






# Search for Higgs Boson Pair Production in the Four b Quark Final State in Proton-Proton Collisions at $\sqrt{s} = 13$ TeV

## Journal Article

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## Search for Higgs Boson Pair Production in the Four $b$ Quark Final State in Proton-Proton Collisions at $\sqrt{s} = 13$ TeV

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A search for pairs of Higgs bosons produced via gluon and vector boson fusion is presented, focusing on the four  $b$  quark final state. The data sample consists of proton-proton collisions at a center-of-mass energy of 13 TeV, collected with the CMS detector at the LHC, and corresponds to an integrated luminosity of  $138 \text{ fb}^{-1}$ . No deviation from the background-only hypothesis is observed. A 95% confidence level upper limit on the Higgs boson pair production cross section is observed at 3.9 times the standard model prediction for an expected value of 7.8. Constraints are also set on the modifiers of the Higgs field self-coupling,  $\kappa_\lambda$ , and of the coupling of two Higgs bosons to two vector bosons,  $\kappa_{2V}$ . The observed (expected) allowed intervals at the 95% confidence level are  $-2.3 < \kappa_\lambda < 9.4$  ( $-5.0 < \kappa_\lambda < 12.0$ ) and  $-0.1 < \kappa_{2V} < 2.2$  ( $-0.4 < \kappa_{2V} < 2.5$ ). These are the most stringent observed constraints to date on the  $HH$  production cross section and on the  $\kappa_{2V}$  coupling.

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The discovery of the Higgs boson ( $H$ ) by the ATLAS and CMS Collaborations [1–3] proves the existence of a fundamental scalar sector of the standard model of particle physics (SM), but the experimental confirmation of the Brout-Englert-Higgs mechanism [4–6] requires the determination of the shape of the postulated scalar potential. This shape is governed by a parameter  $\lambda$  that drives the strength of the Higgs boson self-couplings and can thus be determined experimentally with a measurement of Higgs boson pair ( $HH$ ) production.

At the CERN Large Hadron Collider (LHC), at the energy of  $\sqrt{s} = 13$  TeV, the dominant  $HH$  production mode in the SM is through the gluon fusion mechanism ( $ggF$ ), with a cross section of  $31.1^{+2.1}_{-7.2} \text{ fb}$  [7–14], followed by the vector boson fusion process (VBF), with a cross section of  $1.726 \pm 0.036 \text{ fb}$  [15] and characterized by the presence of two additional hadronic jets,  $j$ , giving a  $b\bar{b}b\bar{b}jj$  final state. Variations of the Higgs boson self-coupling with respect to the SM prediction are parametrized by the modifier  $\kappa_\lambda = \lambda/\lambda^{\text{SM}}$  and affect the  $ggF$  and VBF production modes. The VBF production mode also depends on the strength of the interaction of pairs of vector bosons  $V$  ( $= W, Z$ ) with a single (VVH) and a pair (VVHH) of Higgs bosons, whose values with respect to the SM prediction are parametrized by the modifiers  $\kappa_V$  and  $\kappa_{2V}$ , respectively. Departures from the relation  $\kappa_{2V} = \kappa_V^2$

predicted in the Brout-Englert-Higgs mechanism are possible in models of physics beyond the SM where the Higgs boson is a composite state emerging from the presence of new strong dynamics at the TeV scale [16].

The ATLAS and CMS Collaborations have searched for  $ggF$   $HH$  production with a dataset corresponding to an integrated luminosity of about  $36 \text{ fb}^{-1}$  in a variety of final states [17–26], whose combinations [27,28] set an observed (expected) upper limit at the 95% confidence level (CL) on the SM production cross section of 7 (10) and 22 (13) times theoretical prediction, respectively. Updated searches have been performed with an integrated luminosity of about  $140 \text{ fb}^{-1}$  [29–31], and the most stringent observed limits are from the ATLAS search in the  $b\bar{b}\gamma\gamma$  final state and correspond to 4.2 times the SM prediction, with a value of  $\kappa_\lambda$  between  $-1.5$  and  $6.7$  at the 95% CL. The VBF  $HH$  production process has been studied in the  $b\bar{b}b\bar{b}$  [32] and  $b\bar{b}\gamma\gamma$  [30] final states by the ATLAS and CMS Collaborations, respectively, and the most stringent observed constraints at the 95% CL correspond to  $-0.43 < \kappa_{2V} < 2.56$  from  $b\bar{b}b\bar{b}$  and 225 times the SM cross section prediction from  $b\bar{b}\gamma\gamma$ .

