

CERN-EP-2018-269
2019/04/22

CMS-HIG-17-017

Search for nonresonant Higgs boson pair production in the $b\bar{b}b\bar{b}$ final state at $\sqrt{s} = 13$ TeV

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Abstract

Results of a search for nonresonant production of Higgs boson pairs, with each Higgs boson decaying to a $b\bar{b}$ pair, are presented. This search uses data from proton-proton collisions at a centre-of-mass energy of 13 TeV, corresponding to an integrated luminosity of 35.9 fb^{-1} , collected by the CMS detector at the LHC. No signal is observed, and a 95% confidence level upper limit of 847 fb is set on the cross section for standard model nonresonant Higgs boson pair production times the squared branching fraction of the Higgs boson decay to a $b\bar{b}$ pair. The same signature is studied, and upper limits are set, in the context of models of physics beyond the standard model that predict modified couplings of the Higgs boson.

Published in the Journal of High Energy Physics as doi:10.1007/JHEP04(2019)112.

1 Introduction

The detailed understanding of the properties of the Higgs boson (H) discovered in 2012 by the CERN LHC experiments [1–3] remains an important subject in fundamental physics. Current determinations of the properties of the new particle by the ATLAS and CMS Collaborations are found to be in agreement with standard model (SM) predictions [4, 5]. However, there are still many measurements that could reveal unexpected deviations from the SM. A number of models of physics beyond the SM (BSM) can be tested using their predictions of the properties of the observed state, including the Higgs boson self-coupling and couplings to bosons and fermions [6–10].

The production of Higgs boson pairs (HH) is the most direct way to access the Higgs boson self-coupling [11] and to study in detail the SM Higgs potential. The HH production cross section predicted by the SM for 13 TeV proton-proton (pp) collisions and $m_H = 125.09 \text{ GeV}$ [5, 12] is $33.49^{+4.3\%}_{-6.0\%}(\text{scale}) \pm 2.3\%(\alpha_S) \pm 2.1\%(\text{PDF}) \text{ fb}$ [13–17], where the uncertainty is due to the variation of the renormalization (μ_R) and factorization (μ_F) scales (scale), the strong coupling constant (α_S) uncertainties, and the uncertainty in parton distribution functions (PDF). The predicted cross section results in a low expected event rate, and the acceptance for HH events in the detector is small. This means that the SM HH production process cannot be observed with the data collected so far at the LHC: the expectation is that it will only be possible to set an upper limit on the HH production cross section, as discussed, e.g. in Refs. [18, 19]. However, the cross section can be enhanced by anomalous couplings in BSM models [20] and in some cases the enhancement is large enough that HH production could be observed with the current data.

The first searches for nonresonant HH production were performed by LHC experiments using pp collisions data at $\sqrt{s} = 8 \text{ TeV}$ [21, 22]. The data collected in 2015 and 2016 at $\sqrt{s} = 13 \text{ TeV}$ were used for improved analyses in the decay channels: $b\bar{b}b\bar{b}$ [19], $b\bar{b}l\nu l\nu$ [23], $b\bar{b}l\nu q\bar{q}$ [24], $b\bar{b}\tau\tau$ [18, 25], $b\bar{b}\gamma\gamma$ [26, 27], $\gamma\gamma WW^*$ [28], and WW^*WW^* [29]. An additional search in the $b\bar{b}b\bar{b}$ decay channel focused on the region of phase space where one $b\bar{b}$ pair is highly Lorentz-boosted and is reconstructed as a single large-area jet [30]. In the cases mentioned above, at least one of the two Higgs bosons is required to decay to $b\bar{b}$ to exploit the large branching fraction of this decay. Results were found to be compatible within uncertainties to the expected SM background contribution. The measurement of nonresonant HH production at the LHC with the tightest expected upper limit (15 times the SM rate) was made in the $b\bar{b}\tau\tau$ channel [25], yielding an observed upper limit equivalent to 13 times the SM rate.

This article reports the results of a search for HH production with both Higgs bosons decaying into bottom quark pairs, resulting in four resolved hadronic jets. The search is performed using 13 TeV pp collisions data corresponding to an integrated luminosity of 35.9 fb^{-1} , collected by the CMS detector in 2016. The final state containing four b quarks has the highest branching fraction of all possible HH final states, corresponding to ≈ 0.339 for an SM Higgs boson with a mass of 125 GeV. It is one of the most sensitive signatures for the investigation of HH production, as confirmed by the results of a similar search recently performed by the ATLAS Collaboration [19]. The main challenge for this analysis is the large background from multijet final states produced by quantum chromodynamics (QCD) processes, which collectively yield rates exceeding that of the signal by several orders of magnitude. We address this by fully exploiting the distinctive features of the signal: the presence of four b quarks and the kinematical properties of the decay process. In a sample selected by requiring four b quark jets, a multivariate event classifier is trained to discriminate signal from background. This sample is studied by comparing it to a model of all contributing background processes, which is completely based

on data. Because of the use of different data sets, triggers, and offline selection requirements, this analysis is fully independent from the CMS searches mentioned above [18, 23, 26, 30].

2 Beyond-the-standard-model extensions

In the SM, HH production occurs predominantly by gluon-gluon fusion (ggF) via an internal fermion loop, where the top quark (t) contribution is dominant. In the absence of new light states, the ggF HH production at the LHC can be generally described (considering operators up to dimension 6) by five parameters controlling the tree-level interactions of the Higgs boson. Without considering CP violating effects, the relevant part of the Lagrangian then takes the form:

$$\mathcal{L}_H = \frac{1}{2} \partial_\mu H \partial^\mu H - \frac{1}{2} m_H^2 H^2 - \kappa_\lambda \lambda_{SM} v H^3 - \frac{m_t}{v} (v + \kappa_t H + \frac{c_2}{v} HH) (\bar{t}_L t_R + \text{h.c.}) + \frac{1}{4} \frac{\alpha_S}{3\pi v} (c_g H - \frac{c_{2g}}{2v} HH) G^{\mu\nu} G_{\mu\nu}. \quad (1)$$

This Lagrangian follows from extending the SM with operators of mass dimension between four and six in the framework of an effective field theory [31], encoding the effects of new heavy states currently beyond experimental reach. The five parameters of the Lagrangian, named κ_λ , κ_t , c_g , c_{2g} , and c_2 , are related to the Higgs boson couplings. In particular, the multiplicative factors $\kappa_\lambda = \lambda_{HHH}/\lambda_{SM}$ and $\kappa_t = y_t/y_{SM}$ parametrize deviations from the SM values of, respectively, the Higgs boson trilinear coupling and the top quark Yukawa coupling. The former is given by $\lambda_{SM} = m_H^2/2v^2$, with v being the vacuum expectation value of the Higgs field. The absolute couplings c_g , c_{2g} , and c_2 parametrize contact interactions not predicted by the SM, i.e. the coupling of the Higgs boson to gluons and those of the two Higgs bosons to two gluons or to a top quark-antiquark pair, which could arise through the mediation of very heavy new states. In Eq. (1), m_t is the mass of the top quark, and $G^{\mu\nu}$ the gluon field. We neglect possible modifications of the bottom quark Yukawa coupling κ_b , which is already constrained by LHC data [32]. The Feynman diagrams contributing to HH production in pp collisions at leading order (LO) are shown in Fig. 1. The translation of the above parametrization to the

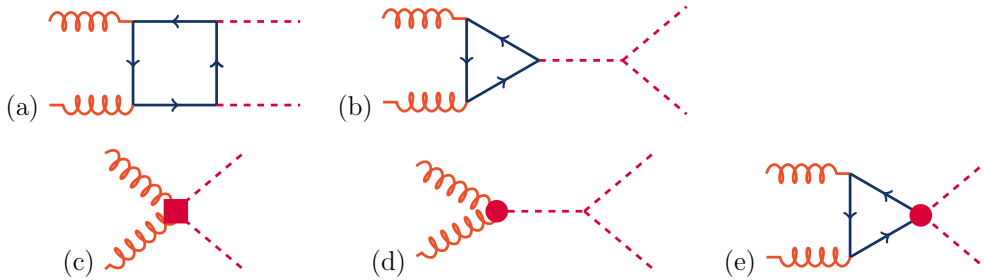


Figure 1: Feynman diagrams that contribute to HH production via gluon-gluon fusion at LO. Diagrams (a) and (b) correspond to SM-like processes, while diagrams (c), (d), and (e) correspond to pure BSM effects: (c) and (d) describe contact interactions between the Higgs boson and gluons, and (e) describes the contact interaction of two Higgs bosons with top quarks.

flavour-diagonal Higgs basis (as discussed in Ref. [31]) is trivial; we use the notation of Eq. (1) for simplicity.

The parameter space for the Higgs boson couplings in a BSM scenario has five dimensions. Constraints on the ranges of the five parameters come from measurements of single Higgs boson production already performed at the LHC, as well as other theoretical considerations [33]. However, the allowed phase space is still large and a precise scan is not feasible. The kinematical properties of the pair-produced Higgs bosons depend strongly on the values of those five couplings. A statistical approach has been developed in order to identify regions of the parameter space that have similar final state kinematical properties. The approach uses the generator-level distributions of the invariant mass of the HH system ($m_{\text{HH}}^{\text{gen}}$) and the modulus of the cosine of the polar angle of one Higgs boson with respect to the beam axis ($|\cos \theta_{\text{gen}}^*|$) to cluster the points in the parameter space. In each region found, a representative benchmark model is selected as the point having most similar kinematical properties to the other points in the region. The procedure, described in Ref. [33], leads to twelve benchmarks that taken together best represent, within a limited uncertainty, the phenomenology of the whole five-dimensional space. An additional benchmark (box), representative of the null Higgs boson self-coupling hypothesis, is also considered. The parameter values of the benchmarks are listed in Table 1. The search for BSM signals presented here is focused on these benchmarks.

