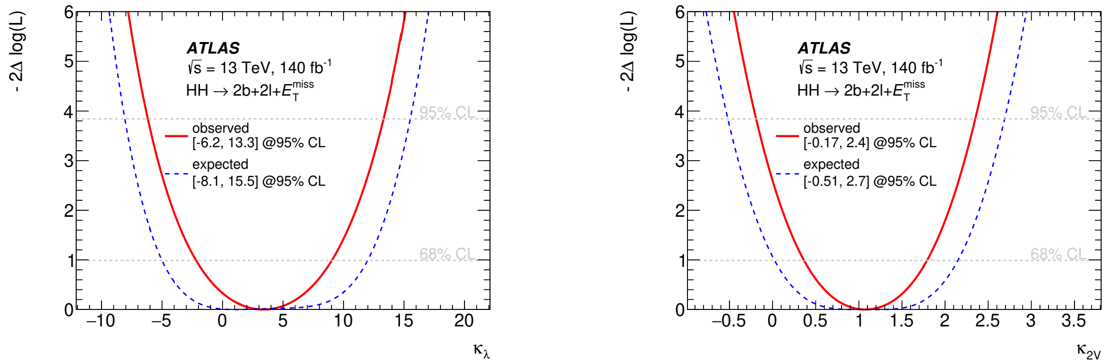


Figure 6. Observed and expected upper limits on the ratios of the Higgs boson pair production cross-section to the corresponding Standard Model prediction $\sigma_{HH}/\sigma_{HH}^{\mathrm{SM}}$ for the ggF HH signal only (top row), the VBF HH signal only while considering ggF HH as background (second row) and the combined ggF+VBF HH signal considering only the ggF SR (third row) and considering all SRs (bottom row) at a 95% confidence level. The relative ratio between the ggF and VBF production modes is fixed to the SM value.



(a) (b)

Figure 7. Likelihood profiles of the (a) κ_λ and (b) κ_{2V} parameters.

9 Conclusion

A search for non-resonant Higgs boson pair production via the ggF and VBF production modes is performed. It probes decay channels with one of the Higgs bosons decaying to $b\bar{b}$ and the other to either WW^*, ZZ^*, or $\tau^+\tau^-$. Selected events contain exactly two b-tagged jets, two light leptons with opposite electric charge and missing transverse energy. The analysis employs 140 fb^{-1} of pp collision data at $\sqrt{s} = 13$ TeV, recorded by the ATLAS detector at the LHC. The results are consistent with the predictions for the SM background processes. An observed (expected) 95% CL upper limit on the cross-section for the production of Higgs boson pairs is set at 9.7 (16.2) times the SM prediction, which is a significant improvement compared to the previous ATLAS search in this channel. The analysis also establishes separate 95% CL limits on the Higgs coupling parameters κ_λ and κ_{2V} excluding values outside the ranges $[-6.2, 13.3]$ and $[-0.17, 2.4]$, respectively. These ranges are obtained under the assumption that all other couplings, except the individual coupling being tested, are set to their SM values.

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