This Letter reports on searches for both the  $ggF$  and VBF  $HH$  production mechanisms in the  $b\bar{b}b\bar{b}$  decay channel. In the SM, this decay mode is characterized by a combined branching fraction of  $0.339 \pm 0.008$  for  $m_H = 125 \text{ GeV}$  [33]. The analysis uses a sample of proton-proton collision (pp) events at  $\sqrt{s} = 13$  TeV recorded between 2016 and 2018 with the CMS detector, corresponding to an integrated luminosity of  $138 \text{ fb}^{-1}$ .

The CMS apparatus [34] is a multipurpose, nearly hermetic detector, designed to trigger on [35,36] and identify electrons, muons, photons, and hadrons [37–41].

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A global event reconstruction “particle-flow” (PF) algorithm [42] combines the information provided by the all-silicon inner tracker and by the crystal electromagnetic and brass-scintillator hadron calorimeters, operating inside a 3.8 T superconducting solenoid, with data from gas-ionization muon detectors embedded in the solenoid iron return yoke, to build  $\tau$  leptons, jets, missing transverse momentum, and other physics objects [43–45].

Hadronic jets are clustered from the PF objects using the anti- $k_T$  algorithm [46,47] with a distance parameter of 0.4. Jet energy corrections are derived from simulation studies and corrected with *in situ* measurements to match the energy scale in data and in simulation [44]. Jets originating from  $b$  quarks are identified using as a discriminant the output of a deep neural network algorithm (DEEPIET) [48,49], trained using as input information the properties of the PF constituents of the jets and of the secondary vertices associated with them. For the jets in this search, two working points (WPs) of the DEEPIET discriminant are considered: the medium WP, which yields a  $b$  jet identification efficiency of 75% with a corresponding misidentification rate of light flavor and gluon (charm) jets of about 1 (10)%, and the tight WP, which corresponds to a  $b$  jet identification efficiency of 58% and to a misidentification rate of about 0.1(2)%.

Signal processes from  $ggF$   $HH$  production are simulated at next-to-leading order (NLO) accuracy in quantum chromodynamics (QCD) with POWHEG2.0 [50–52], and samples for VBF  $HH$  production are generated at leading order (LO) accuracy in QCD using MADGRAPH5\_aMC@NLO2.6.5 [53] for various combinations of couplings. The distributions are scaled by functions of the couplings defined according to the known dependence of the theoretical cross section [54] and added together to model arbitrary coupling combinations, and the total predictions are normalized to the corresponding next-to-NLO (NNLO) cross section [13] for  $ggF$  and by the ratio of the next-to-NNLO [15] to LO SM cross sections for VBF. Although not used to model the background, simulated samples for the QCD multijet,  $t\bar{t}$ , and  $ZZ$  backgrounds are used for the optimization of the analysis. For all simulations, the generators are interfaced with PYTHIA8.226 (2016) and 8.230 (2017–2018) [55], and the CMS detector response is modeled with GEANT4 [56]. The simulated events are weighted to match the distribution of additional pp interactions (pileup) within the same or nearby bunch crossings, relative to the collision of interest, to the one observed in data. See Supplemental Material [57] for further details on the simulated samples.

The trigger selection for events collected in 2016 requires the presence of four jets with transverse momentum  $p_T > 45$  GeV or of two jets with  $p_T > 30$  GeV and two jets with  $p_T > 90$  GeV. For 2017 (2018) data, the presence of four jets above the  $p_T$  thresholds of 40, 45, 60, and 75 GeV is required together with  $H_T > 300(330)$  GeV,

respectively, where  $H_T$  denotes the scalar sum of the transverse momentum of the jets reconstructed in the event. As a consequence of the change in jet trigger thresholds, data collected in 2017 and 2018 are analyzed separately from those collected in 2016.

Offline, events are required to contain at least four jets with pseudorapidity  $|\eta| < 2.4(2.5)$  and  $p_T > 30(40)$  GeV for the 2016 (2017–2018) data, respectively. Jets are required to satisfy the tight WP of the PF jet identification algorithm [58,59], corresponding to an efficiency larger than 99%. If their  $p_T$  is below 50 GeV, the medium WP of the pileup discriminant [58] is also required, for a signal jet efficiency of about 90%. If more than four jets satisfy these criteria, the four objects with the largest DEEPIET output are selected. The  $p_T$  of these four jets are corrected with a multivariate regression method developed for  $b$  jets that improves the determination of the momentum by up to 15% and simultaneously estimates the per jet resolution achieved [60]. After the application of this method, the resolution on the dijet invariant mass for  $H \rightarrow b\bar{b}$  events reconstructed in this analysis ranges between 11% and 14%. At least three of the selected jets are required to satisfy the medium WP of the DEEPIET discriminant.