Table 1: The values of the anomalous coupling parameters for the 13 benchmark models studied [33]. For reference, the values of the parameters in the SM are also included.

Benchmark point	κ_λ	κ_t	c_2	c_g	c_{2g}
1	7.5	1.0	-1.0	0.0	0.0
2	1.0	1.0	0.5	-0.8	0.6
3	1.0	1.0	-1.5	0.0	-0.8
4	-3.5	1.5	-3.0	0.0	0.0
5	1.0	1.0	0.0	0.8	-1.0
6	2.4	1.0	0.0	0.2	-0.2
7	5.0	1.0	0.0	0.2	-0.2
8	15.0	1.0	0.0	-1.0	1.0
9	1.0	1.0	1.0	-0.6	0.6
10	10.0	1.5	-1.0	0.0	0.0
11	2.4	1.0	0.0	1.0	-1.0
12	15.0	1.0	1.0	0.0	0.0
Box	0.0	1.0	0.0	0.0	0.0
SM	1.0	1.0	0.0	0.0	0.0

3 The CMS detector

The CMS detector is a multipurpose apparatus designed to reconstruct the high-energy interactions produced by the LHC. Its central feature is a superconducting solenoid with an internal diameter of 6 m. The solenoid generates a magnetic field of 3.8 T inside a volume occupied by four main sub-detectors, each composed of a barrel and two endcap sections: silicon pixel and strip tracker detectors, a lead tungstate crystal electromagnetic calorimeter (ECAL), and a brass and scintillator hadron calorimeter (HCAL). The pixel tracker provides an impact parameter resolution for charged tracks of about $15 \mu\text{m}$, which allows for a precise reconstruction of secondary vertices, crucially used to identify jets originating from the hadronization of b quarks (b jets). Muons are measured in gas-ionization detectors embedded in a steel flux return yoke outside the solenoid. Information from the calorimeters and muon detectors is used by the first level of the CMS trigger [34], a system based on custom hardware processors that provides the first online event selection. The second level of the CMS trigger, also called high-level trigger

and consisting of a farm of processors running a version of the full event reconstruction software optimized for fast processing, further selects events using information from the whole detector before sending them downstream for detailed processing and storage. Particles produced in the pp collisions are detected in the pseudorapidity range $|\eta| < 5$. Pseudorapidity is defined as $|\eta| = -\ln \tan(\theta/2)$, where the polar angle θ is measured from the z-axis, which points along the beam direction toward the Jura mountains from LHC Point 5. A more detailed description of the CMS detector can be found in [35].

4 Data sets

The online event selection for the data used in this analysis is designed to select a sample of multijet events enriched with b quark decays, reducing the rate from the QCD multijet background with light quarks and gluons. The combined secondary vertex (CSVv2) algorithm [36] is used to identify b jets. This algorithm exploits the relatively long lifetime of hadrons containing b quarks ($c\tau \sim 450 \mu\text{m}$), which results in a displaced decay point of the produced b hadrons. The reconstructed trajectories of charged decay products from b hadrons thus exhibit significant impact parameters with respect to the b quark production point. The CSVv2 algorithm uses the impact parameter information together with information on other characteristics of the jets to discriminate jets originating from b quarks from those produced by the hadronization of light quarks or gluons. Two trigger paths contribute to the online selection. In the first trigger path jets are considered if their momentum transverse to the beam direction, p_T , is above 30 GeV and $|\eta| < 2.6$. Selected events must contain at least four such jets of which at least three are tagged as b jets by the CSVv2 algorithm and at least two have $p_T > 90$ GeV. The second trigger path requires at least four jets with $p_T > 45$ GeV with at least three tagged as b jets by the CSVv2 algorithm. The logical OR between these two selections provides the data used in this analysis.

The production of nonresonant HH in the SM is simulated following the prescriptions of Ref. [37] at LO with MADGRAPH5_aMC@NLO 2.2.2 [38] used as the generator. Loop factors are calculated on an event-by-event basis and applied to an effective model, from Ref. [37]; the NNPDF30_lo_as_0130_nf4 PDF set [39] is used. In addition, for the study of BSM models involving anomalous Higgs boson couplings, we generate for each of the parameter space points listed in Table 1 a set of 300 000 simulated events.

The 14 simulated signal samples are added together to obtain a larger signal sample. We will refer to this ensemble of events as the Pangea sample. This sample is then reweighted to reproduce the physics of any particular point in the BSM phase space. The weights are obtained by looking at the matrix element information for m_{HH}^{gen} and $\cos \theta_{\text{gen}}^*$ from dedicated simulations, as described in Ref. [40]. The numbers of events used to determine the weights at generator level are 3 000 000 for the SM sample and 50 000 for each BSM benchmark. In the following, we always use the Pangea sample instead of the 14 original samples to study signal properties in each model considered.

Although our search employs an approach fully based on data to model backgrounds, we make use of a simulation of QCD processes for several cross-checks. This simulation consists of a collection of seven simulated data sets of contiguous ranges in the H_T^{gen} variable, which is defined as the scalar sum of the p_T of all partons that originate from the hard-scattering process in a simulated event. The samples are generated by MADGRAPH5_aMC@NLO 2.2.2 at LO, using the NNPDF30_lo_as_0130 set, and are then interfaced with PYTHIA 8.212 [41] for fragmentation and parton showering, using the MLM matching [42]; their equivalent integrated

luminosity depends on the H_T^{gen} range considered and increases from 0.06 to 400 fb⁻¹ as H_T^{gen} varies between 200 and 2000 GeV. For additional studies of the sub-dominant background from top quark pairs, a large next-to-leading order (NLO) POWHEG 2.0 [43–45] sample of inclusive $t\bar{t}$ [46] events is used. The behaviour of minor backgrounds is verified and a study of their contamination of our selected sample is carried out using POWHEG 2.0 NLO samples of single top quark t channel [47], $t\bar{t}H$ [48], single Higgs boson production [49], and associated ZH production [50]. In addition, we use single top quark s channel, $t\bar{t}t\bar{t}$, $t\bar{t}b\bar{b}$, and $b\bar{b}H$ samples generated with MADGRAPH5_aMC@NLO 2.2.2 at NLO. All of those samples are interfaced with PYTHIA 8.212 for parton showering and fragmentation. The $t\bar{t}$ sample utilises the generator tune CUETP8M2T4 [51] for the underlying event activity, other samples interfaced with PYTHIA use the tune CUETP8M1 [52]. The $t\bar{t}$, $t\bar{t}H$, single Higgs boson, and ZH samples are generated using the NNPDF30_nlo_as.0118 PDF set. The single top quark, $t\bar{t}b\bar{b}$, and $b\bar{b}H$ samples are generated with the NNPDF30_nlo_nf.4.pdfas set. The NNPDF30_nlo_nf.5.pdfas set is used to generate the $t\bar{t}t\bar{t}$ sample. All of the PDF sets are taken from the LHAPDF6 set [53]. The response of the CMS detector is modelled using GEANT4 [54].

Finally, in order to study possible discrepancies between the efficiency of the triggers used in our data selection and their modelling by the simulation, we compare the effect of b jet selection requirements on data collected by a trigger requiring a single isolated muon of $p_T > 18$ GeV with its simulation, using a mixture of events from $t\bar{t}$ /single-top described above and a MADGRAPH5_aMC@NLO 2.2.2 W+jets LO sample using the MLM matching, weighted appropriately, and a W+jets sample generated using the NNPDF30_lo_as.0130 PDF set.

5 Event reconstruction

Global event reconstruction is performed by the particle-flow (PF) algorithm [55], which aims to reconstruct and identify each individual particle in an event, with an optimized combination of information from the various elements of the CMS detector. In this process, the identification of the particle type (photon, electron, muon, charged hadron, neutral hadron) plays an important role in the determination of the particle direction and energy. Electrons (e.g. coming from photon conversions in the tracker material or from b hadron semileptonic decays) are identified as a primary charged particle track and one or more ECAL energy clusters corresponding to this track extrapolation to the ECAL and to possible bremsstrahlung photons emitted along the way through the tracker material. Muons (e.g. from b hadron semileptonic decays) are identified as a track in the central tracker consistent with either a track or several hits in the muon system, associated with an energy deficit in the calorimeters. The objects primarily considered in this analysis are hadronic jets, composed of particles produced by quark fragmentation and hadronization. The energy of charged hadrons is determined from a combination of their momentum measured in the tracker and the matching ECAL and HCAL energy deposits, corrected for zero-suppression effects and for the response function of the calorimeters to hadronic showers. The energy of neutral hadrons is obtained from the corresponding corrected ECAL and HCAL energy. Jets are reconstructed from PF candidates using the anti- k_T clustering algorithm [56] with a distance parameter of 0.4, as implemented in the FASTJET package [57]. Jet energy corrections are applied to both data and simulation to scale the energy and correct for differences in the detector response in real and simulated collisions [58]. Jet identification criteria are also applied in order to reject fake jets from detector noise and jets originating from primary vertices not associated with the hard interaction [59]. The combined multivariate algorithm (cMVA_{v2}) [36] is used in the offline analysis to identify jets that originate from the hadronization of b quarks. The cMVA_{v2} builds on the CSV algorithm by adding soft-lepton information to the combined discriminant. The value of the multivariate discriminant used de-

depends on the required suppression of jets from light quarks and gluons. The medium working point of the cMVA_{v2}, defined such that the misidentification rate of light quarks and gluons as b jets is 1%, is used in this analysis. For jets produced by the hadronization of b quarks emitted in HH production events, the medium working point corresponds to a b-tagging efficiency of about 65% for the jets of interest of this analysis.

A weight is applied to each Monte Carlo (MC) event in order to match the distribution of the number of primary interactions per event in data (pileup correction), thus reproducing the effect on the selection efficiency of the varying instantaneous luminosity conditions incurred during data taking. The simulated events are also weighted to account for measured differences in the b tagging efficiency between data and simulation [36]. The trigger efficiency for signal events is evaluated using a full simulation of the trigger [34]. The correction factor for the efficiency is found to be 0.96 ± 0.02 based on measurements performed in b-tag multiplicity categories, using a top-pair enriched sample collected with an inclusive muon trigger.

6 Analysis strategy

The focus of this search is the study of nonresonant production of HH in the $b\bar{b}b\bar{b}$ final state, as predicted by the SM and by several BSM extensions. The analysis is optimized for sensitivity to the SM signal. We use the same selection to extract limits on the HH production cross section for the BSM models.

The offline selection, performed on all data events passing one of the two trigger paths described in Section 4, aims at increasing the fraction of data events containing two Higgs boson candidates decaying into b quark jet pairs. This includes a preliminary selection of events where four or more jets have been b-tagged by the cMVA_{v2}. Although this selection significantly reduces the QCD multijet background rate, this background still dominates the selected data, with contributions from events where light quark or gluon jets are mistagged by the cMVA_{v2} and events containing heavy quarks.

After the selection of events with four or more b tags, each reconstructed Higgs boson candidate is composed of a pair of b jets, referred to in the following as “a dijet system” or simply “dijet”. A boosted decision tree (BDT) classifier [60] is then trained to exploit the observable differences between the SM signal and the background. Finally, a search for a signal contribution to the selected data and an extraction of an upper limit in the number of selected signal events is performed by means of a binned fit to the distribution of the BDT classifier output. The limit on the number of events is converted to a limit on the HH production cross section times the square of the branching fraction of the Higgs boson into a $b\bar{b}$ pair, using the corresponding integrated luminosity and the computed signal efficiency.

Both the optimization of the BDT classifier and the extraction of upper limits on HH production require an accurate modelling of the multijet background. Unfortunately, the precise simulation of QCD processes yielding a large number of final-state partons is notoriously hard, as MC simulations are not complete to beyond LO; in addition, the very large production cross section for those processes makes it wholly impractical to produce simulated data sets corresponding to an integrated luminosity comparable to that of collision data. To address these issues, a dedicated method, fully based on data, was developed to produce a precise model of the kinematical behaviour of background events. This is described in detail in Section 8.

7 Event selection

The events of interest are identified by a jet-based selection applied to data collected by the triggers described in Section 4, as well as to all simulated samples. Jets are required to have $p_{Tj} > 30 \text{ GeV}$ and $|\eta_j| < 2.4$. We require at least four such jets ($N_j \geq 4$) and these need to be defined as b-tagged jets by the medium working point of the cMVA2 ($N_b \geq 4$). These criteria strongly reduce the QCD multijet background and select HH production events where the final state can be fully reconstructed. The number of selected events in the data set studied is 184 879.

The efficiencies for the SM signal are listed in Table 2. The efficiency for the 13 BSM points varies from -40% to +10% compared to the SM values. The average number of jets per selected event is ≈ 5 . The four jets with the highest cMVA2 discriminant values are considered as the decay products of two Higgs boson candidates. The pairing of the four jets into Higgs boson candidates is performed by considering the invariant mass of the two dijet candidates calculable for the three possible pairings, and computing the absolute mass differences $\Delta M_{klmn} = |M_{kl} - M_{mn}|$, where the $klmn$ indices run on the three permutations of the four jets. The combination resulting in the smallest mass difference between the two dijet systems is chosen as the one best describing the decay topology. This procedure results in a correct pairing of the b quarks to Higgs bosons in 54% of the cases, as tested on the Pangea MC signal sample. The two selected dijets are then labelled as “leading” and “trailing” according to their invariant mass value. This procedure, which does not explicitly use the known mass of the Higgs boson, allows the dijet masses for the selected combinations to retain the power to discriminate the HH production signal from the background.

Table 2: Cut-flow efficiency for the SM signal $pp \rightarrow HH \rightarrow b\bar{b}b\bar{b}$; the efficiency and the relative reduction of each successive selection step is shown. The number of expected SM signal events for an integrated luminosity of 1 fb^{-1} is also reported.

	Produced	Trigger	$\geq 4 \text{ b tags}$
N events / fb	11.4	3.9	0.22
Relative eff.		34%	5.6%
Efficiency		34%	1.9%

A multivariate technique is used in order to improve the sensitivity of the analysis. A BDT discriminator is trained to distinguish the SM signal from backgrounds (as described in Section 8), using the XGBOOST library [60]. All 13 BSM models use the same BDT as the SM to distinguish signal from background. We supply the BDT algorithm with a set of variables describing the kinematical properties of the event. The list of variables is pruned to discard those not contributing to the overall discrimination power of the algorithm. In Table 3 we list the variables chosen to build the classifier. In order to characterise the HH system we use as mass variables the invariant mass of the HH system (M_{HH}), an estimator of the combined mass of the HH system, M_X (defined by Eq. 2 below), and the invariant masses of the reconstructed Higgs boson candidates (M_{H_1}, M_{H_2}). The p_T of the HH system and of each Higgs boson candidate ($p_T^{H_1 H_2}, p_T^{H_1}$ and $p_T^{H_2}$) are used as well as the $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$ and $\Delta\phi$ angles between the jets that form each reconstructed Higgs boson ($\Delta R_{jj}^{H_1}, \Delta R_{jj}^{H_2}, \Delta\phi_{jj}^{H_1}$ and $\Delta\phi_{jj}^{H_2}$). Additionally, we use the θ^* angles between the HH system and the leading Higgs boson candidate, $\cos\theta_{H_1 H_2 - H_1}^*$, and between the leading Higgs boson candidate and the leading jet, $\cos\theta_{H_1 - j_1}^*$. We further use the following jet-related variables: the p_{Tj}^i and η_j^i ($i = 1-4$) of the four jets with the highest values of the cMVA2 discriminant, the scalar p_T sum of the jets in the event (H_T), and of the jets that are not part of the reconstructed HH system (i.e. the rest of the jets, H_T^{rest}). The cMVA2 values

of the third and fourth jets sorted by cMVA_{v2} value ($CMVA_3$ and $CMVA_4$) are also used. The estimator, M_X , of the mass of the system of two Higgs bosons is constructed as:

$$M_X = m_{4j} - \left(M_{H_1} - m_H \right) - \left(M_{H_2} - m_H \right), \quad (2)$$

where $m_H = 125 \text{ GeV}$. Even though M_X is strongly correlated with other variables used in the BDT, its use improves the discrimination power.

The invariant masses of the reconstructed Higgs boson candidates are the variables with the largest discrimination power, but all the variables used make significant contributions to the classifier.

Table 3: List of BDT input variables.

HH system	H candidates	Jet variables
$M_X, M_{HH},$ $p_T^{H_1 H_2}$ $\cos \theta_{H_1 H_2 - H_1}^*$	M_{H_1}, M_{H_2} $p_T^{H_1}, p_T^{H_2}$ $\cos \theta_{H_1 - j_1}^*$ $\Delta R_{jj}^{H_1}, \Delta R_{jj}^{H_2}, \Delta \phi_{jj}^{H_1}, \Delta \phi_{jj}^{H_2}$	$p_{Tj}^{(i=1-4)}, \eta_j^{(i=1-4)},$ H_T^{rest}, H_T $CMVA_3, CMVA_4$

We use 60% of the Pangea sample for training the classifier. The remaining 40% of the Pangea sample is employed for the validation (20%) and application (20%) steps; this splitting has been found to produce maximal sensitivity to a possible HH signal. As a background sample, an artificial data set constructed with a custom mixing procedure, as described in Section 8, is employed.

8 The background model

A method exploiting collision data only, based on hemisphere mixing, has been developed [61] to perform two separate tasks: first, to provide input to the training of the BDT classifier; and second, to reproduce the expected shape of the BDT output in background-only events. The method does not require the presence of signal-depleted sidebands in order to extract a background estimation; in fact, it aims at creating an artificial background data set using the whole original data set as the input. Thus, rather than a model of a single distribution, a full model of the original data is produced.