Events are rejected if they contain an electron or a muon with  $p_T > 15$  and 10 GeV, respectively, and  $|\eta| < 2.4$ , where these objects must satisfy identification discriminants and criteria that include isolation and impact parameter with respect to the primary interaction vertex. This selection suppresses background events containing leptonic top quark decays.

The two Higgs boson candidates are formed by pairing the four jets. There are three possible pairings of jets, and in each the two Higgs boson candidates, denoted as  $H_1$  and  $H_2$ , are defined by the relation  $p_T(H_1) > p_T(H_2)$ . The  $(H_1, H_2)$  pairings are ordered according to the increasing value of a distance parameter  $d = |m_{H_1} - km_{H_2}|/\sqrt{1+k^2}$ . The constant  $k$  is the ratio of the expected peak positions of the reconstructed Higgs boson masses for events that are correctly paired,  $k = c_1/c_2 = (125 \text{ GeV})/(120 \text{ GeV}) = 1.04$ . Its value differs from 1 because of the residual jet momentum dependence of the multivariate energy regression that more strongly impacts the softer  $H$  candidate. If the difference in the distance parameter of the first and second pairing,  $\Delta d$ , is larger than 30 GeV, corresponding to about 2 times the resolution on the Higgs boson mass, the pairing with the smallest  $d$  is chosen. Conversely, if  $\Delta d \leq 30$  GeV, the experimental resolution limits the capability to identify the correct pairing based on the invariant masses, and a choice is made between the first and second pairing as the one that maximizes the  $p_T$  of the two Higgs boson candidates in the four-jet center-of-mass reference frame. This procedure results in a correct jet pairing of about 96% of the selected events in a  $ggF$  SM  $HH$  sample, and amounts to 82%–96% (91–98)% for the different couplings studied in  $ggF$  (VBF) signal events.

The two non- $b$  jets in the VBF production events are selected with  $p_T > 25$  GeV and  $|\eta| < 4.7$ , and they must satisfy the tight WP of the jet identification algorithm and the medium WP of the pileup discriminant if  $p_T < 50$  GeV. For the 2017 data, affected by large noise in the end caps of the electromagnetic calorimeter (ECAL), jets in the region  $2.6 < |\eta| < 3.1$  are additionally required to satisfy the tight WP of the pileup discriminant to mitigate the noise effects. The two VBF jet candidates  $j_1$  and  $j_2$  are chosen as the highest  $p_T$  jet and the second-highest  $p_T$  jet that has an opposite  $\eta$  sign with respect to the former.

Events that do not contain such a VBF jet pair are assigned to the  $ggF$  category. About 26%–28% of  $ggF$  events contain additional jets that satisfy the above requirements on the VBF jet candidates, and in order to correctly classify them, a boosted decision tree (BDT) discriminant is trained to separate  $ggF$  and VBF  $HH$  signal events. The discriminant uses  $p_T(H_1)$ ,  $p_T(H_2)$ ,  $p_T(j_1)$ ,  $p_T(j_2)$ , the invariant mass and absolute value of pseudorapidity of the  $jj$  system, the angular separation  $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$ , where  $\phi$  is the azimuthal angle, between the two  $H$  candidates and between each  $H$  and VBF jet, the absolute value of the polar angles with respect to the beam direction of the two VBF jets in the center-of-mass frame of the six selected jets and the product of the two Higgs boson centralities  $\exp[-([\eta(H_1) - \eta_{\text{avg}}]/\Delta\eta)^2 - ([\eta(H_2) - \eta_{\text{avg}}]/\Delta\eta)^2]$ , where  $\Delta\eta = \eta(j_1) - \eta(j_2)$  and  $\eta_{\text{avg}} = [\eta(j_1) + \eta(j_2)]/2$ . The discriminant is trained to separate the SM  $ggF$   $HH$  signal from the  $\kappa_{2V} = 2$  VBF signal, in order to optimize both the sensitivity to the anomalous  $\kappa_{2V}$  coupling hypotheses and the correct classification of SM  $ggF$  signal events. The value  $\kappa_{2V} = 2$  is chosen because it is representative of the event kinematics in the presence of anomalous couplings, characterized by the large invariant mass of the  $jj$  and  $HH$  systems. These signals are associated with a large increase of the total cross section that would make them detectable with the available dataset. A threshold on the BDT output is chosen to assign events to either the  $ggF$  or VBF category. It results in the correct assignment of about 97% of all  $ggF$   $HH$  signal events to the  $ggF$  category and of about 60% (80)% of SM ( $\kappa_{2V} = 2$ ) VBF  $HH$  events that contain the additional jets to the VBF category.