8.1 The hemisphere mixing technique

The basic concept at the heart of the method is to divide each data event in two hemispheres. The collection of hemispheres can then be used to create new events by recombining them in pairs. To create a good background model, the kinematical properties of the new events must be as similar as possible to the ones of the original data but also insensitive to the possible presence of signal. In order to define the hemispheres, we use the transverse thrust axis. This is defined as the axis on which the sum of the absolute values of the projections of the p_T of the jets is maximal, and correspondingly, transverse thrust (T) is the value of this sum. Once the transverse thrust axis is identified, the event is divided into two halves by cutting perpendicular to the transverse thrust axis. One such half is called a hemisphere (h). In a preliminary step, each event in the original N -event data set is split into two hemispheres that are collected in a library of $2N$ elements. Once the library is created, each event is used as a basis for creating artificial events. These are constructed by picking two hemispheres from the library that

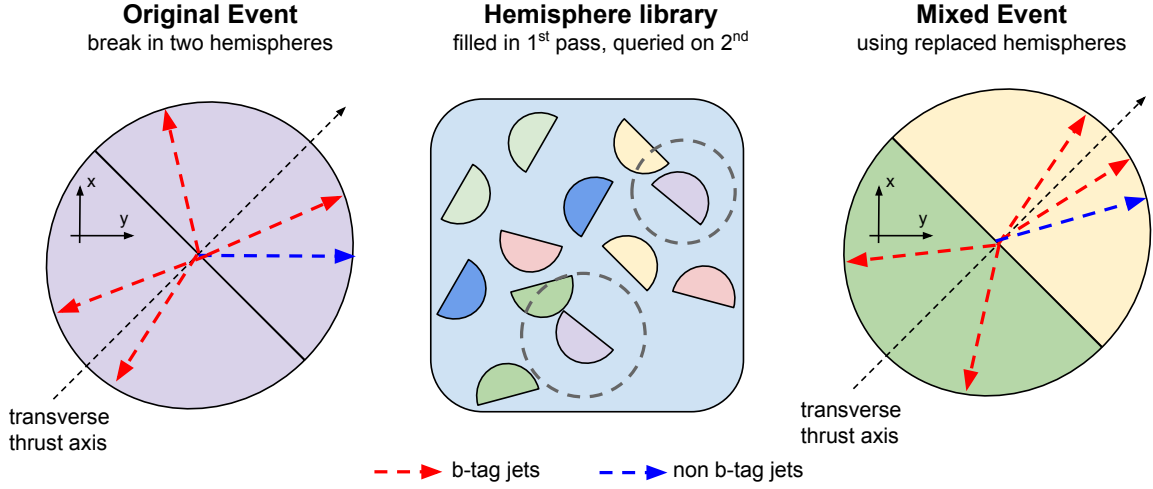


Figure 2: An illustration of the hemisphere mixing procedure. The transverse thrust axis is defined as the axis on which the sum of the absolute values of the projections of the p_T of the jets is maximal. Once the thrust axis is identified, the event is divided into two halves by cutting along the axis perpendicular to the transverse thrust axis. One such half is called a hemisphere (h). In a preliminary step, each event in the original N -event data set is split into two hemispheres that are collected in a library of $2N$ hemispheres. Once the library is created, each event is used as a basis for creating artificial events. These are constructed by picking two hemispheres from the library that are similar to the two hemispheres that make up the original event.

are *similar*, according to a measure defined below, to the two hemispheres that make up the original event. An illustration of the procedure can be found in Fig. 2.

The number of jets N_j^h and number of b-tagged jets N_b^h in each hemisphere, together with four jet-related variables, are used to define a hemisphere similarity criterion. The four variables are the combined invariant mass of all jets contained in the hemisphere M_{tot}^h , transverse thrust of the hemisphere T^h , the scalar sum of the projections of the p_T of all the jets onto the axis orthogonal to the thrust axis on the transverse plane, T_a^h , the projection of the vectorial sum of the momenta of the jets along the beam axis, Σp_z^h . If we label the original hemisphere o , and q the one in the library that is compared to o , the number of jets in o and q is required to be equal, $N_j^o = N_j^q$, and also the number of b-tagged jets are required to be equal, $N_b^o = N_b^q$. These two requirements are used to maintain the topology of the original events and to avoid introducing events that would not pass the selection described in Section 7 (e.g. by combining a hemisphere with 2 jets with a hemisphere with 1 jet, resulting in an event with 3 jets). The requirement for equal numbers of jets is waived for the infrequently occurring pairs of hemispheres that both have at least four jets and at least four b-tagged jets. For each hemisphere q in the library fulfilling the above criteria, a multidimensional distance from hemisphere o is computed using the four jet-related variables, as follows:

$$D(o, q)^2 = \frac{(M_{\text{tot}}^o - M_{\text{tot}}^q)^2}{V(M_{\text{tot}})} + \frac{(T^o - T^q)^2}{V(T)} + \frac{(T_a^o - T_a^q)^2}{V(T_a)} + \frac{(|\Sigma p_z^o| - |\Sigma p_z^q|)^2}{V(\Sigma p_z)}. \quad (3)$$

In the equation above, $V(x)$ represents the variance for the variable x , within the subset of events of given N_b and N_j characterizing the hemisphere in question. Once all $D(o, q)$ are computed, the k th nearest-neighbour hemisphere in the library, with $k \geq 1$ (i.e. the one such

that $0 = D(o, 0) < \dots < D(q, k)$ can be chosen to model the corresponding hemisphere of the original event; the nearest hemisphere, corresponding to $k = 0$, is by construction the original one. We match the Σp_z variables by considering only their absolute value (assuming forward-backward symmetric detector acceptance to jets, as is safe to do in the case of the CMS detector) and invert the sign of jet Σp_z components in one of the two matched hemispheres (q_1 and q_2) if $\text{sgn}(\Sigma p_z^{o_1} \Sigma p_z^{o_2}) \neq \text{sgn}(\Sigma p_z^{q_1} \Sigma p_z^{q_2})$, where indices o_1 and o_2 are the two hemispheres of the original event. Finally, the four-vectors of the jets contained in the two hemispheres are rotated along the ϕ coordinate to match the original transverse thrust axis of the modelled event. To keep track of the distance criterion used to choose each hemisphere, the artificial event may be labelled as (k_1, k_2) using the neighbour indices, indicating that one hemisphere of the original event was replaced by its k_1 th neighbour and the other hemisphere of the original event by its k_2 th neighbour and these were used to form the artificial event. By applying this procedure to the whole set of events of the data to be modelled, and by choosing a limiting value K for k , we obtain a total of K^2 data sets, each equal in size to the original one, and each featuring very similar characteristics to the original one, despite being made up entirely of artificial events.

The procedure described above is successful at modelling multijet events because it exploits the fact that their production can be idealized at LO as a $2 \rightarrow 2$ process, which is made complex by a number of sub-leading effects (QCD radiation, pileup, multiple interactions). The reconstruction of the transverse thrust axis, and the decomposition of events into hemispheres using that axis as a seed, uses the independent fragmentation of the two final state partons as a working hypothesis to create artificial replicas of the original events. The method destroys any correlation in the jet distribution between the two hemispheres, so that any physical effect, such as the decay of a heavy object into jet pairs, is washed out in the artificial samples. Because of this, the resulting artificial data sets are unaffected by the presence of a small signal contamination in the original data. This has been verified by signal injection tests. We started with an original data set composed of simulated QCD multijet events to which is added an additional component of signal corresponding to a cross section 100 times larger than the one expected by the SM. After hemisphere mixing, the kinematical properties of the resulting artificial samples are found to resemble closely those from the QCD multijet part of the original data set, which is its dominant component, and unaffected by the minority component (the signal contamination). Naively this can be understood if we note that, if the signal fraction in the original sample amounts to e.g. 0.1%, the probability that a signal event is modelled using two different hemispheres both originally belonging to signal events is of the order of 0.0001%. Event-based variables such as the two Higgs boson candidate masses, which are obtained by the minimum ΔM criterion described in Section 7 and are thus sensitive to the characteristics of both hemispheres together, do not retain their distribution in events where only one hemisphere is taken from an HH decay event.

We apply the hemisphere mixing technique to data events selected with the $N_j \geq 4$, $N_b \geq 4$ criteria, using $K = 10$ neighbour hemispheres to each hemisphere of the original event, which were found to still provide good modelling. The resulting artificial samples are used to provide a background model in the training of the BDT classifier (training sample), as well as an independent set for the BDT validation and optimization (validation sample), and a third data set used to extract the predicted shape of the optimized BDT (application sample). Not all of the data sets are fully independent so only a subset can be safely employed for further studies. We use the following collections of artificial events in the measurement: for the training sample, we use all artificial events of types (1, 1), (1, 2), (2, 1), and (2, 2); for the validation sample, all artificial events of types (3, 4), (5, 6), (7, 8), and (9, 10); and for the application sample, all artificial events of types (4, 3), (6, 5), (8, 7), and (10, 9). This split guarantees that the three samples

have equal number of events, and that the validation and application samples are independent of each other, being constituted of artificial events made up of different hemispheres. For the training sample the partial use of the same hemispheres in modelling different artificial events might at most slightly degrade the discrimination power but does not have a detrimental effect on the subsequent steps of the analysis. A study is performed by switching the validation and application samples and we find that this does not change the results. The fraction of data events that are totally replicated in the background template is completely negligible. A comparison between the distributions obtained through the procedure described above and by using MC simulation for QCD multijet processes can be seen in Fig. 3 for a number of variables. The compatibility is good, although the statistical uncertainties in the model from MC simulation are large.

8.2 The background template validation

We perform a number of stringent checks to verify that the background is well modelled by the hemisphere mixing procedure. For this purpose, we define two control regions (CRs): the first one, called the m_H CR, is obtained by removing from the data events where the leading and trailing dijet masses are in the region $90 < M_{H_1} < 150$ GeV, $80 < M_{H_2} < 140$ GeV. This avoids using events belonging to the signal-enriched region. In the second region, the b tag CR, fully orthogonal to the default selection, we select events with at least four b-tagged jets as defined by the loose working point of the cMVA_{v2}, while vetoing events with any jets that are defined as b-tagged jets according to the medium working point of the cMVA_{v2}. The loose working point of the cMVA_{v2} has a misidentification rate of $\approx 10\%$ and a b-tagging efficiency of $\approx 85\%$ for jets produced by the hadronization of b quarks emitted in HH production events. The distributions of all individual event variables for the artificial data sets are compared to those from the original data set in these two CRs and are found to be in agreement. This is illustrated for a number of variables in Figs. 4 and 5. However, the power of the technique rests in its ability to provide fully multidimensional modelling. To verify this, a first cross-check consists of comparing the full BDT shape for data and the artificial model in the m_H CR. We observe an agreement in the shape of the BDT discriminator with a slight excess of background events in the lower range of the BDT output (as can be seen in Fig. 6, left). A similar trend is seen in the b tag CR.

A high-precision study is required to investigate the need for a correction to the background shape of the BDT discriminator and a corresponding systematic uncertainty. For this purpose, all the possible combinations of neighbouring hemispheres in the range 1 to 10, except the ones used for training $((1, 1), (1, 2), (2, 1), (2, 2))$, are merged into a unique sample M . We re-sample 200 new replicas with the same number of events as the original data set without replacement from M , each time starting from the full sample M . Each of the replicas is then used as a new original data set, and artificial samples are created from it using the hemisphere mixing procedure. The output distribution of a previously trained BDT for the large sample M is then compared to that for its artificial counterpart, obtaining a distribution of differences between actual and predicted data in each of the 80 BDT bins. A schematic of the procedure and the results are available in Appendix A. A systematic bias is detected and the background template is corrected for the value obtained from this comparison. The variance related to the background bias extraction, together with expected statistical uncertainty, are estimated and accounted for as a systematic uncertainty in the final fit described in Section 10. The validity of this background bias extraction procedure has been checked by applying it to the data in the two CRs previously mentioned. The means of the per bin expectation values minus the observed values are compatible with zero after the bias correction in both control regions, the root-mean-square

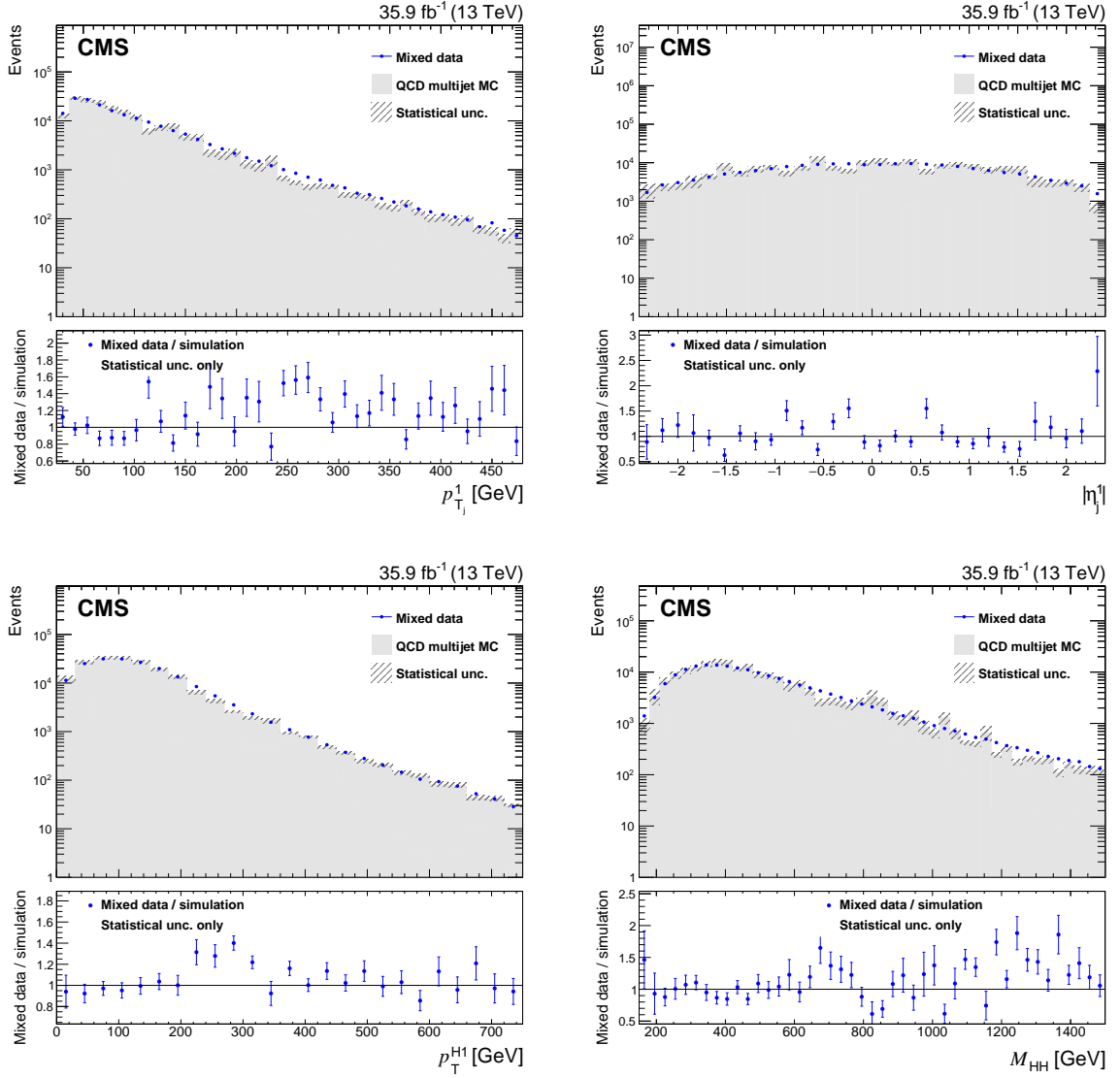


Figure 3: Comparison between the background model obtained with the hemisphere mixing technique and MC simulation of QCD multijet processes for $p_{T_1}^1$ (upper left), η_j^1 (upper right), $p_T^{H_1}$ (lower left), and M_{HH} (lower right). Bias correction for the background model, described in Section 8.2, is applied by rescaling the weight of each event using the event yield ratio between corrected and uncorrected BDT distributions. Only statistical uncertainties are shown as the uncertainties related to the bias correction can not be propagated from the BDT classifier to a different variable.