Events classified as  $ggF$  or VBF signal are further divided into subcategories to optimize the sensitivity of the search for anomalous coupling hypotheses. Events in the  $ggF$  category are divided into a low- and high-mass category if the reconstructed invariant mass of the  $HH$  system,  $m_{HH}$ , is below or above 450 GeV, where the boundary is defined according to the kinematic properties of the signal. The latter category efficiently collects SM  $ggF$   $HH$  events, while the former increases the acceptance to signals with anomalous  $\kappa_\lambda$  values. Events in the VBF category are instead divided into a “SM-like” and an “anomalous  $\kappa_{2V}$ -like” category depending on the value

of the discriminant trained to separate  $ggF$  and VBF. The categorization thresholds were chosen to maximize the expected sensitivity to VBF  $HH$  signals, and result in the assignment of about 25%–30% of the VBF  $\kappa_{2V} = 2$  events to the anomalous  $\kappa_{2V}$ -like category and 95% of SM VBF events to the SM-like category.

The large multijet background that originates from QCD and  $t\bar{t}$  hadronic processes is estimated from the data using background-dominated regions. Analysis signal ( $A_{\text{SR}}$ ) and control ( $A_{\text{CR}}$ ) regions are defined by requiring  $\chi < 25$  GeV and  $25 \leq \chi < 50$  GeV, respectively, where  $\chi$  is the distance from the expected peak position of the two Higgs boson candidates’ invariant masses and is defined as  $\chi = \sqrt{(m_{H_1} - c_1)^2 + (m_{H_2} - c_2)^2}$ , where  $c_1$  and  $c_2$  are as defined for the pairing of the four jets. Both  $A_{\text{SR}}$  and  $A_{\text{CR}}$  are divided into a four  $b$  jet ( $4b$ ) and three  $b$  jet ( $3b$ ) region by requiring the  $b$  jet candidate with the lowest DEEPIET output to satisfy or fail the medium WP of the discriminant, respectively. There are between 5.5 and 11 times more events in the  $3b$  region than in the  $4b$  region, depending on the topological category and data taking year considered. The overall efficiency for both  $ggF$  and VBF signal events to be selected in the  $A_{\text{SR}}^{4b}$  region ranges from 0.3% to 3% depending on the couplings considered and is minimal for the SM VBF production and for the  $ggF$  production with  $\kappa_\lambda \approx 5$  due to the interference effects in the  $HH$  production that result in low momenta of the Higgs bosons. The signal acceptance is mostly limited by the trigger acceptance and the jet  $b$  tagging efficiency.

Background events in the  $A_{\text{SR}}^{4b}$  region are modeled from events in the  $A_{\text{SR}}^{3b}$  region. The former represents the sensitive region of the analysis, while the latter provides a sample enriched in multijet background events with similar kinematic properties. Events in  $A_{\text{SR}}^{4b}$  were analyzed only after all the methods were defined and validated. The normalization is determined by scaling the observed number of events in  $A_{\text{SR}}^{3b}$  by a transfer factor computed as the ratio of the number of events in the  $A_{\text{CR}}^{4b}$  and  $A_{\text{CR}}^{3b}$  regions. Variations of the transfer factor depending on the position in the  $(m_{H_1}, m_{H_2})$  plane are accounted for by measuring it as a function of  $m_{\parallel}$ , defined as the projection of the point in the plane on the line  $m_{H_1} = (c_1/c_2)m_{H_2}$  that is used for the  $H$  candidate reconstruction. Higher values of  $m_{\parallel}$  are correlated with a higher average  $p_T$  of the selected jets.

Differences in the distributions of several variables between the  $3b$  and the  $4b$  regions are addressed with the BDT-based reweighting method described in Ref. [61], which uses a dedicated metric to identify the phase space regions with the largest differences in the distributions and compute an event weight to correct for them. This method accurately models multiple variables and their correlations, while minimizing issues related to the statistical uncertainties arising from the limited number of events in the two



regions. The BDT is trained in the  $A_{\text{CR}}^{4b}$  and  $A_{\text{CR}}^{3b}$  regions, and applied to events in  $A_{\text{SR}}^{3b}$  to model  $A_{\text{SR}}^{4b}$ .

Trainings of this BDT are performed separately for each  $ggF$  and VBF category. All trainings use as inputs the following ten variables:  $p_T$  of the four  $b$  jets,  $m_{HH}$ , the invariant masses and  $p_T$  of the  $H_1$  and  $H_2$  candidates, and the absolute value of their pseudorapidity difference ( $|\Delta\eta(H_1, H_2)|$ ). In the  $ggF$  category, ten additional variables are used: the magnitude of the scalar ( $\sum p_T$ ) and vector ( $p_T(HH)$ ) sums of the  $p_T$  of the four  $b$  jets, the angular  $\Delta R$  separations between the two jets that constitute  $H_1$  and  $H_2$  [ $\Delta R^{H_1}(bb)$ ,  $\Delta R^{H_2}(bb)$ ], the minimal  $\Delta R$  ( $\Delta R^{\text{min}}$ ) and the maximal  $|\Delta\eta|$  ( $|\Delta\eta|^{\text{max}}$ ) between all the possible  $b$  jet pairs, the absolute value of the angle with respect to the beam line of one Higgs boson in the four-jet reference frame ( $|\cos\theta^*|$ ) and of one jet of  $H_1$  in the  $H_1$  candidate reference frame ( $|\cos\theta_b^{H_1}|$ ), the sum of the resolution estimators of the three  $b$ -tagged jets with the best DEEPIET value ( $\sum R_e$ ), and the number of these three jets that satisfy the tight DEEPIET WP ( $N_b^T$ ). In the VBF category, four additional variables are used: the absolute value of the  $\phi$  separation between the two Higgs bosons, the VBF jets invariant mass and absolute value of the  $\eta$  separation, and the output of the production mode BDT discriminant. These variables are chosen as those that best represent the kinematic properties of the events in the  $3b$  and the  $4b$  regions and that provide separation between signal and background and are used in subsequent steps of the analysis.

The training parameters are optimized with a two-step procedure. First, a Kolmogorov-Smirnov distance test is used to ensure that the distributions of the BDT input variables in the target  $A_{\text{CR}}^{4b}$  region are compatible with the ones in the reweighted  $A_{\text{CR}}^{3b}$  region. Once that is verified, a BDT is trained to separate the  $A_{\text{CR}}^{4b}$  and reweighted  $A_{\text{CR}}^{3b}$  data, thus testing also the correlations of variables. All the training configurations that are chosen are required to have an area of 0.5 under the receiver operating curve of the discriminant, corresponding to no separation.

The procedure is validated by applying it to a signal-depleted region, defined by shifting the signal and control regions according to the definition of  $\chi$ , using as values of the center position  $c_1 = 179$  and  $c_2 = 172$  GeV. The center of this validation region is chosen to be along the  $m_{H_1} = 1.04m_{H_2}$  line used in the reconstruction of the  $H$  candidates to provide an accurate proxy of the analysis region. In analogy to the analysis regions, signal and control validation regions,  $V_{\text{SR}}$  and  $V_{\text{CR}}$ , are defined as  $\chi < 25$  GeV and  $25 \leq \chi < 50$  GeV, respectively. After training and applying the reweighting BDT in these regions and computing the normalization transfer factors, the data in  $V_{\text{SR}}^{4b}$  were found to be compatible within uncertainties with the predicted background, validating the modeling method. The agreement is quantified with a goodness-of-fit

test based on a saturated model [62] performed on the observables used in the analysis. For a fit under the background-only hypothesis, a  $p$  value of 53% is observed, ranging between 12% and 83% for the individual categories.

The impact on the estimated background from the presence of signal events in the  $A_{\text{SR}}^{3b}$  region due to jets failing the  $b$  tagging requirement is estimated by generating pseudodata in  $A_{\text{SR}}^{4b}$  according to the modeled background plus simulated  $HH$  signal, and fitting them under a different background hypothesis that includes the contribution from signal events in  $A_{\text{SR}}^{3b}$  weighted as done for background events. This study is repeated for signal yields up to five times larger than the expected sensitivity of this search, and in all cases a signal yield compatible with the true one is observed. We conclude that signal events in  $A_{\text{SR}}^{3b}$  do not have any significant impact on the background model and on the results.