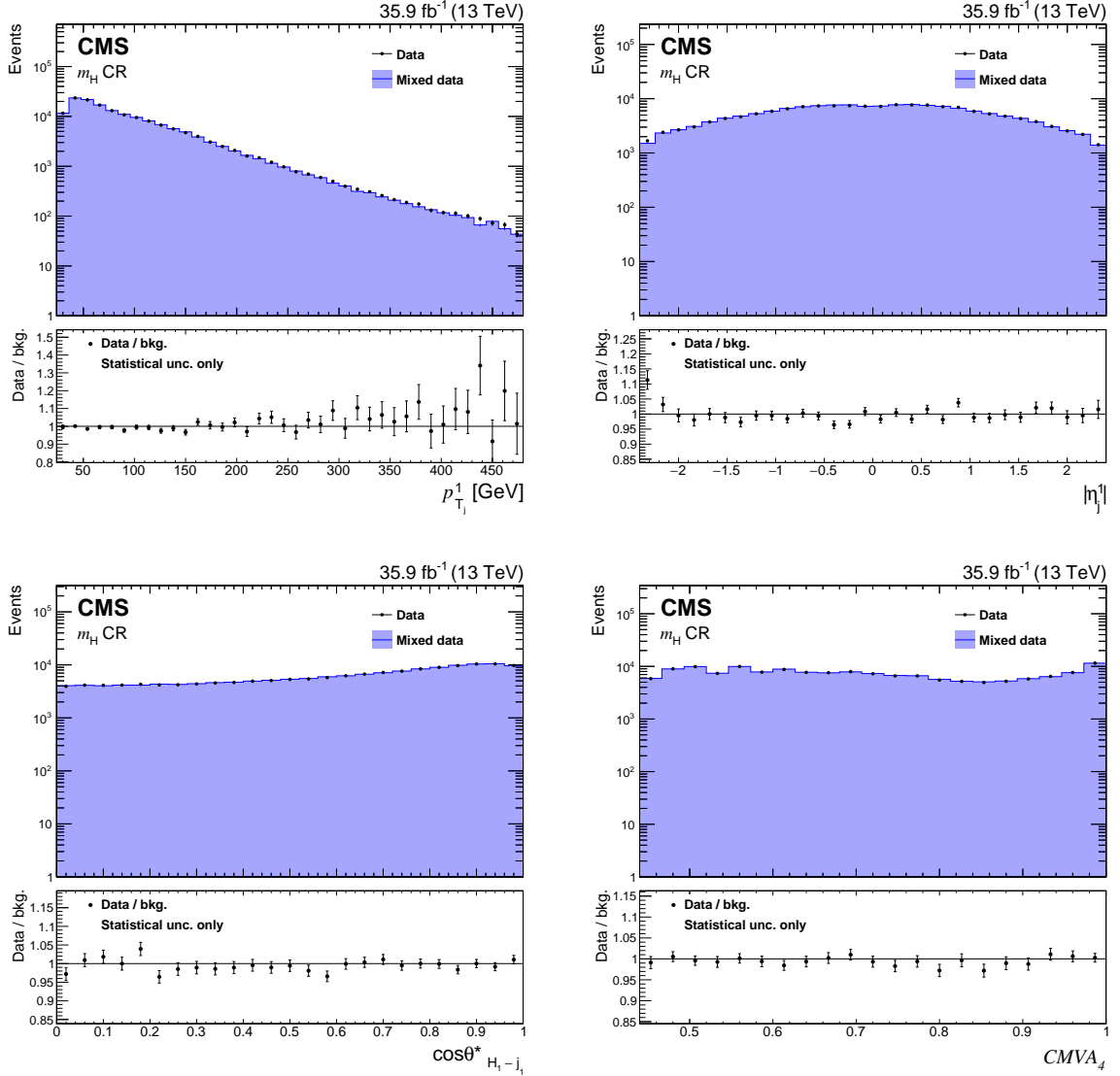


Figure 4: Comparison between the background model obtained with the hemisphere mixing technique and data in the m_H CR for the variables p_{Tj}^1 (upper left), η_j^1 (upper right), $\cos\theta_{H1-j1}^*$ (lower left), and $CMVA_4$ (lower right). Bias correction for the background model, described in Section 8.2, is applied by rescaling the weight of each event using the event yield ratio between corrected and uncorrected BDT distributions in this CR. Only statistical uncertainties are shown as the uncertainties related to the bias correction can not be propagated from the BDT classifier to a different variable.

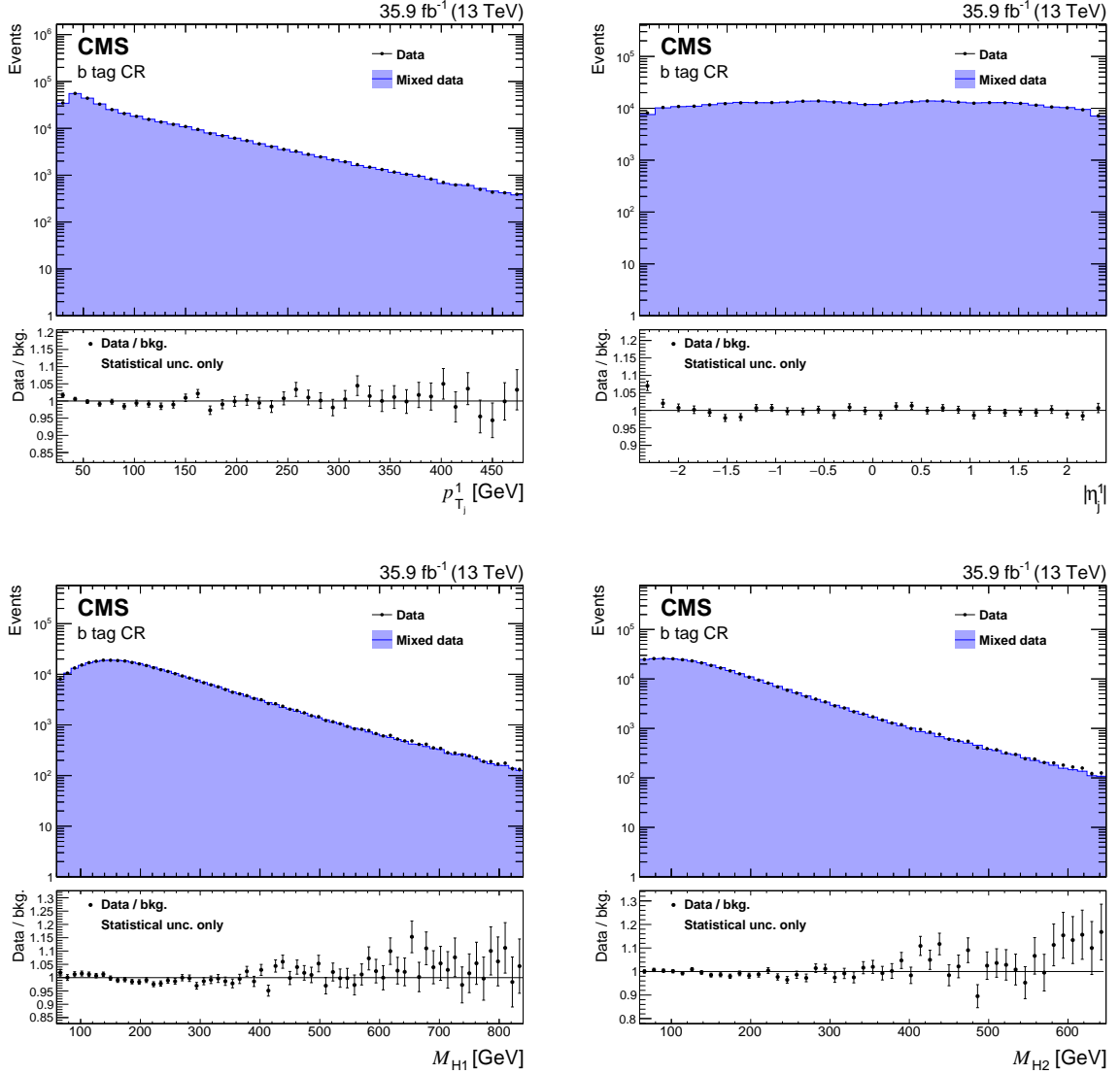


Figure 5: Comparison between the background model obtained with the hemisphere mixing technique and data in the b tag CR for the variables $p_{T_1}^1$ (upper left), η_1^1 (upper right), M_{H_1} (lower left), and M_{H_2} (lower right). Bias correction for the background model, described in Section 8.2, is applied by rescaling the weight of each event using the event yield ratio between corrected and uncorrected BDT distributions in this CR. Only statistical uncertainties are shown as the uncertainties related to the bias correction can not be propagated from the BDT classifier to a different variable.

of the pulls is compatible with one after the bias correction in the b tag CR, but not in the m_H CR, as shown on Fig. 6 (upper right). To account for this, we increase the uncertainty in the background such that the value of standard deviation (s.d.) becomes 1.0 in the m_H CR after the bias correction is applied (Fig. 6, lower right).

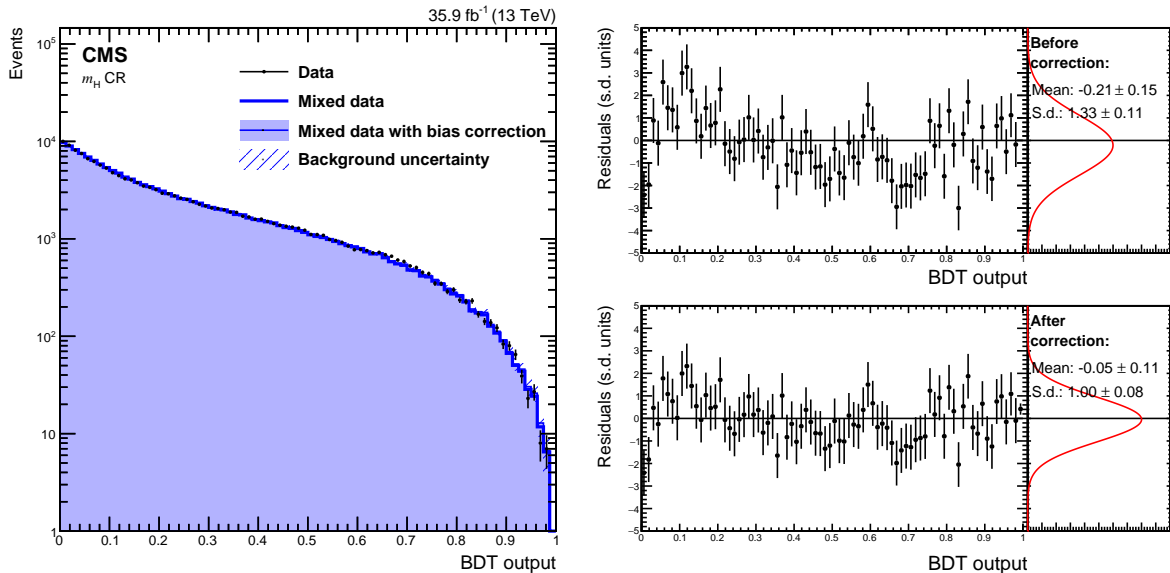


Figure 6: Left: comparison of the distribution of BDT output for data (left) selected in a region of the leading versus trailing Higgs boson candidate mass plane that excludes a 60-GeV-wide box around the most probable values of the dijet masses of signal events, with the corresponding output on an artificial sample obtained from the same data set by hemisphere mixing. Right: bin-by-bin differences between data and model, in s.d. units before (upper right) and after (lower right) bias correction; pull distribution for the differences, fit to a Gaussian distribution. The bias correction uncertainty is increased to take the s.d. of the residuals to 1.0.