For the background model, systematic uncertainties are considered for the limited number of events in the  $A_{\text{SR}}^{3b}$ . These uncertainties are uncorrelated across the individual bins of the background templates used for the statistical analysis, and correspond to the propagation of a bin-by-bin Poisson uncertainty from the  $A_{\text{SR}}^{3b}$  to the  $A_{\text{SR}}^{4b}$  region. The uncertainty in the estimation of the transfer factor from the  $3b$  to the  $4b$  region is computed from the statistical uncertainty in  $A_{\text{CR}}^{3b}$  and  $A_{\text{CR}}^{4b}$  and is 1%–2% for the  $ggF$  categories, 2%–3% for the SM-like VBF category and 18%–32% for the anomalous  $\kappa_2$   $\nu$ -like VBF category. An uncertainty is also considered for the limited number of events in the validation region, in some cases lower than the number of events in the analysis region. It is large (30%–33%) for the anomalous  $\kappa_2$   $\nu$ -like VBF category while it is about 2%–3% and below 1% for the other VBF category and the  $ggF$  categories, respectively, and represents the inherent limitation on the capability to validate the performance of the background model. For analysis categories where the agreement between the observed and predicted background yields in the validation region differs by more than 1 standard deviation, an additional uncertainty is included and ranges between 1.5% and 4.7%, depending on the category and year. Finally, the uncertainty in the performance of the reweighting method to interpolate the kinematics from  $A_{\text{CR}}$  into  $A_{\text{SR}}$  is estimated by performing alternative trainings in two regions of  $A_{\text{CR}}$ . The two regions are defined by requiring the product of  $m_{\perp}$  and  $m_{\parallel}$  to be either positive or negative, where  $m_{\perp}$  is defined as the projection of the point in the  $(m_{H_1}, m_{H_2})$  plane onto the axis perpendicular to the one corresponding to  $m_{\parallel}$  previously defined. The two regions correspond to four quadrants in the  $(m_{H_1}, m_{H_2})$  plane, and allow for tests of the capability of the reweighting method to model  $A_{\text{SR}}$ , starting from events with kinematic properties that are either similar ( $m_{\perp}m_{\parallel} < 0$ ) or that are harder or softer ( $m_{\perp}m_{\parallel} > 0$ )

compared to  $A_{\text{SR}}$ , thus testing the capability of the model to interpolate across different learning domains. The alternative background templates obtained from trainings in these regions represent the uncertainty on the shape of the predicted background distribution. All the uncertainties are independent between the 2016 and 2017–2018 background models. The dominant uncertainties in this search are those associated to the background modeling, and in particular the bin-by-bin and the normalization uncertainties due to the limited number of events in  $A_{\text{SR}}^{3b}$ ,  $A_{\text{CR}}^{3b}$ , and  $A_{\text{CR}}^{4b}$ .

The effects of the imperfect modeling of the detector response and the inaccurate simulation of signal processes are accounted for as systematic uncertainties. The most important sources of systematic uncertainty are the total integrated luminosity, the jet energy scale and resolution, the efficiency of the trigger and of the  $b$ -tagging requirements, the modeling of the pileup distribution, the  $HH \rightarrow b\bar{b}b\bar{b}$  branching fraction, and the parameters used for the generators. A specific uncertainty on the parton shower is considered for the VBF production mode. Uncertainties on the theoretically determined  $HH$  cross section are considered only when quoting a limit on the  $HH$  signal strength ( $\mu$ ), defined as the ratio of the value of the cross section limit relative to the theoretical cross section expectation in

the SM ( $\sigma_{HH}/\sigma_{HH}^{\text{SM}}$ ). These uncertainties are negligible in comparison to the background uncertainties. See Supplemental Material [57] for more details.

A multivariate BDT discriminant is trained with the XGBOOST software [63] in the two  $ggF$  subcategories to separate the signal from the weighted  $A_{\text{SR}}^{3b}$  background events. The discriminant uses as inputs  $p_T(H_1)$ ,  $p_T(H_2)$ ,  $m_{H_1}$ ,  $m_{H_2}$ ,  $|\Delta\eta(H_1, H_2)|$ ,  $m_{HH}$ ,  $p_T(HH)$ ,  $\Delta R^{H_1}(bb)$ ,  $\Delta R^{H_2}(bb)$ ,  $\Delta R^{\text{min}}$ ,  $|\Delta\eta|^{\text{max}}$ ,  $\sum p_T$ ,  $N_b^T$ ,  $\sum R_e$ ,  $|\cos\theta^*|$ , and  $|\cos\theta_b^*|$ . For each subcategory, a separate training is performed to separate the SM  $ggF$   $HH$  signal from the weighted  $A_{\text{SR}}^{3b}$  region data. Since the same  $A_{\text{SR}}^{3b}$  data are also used to model the background, this dataset is divided in two equal-size subsamples. Two trainings are performed on each half and applied to the other half, and the two partial background templates are added together. In this way, the full dataset can be used for the modeling, while the BDT discriminant is not evaluated on events used for its training. In the VBF SM-like category,  $m_{HH}$  is used as the discriminating variable, while in the anomalous  $\kappa_2$  V-like category, a counting experiment is performed because of the small number of expected background events. The distributions of these variables are shown in Fig. 1. For the

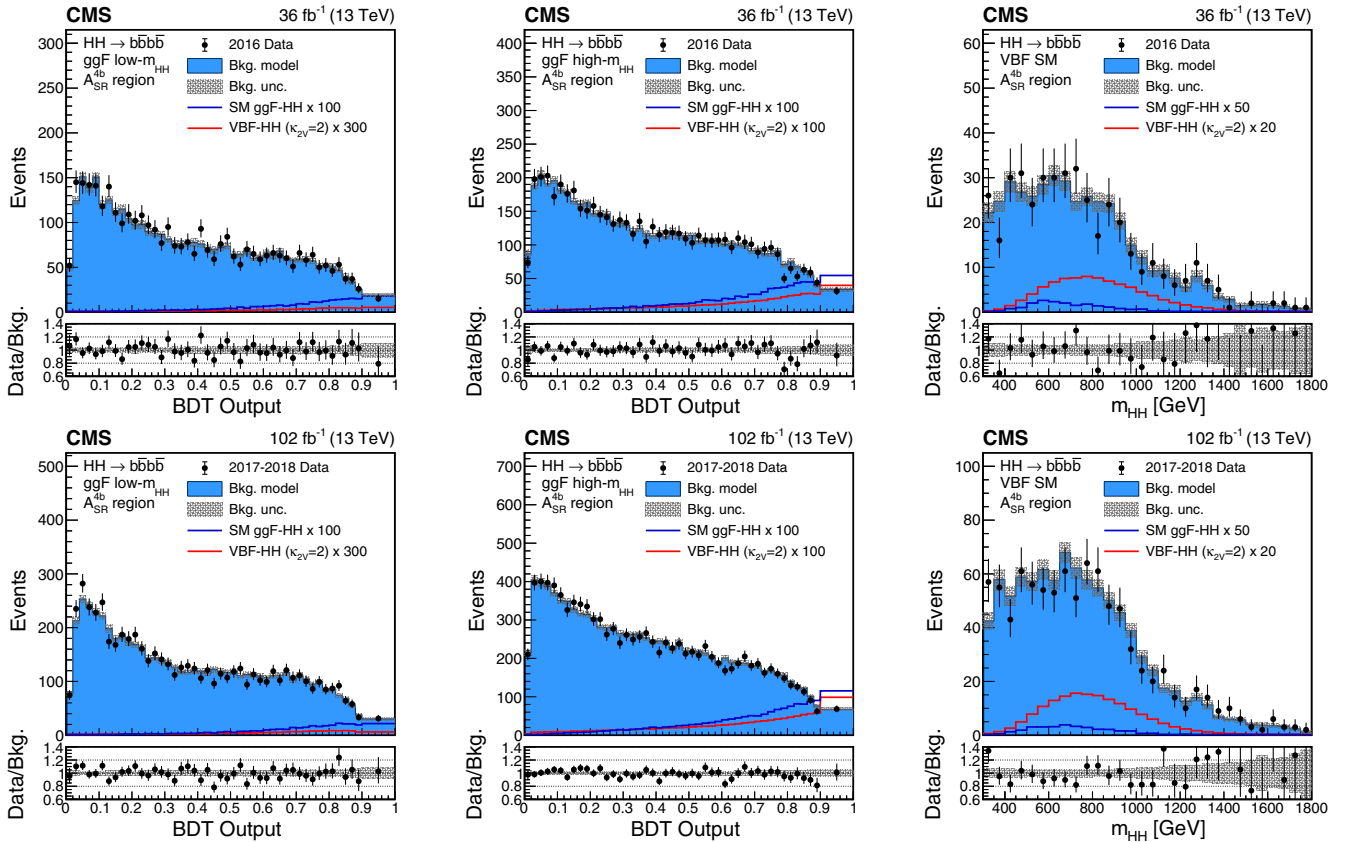


FIG. 1. Distributions of the events observed in the  $A_{\text{SR}}^{4b}$  signal region for 2016 (top) and 2017–2018 (bottom) data. The two leftmost columns show the BDT output in the low- and high-mass categories, and the rightmost column shows the  $m_{HH}$  distribution in the VBF SM-like category.

VBF anomalous  $\kappa_{2V}$ -like category in the 2016 (2017–2018) data set, 4 (13) events are observed for a total of  $4.0 \pm 1.3$  ( $15.0 \pm 3.4$ ) background and 1.5 (3.5) VBF  $\kappa_{2V} = 2$  signal events expected.

A binned maximum likelihood fit is simultaneously performed in all analysis categories, where the systematic uncertainties previously discussed are introduced as nuisance parameters. No deviation from a background-only hypothesis is observed. Results are used to set 95% CL upper limits on the  $HH$  production cross section using the modified frequentist  $CL_s$  criterion [64,65] with the profile likelihood ratio modified for upper limits [66] as the test statistics, and making use of the asymptotic approximation [67].