9 Systematic uncertainties

The sources of systematic uncertainties found to be relevant to this analysis are listed in Table 4. The systematic uncertainty in the shape of the background model is accounted for by assigning an uncertainty to each BDT output bin that includes the statistical uncertainty and the systematic uncertainty related to the bias extraction discussed in the previous section. The background normalization is left freely floating in the BDT distribution fit. The uncertainty due to the b tagging efficiencies is estimated by varying them within their uncertainties. The uncertainty due to the pileup modelling is computed by considering a $\pm 4.6\%$ variation in the total inelastic cross section value at 13 TeV [62]. The effect of jet energy resolution is evaluated by smearing jet energies according to their estimated uncertainty. The jet energy scale is varied within one s.d. as a function of jet p_T and $|\eta|$, and the efficiency of the selection criteria is recomputed. The trigger efficiency correction factor discussed in Section 5 is affected by a 2% uncertainty that is taken as a systematic uncertainty in the related source. In the mentioned sources of systematic uncertainty, both shape and normalization shifts are considered in the model. The signal yield for a given production cross section is affected by a systematic uncertainty in the measured integrated luminosity of 2.5% [63]. The effect of variation of the μ_R and μ_F scales on the signal acceptance is estimated by taking the maximum and the minimum difference with respect to the nominal acceptance when varying μ_F and μ_R each individually as

well as both together up and down by a factor of two. Lastly, to estimate the signal acceptance uncertainty due to PDF uncertainties, the PDF4LHC [64] recommendation is followed, using as the uncertainty the s.d. in the acceptance for a set of 100 MC replicas of the NNPDF 3.0 set [39].

Table 4: Systematic uncertainties considered in the analysis and relative impact on the expected limit for the SM HH production. The relative impact is obtained by fixing the nuisance parameters corresponding to each source and recalculating the expected limit.

Source	Affects	Exp. limit variation
Bkg. shape	bkg.	30%
Bkg. norm.	bkg.	8.6%
b tagging eff.	sig	2.8%
Pileup	sig	<0.01%
Jet energy res.	sig	<0.01%
Jet energy scale	sig	<0.01%
Int. luminosity	sig	<0.01%
Trigger eff.	sig	<0.01%
μ_F and μ_R scales	sig	<0.01%
PDF	sig	<0.01%

10 Results

We search for the presence of HH events in CMS data collected in the 2016 run of the LHC using the BDT discriminant trained on the SM signal simulation and artificial background data. Two-component likelihood fits to the binned BDT output distributions are performed, using the BDT distribution for the background resulting from the artificial data set described in Section 8 and the signal simulations corresponding to the SM and each of the BSM benchmark points. The validation samples were used to study the dependence of both the expected limit and the compatibility of the data and background distributions on the value of the BDT discriminator used for the selection. Selecting BDT discriminator values >0.2 results in a small loss of sensitivity ($\approx 1.5\%$) with improved data-background compatibility. As a result, the 64 bins with BDT >0.2 are used to extract the limits. The fit to the SM signal is shown in Fig. 7 and the postfit distributions of reconstructed Higgs boson masses are shown in Fig. 8. Minor background contamination arising from $t\bar{t}H$, ZH , $b\bar{b}H$, and single Higgs boson production processes do not show a signal-like BDT distribution and their effect is found to be negligible in the selected data at our level of sensitivity.

The observed and expected 95% confidence level (CL) upper limits on the cross section for $pp \rightarrow HH \rightarrow b\bar{b}b\bar{b}$ nonresonant production, are computed using the asymptotic approximation [65] of the CL_s criterion [66–68], using a test statistic based on the profile likelihood ratio (the LHC test statistic) [65]. The systematic uncertainties are treated as nuisance parameters and are profiled in the minimization. The limits are shown in Table 5 together with the 1 s.d. and 2 s.d. CL intervals around the expected limits. For the SM process, the expected limit is 419 fb, which corresponds to ≈ 37 times the SM HH production cross section times the square of the branching fraction for the $H \rightarrow b\bar{b}$ decay. The observed upper limit obtained is 847 fb, which is ≈ 2 s.d. above the expected upper limit. This corresponds to an observed limit of 2496 fb for $\sigma(pp \rightarrow HH)_{SM}$.

We perform the procedure described above in turn on the 13 BSM benchmark models considered. The results are shown in Fig. 9 and reported in Table 6. The difference between observed and expected limits is similar for SM and all the benchmark models. This is explained by the

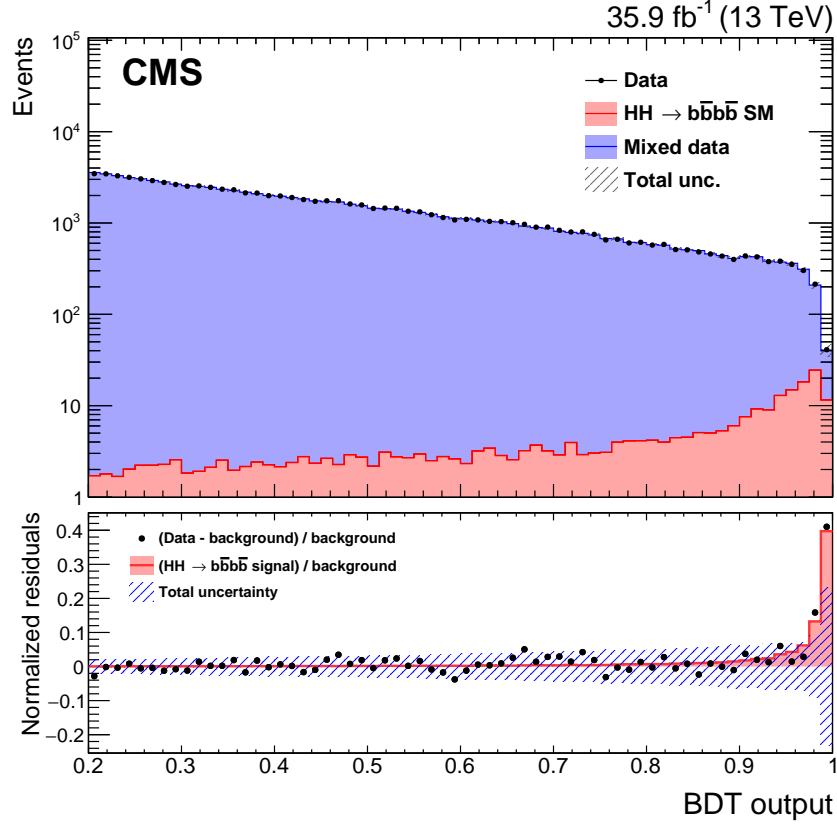


Figure 7: Results of the fit to the BDT distribution for the SM HH production signal. In the bottom panel a comparison is shown between the best fit signal and best fit background subtracted from measured data. The band, centred at zero, shows the total uncertainty.

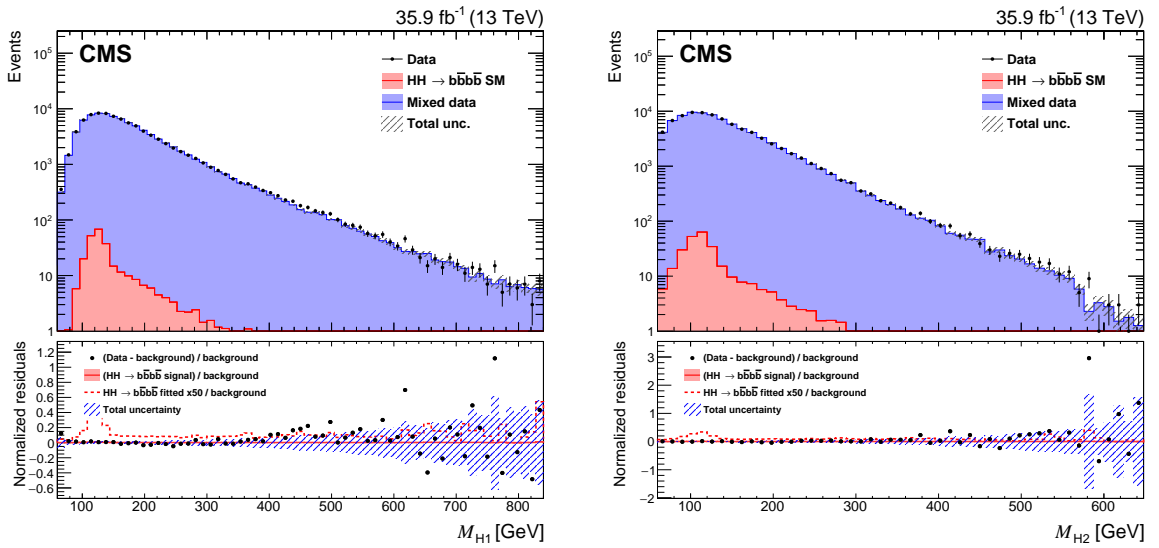


Figure 8: Post-fit distribution of M_{H_1} (left) and M_{H_2} (right). Bias correction for the background model is applied by rescaling the weight of each event using the event yield ratio between corrected and uncorrected BDT distributions.

Table 5: The observed and expected upper limits on $\sigma(\text{pp} \rightarrow \text{HH} \rightarrow \text{b}\bar{\text{b}}\text{b}\bar{\text{b}})$ in the SM at 95% CL in units of fb.