Figure 2 shows the 95% CL cross section upper limits as functions of the  $\kappa_\lambda$  and  $\kappa_{2V}$  values. The value of  $\kappa_\lambda$  is observed (expected) to be in the range  $-2.3 < \kappa_\lambda < 9.4$

( $-5.0 < \kappa_\lambda < 12.0$ ) at the 95% CL, while the value of  $\kappa_{2V}$  is observed (expected) to be in the range  $-0.1 < \kappa_{2V} < 2.2$  ( $-0.4 < \kappa_{2V} < 2.5$ ) at the 95% CL. The total  $HH$  production cross section, defined as the sum of the  $ggF$  and VBF production modes, is observed (expected) to be smaller than 120 (238) fb, corresponding to 3.9 (7.8) times the SM prediction, when uncertainties on the theoretical production cross section are included. The  $HH$  VBF production cross section is observed (expected) to be smaller than 226 (412) times the SM prediction. The deficit in the observed number of events localized around the BDT discriminant values of 0.85–0.9 in the  $ggF$  high-mass category in the 2017–2018 dataset, which provides the largest sensitivity to the signal, results in the observed limit to be below the expected one. Studies of the background model for the individual BDT input variables and the absence of deficit in the 2016 data in the same high-sensitivity region, and in the other categories suggest that this under fluctuation is of statistical nature.

The intervals containing 68% and 95% of the expected signal strength upper limits correspond to [5.5, 12.3] and [4.0, 18.7] ([291, 598] and [216, 846]) for the  $ggF$  (VBF) production modes, and the observed limit is thus compatible with the expectation within about 2 standard deviations. The sensitivity is mostly limited by the number of events in the signal and control regions of the analysis.

Tabulated results are available in the HEPData record of this analysis [68].

In summary, a search for the production of Higgs boson pairs via gluon and vector boson fusion in the four  $b$  quark decay channel has been presented. The data are found to be statistically compatible with the background-only hypothesis, and an observed (expected) upper limit at the 95% confidence level is set to 3.9 (7.8) times the SM prediction for the combined  $ggF$  and VBF  $HH$  cross section. The value of the Higgs boson self-coupling, normalized to the SM expectation, is observed (expected) to be in the range  $-2.3 < \kappa_\lambda < 9.4$  ( $-5.0 < \kappa_\lambda < 12.0$ ), and the value of the coupling of Higgs boson pairs to vector boson pairs, normalized to the SM expectation, to be in the range  $-0.1 < \kappa_{2V} < 2.2$  ( $-0.4 < \kappa_{2V} < 2.5$ ). These are the most stringent observed constraints to date on the  $HH$  production cross sections and on the  $\kappa_{2V}$  coupling.

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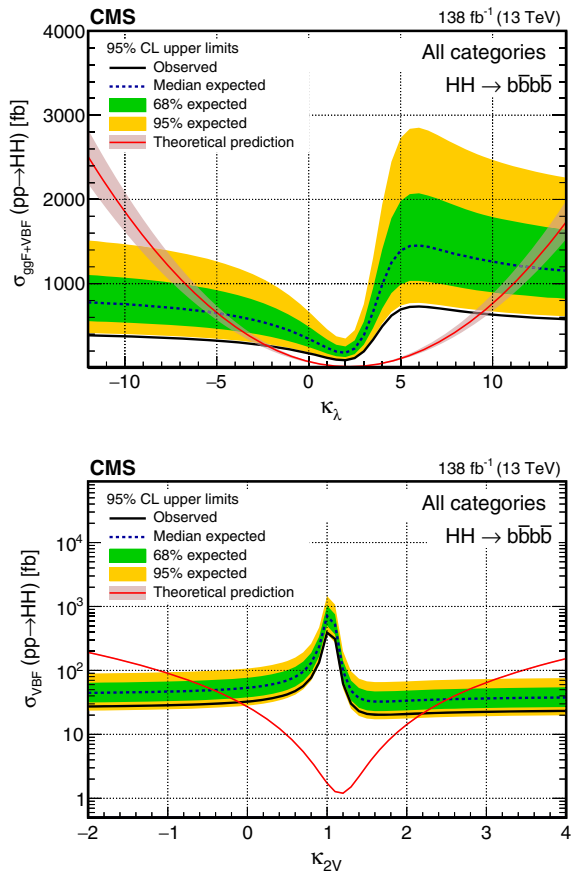


FIG. 2. Observed and expected 95% CL upper limits on the  $\sigma_{ggF+VBF} HH$  cross section as a function of  $\kappa_\lambda$  (left), and on the  $\sigma_{VBF} HH$  cross section as a function of  $\kappa_{2V}$  (right). The green (yellow) band indicates the regions containing 68% (95%) of the limit values expected under the background-only hypothesis. The red lines denote the theoretical cross section expectation assuming that other couplings are set to the SM prediction. For the cross section limit as a function of  $\kappa_{2V}$ , the  $ggF$   $HH$  production is assumed to correspond to the SM prediction.



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