Category	Observed	Expected	-2 s.d.	-1 s.d.	+1 s.d.	+2 s.d.
SM $\text{HH} \rightarrow \text{b}\bar{\text{b}}\text{b}\bar{\text{b}}$	847	419	221	297	601	834

fact that the benchmark points use the same BDT as SM, resulting in the same background shape as an input to the fit. The background shape has a deficit of events compared to data in the last bins of the BDT distribution, as seen in Fig. 7. We also search for HH production with values of κ_λ in the range $[-20, 20]$, assuming $\kappa_t = 1$, and the results are shown in Fig. 10. The kinematic properties vary significantly across the points in this range. We do not exclude any values of κ_λ , assuming $\kappa_t = 1$.

Table 6: The observed and expected upper limits on the $\sigma(\text{pp} \rightarrow \text{HH} \rightarrow \text{b}\bar{\text{b}}\text{b}\bar{\text{b}})$ cross section for the 13 BSM benchmark models at 95% CL in units of fb.

Benchmark point	Observed	Expected	-2 s.d.	-1 s.d.	+1 s.d.	+2 s.d.
1	602	295	155	209	424	592
2	554	269	141	190	389	548
3	705	346	182	245	497	691
4	939	461	244	327	662	920
5	508	248	131	176	357	501
6	937	457	240	323	657	916
7	3510	1710	905	1210	2440	3390
8	686	336	177	238	483	674
9	529	259	136	183	373	520
10	2090	1000	527	709	1440	2010
11	1080	525	277	372	755	1050
12	1744	859	455	611	1230	1710
Box	1090	542	286	384	775	1080

11 Summary

This paper presents a search for nonresonant Higgs boson pair (HH) production with both Higgs bosons decaying into $\text{b}\bar{\text{b}}$ pairs. The standard model (SM) production has been studied along with 13 beyond the SM (BSM) benchmark models, using a data set of $\sqrt{s} = 13$ TeV proton-proton collision events, corresponding to an integrated luminosity of 35.9 fb^{-1} collected by the CMS detector during the 2016 LHC run. The analysis of events acquired by a hadronic multijet trigger includes the selection of events with 4 b-tagged jets and a classification using boosted decision trees, optimized for discovery of the SM HH signal. Limits at 95% confidence level on the HH production cross section times the square of the branching fraction for the Higgs boson decay to b quark pairs are extracted for the SM and each BSM model considered, using binned likelihood fits of the shape of the boosted decision tree classifier output. The background model is derived from a novel technique based on data that provides a multidimensional representation of the dominant quantum chromodynamics multijet background and also models well the overall background distribution. The expected upper limit on $\sigma(\text{pp} \rightarrow \text{HH} \rightarrow \text{b}\bar{\text{b}}\text{b}\bar{\text{b}})$ is 419 fb, corresponding to 37 times the expected value for the SM process. The observed upper limit is 847 fb. Anomalous couplings of the Higgs boson are also investigated. The upper limits extracted for the HH production cross section in the 13 BSM benchmark models range from 508 to 3513 fb.

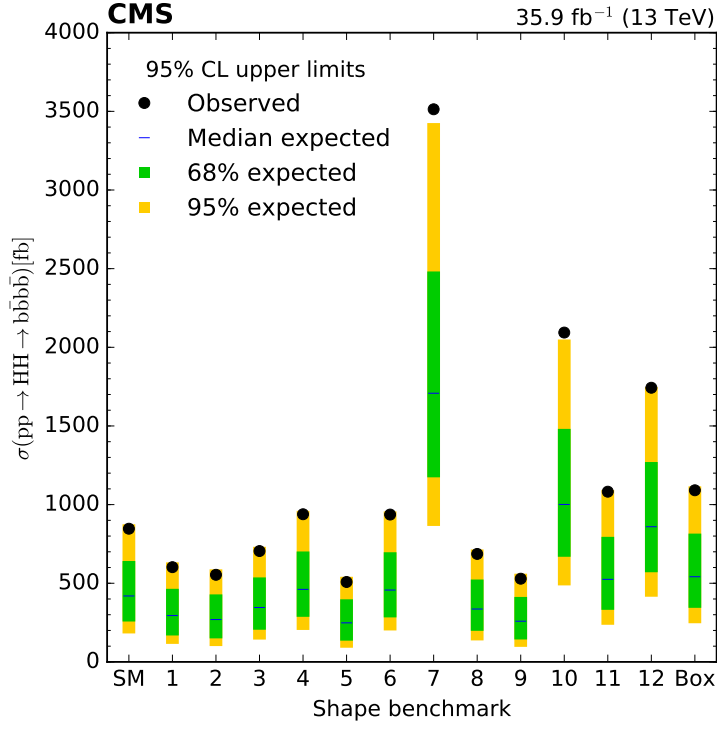


Figure 9: The observed and expected upper limits at 95% CL on the $\sigma(pp \rightarrow HH \rightarrow b\bar{b}b\bar{b})$ cross section for the 13 BSM models investigated. See Table 1 for their respective parameter values.

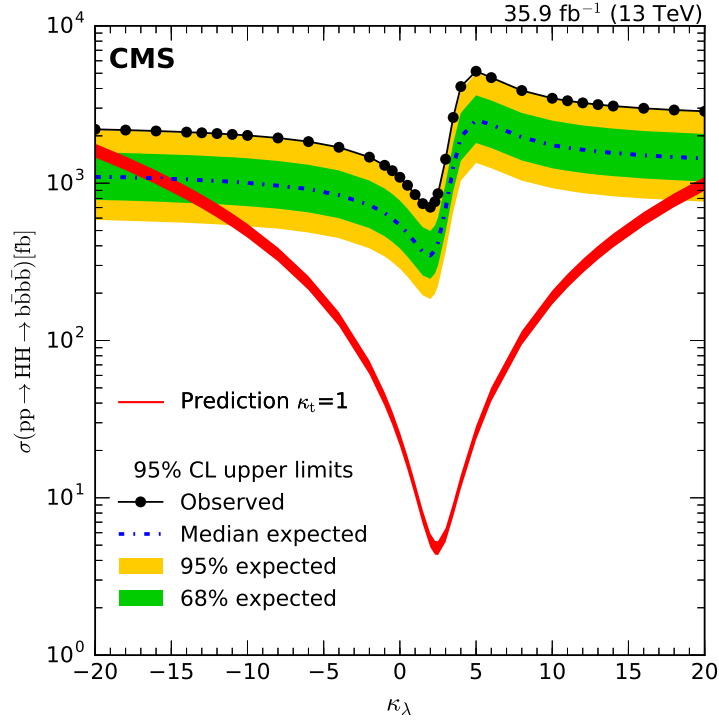


Figure 10: 95% CL cross section limits on $\sigma(pp \rightarrow HH \rightarrow b\bar{b}b\bar{b})$ for values of κ_λ in the $[-20, 20]$ range, assuming $\kappa_t = 1$; the theoretical prediction with $\kappa_t = 1$ is also shown.

Acknowledgments

We congratulate our colleagues in the CERN accelerator departments for the excellent performance of the LHC and thank the technical and administrative staffs at CERN and at other CMS institutes for their contributions to the success of the CMS effort. In addition, we gratefully acknowledge the computing centres and personnel of the Worldwide LHC Computing Grid for delivering so effectively the computing infrastructure essential to our analyses. Finally, we acknowledge the enduring support for the construction and operation of the LHC and the CMS detector provided by the following funding agencies: BMBWF and FWF (Austria); FNRS and FWO (Belgium); CNPq, CAPES, FAPERJ, FAPERGS, and FAPESP (Brazil); MES (Bulgaria); CERN; CAS, MoST, and NSFC (China); COLCIENCIAS (Colombia); MSES and CSF (Croatia); RPF (Cyprus); SENESCYT (Ecuador); MoER, ERC IUT, and ERDF (Estonia); Academy of Finland, MEC, and HIP (Finland); CEA and CNRS/IN2P3 (France); BMBF, DFG, and HGF (Germany); GSRT (Greece); NKFI (Hungary); DAE and DST (India); IPM (Iran); SFI (Ireland); INFN (Italy); MSIP and NRF (Republic of Korea); MES (Latvia); LAS (Lithuania); MOE and UM (Malaysia); BUAP, CINVESTAV, CONACYT, LNS, SEP, and UASLP-FAI (Mexico); MOS (Montenegro); MBIE (New Zealand); PAEC (Pakistan); MSHE and NSC (Poland); FCT (Portugal); JINR (Dubna); MON, RosAtom, RAS, RFBR, and NRC KI (Russia); MESTD (Serbia); SEIDI, CPAN, PCTI, and FEDER (Spain); MOSTR (Sri Lanka); Swiss Funding Agencies (Switzerland); MST (Taipei); ThEPCenter, IPST, STAR, and NSTDA (Thailand); TUBITAK and TAEK (Turkey); NASU and SFFR (Ukraine); STFC (United Kingdom); DOE and NSF (USA).

Individuals have received support from the Marie-Curie programme and the European Research Council and Horizon 2020 Grant, contract No. 675440 (European Union); the Leventis Foundation; the A. P. Sloan Foundation; the Alexander von Humboldt Foundation; the Belgian Federal Science Policy Office; the Fonds pour la Formation à la Recherche dans l'Industrie et dans l'Agriculture (FRIA-Belgium); the Agentschap voor Innovatie door Wetenschap en Technologie (IWT-Belgium); the F.R.S.-FNRS and FWO (Belgium) under the "Excellence of Science - EOS" - be.h project n. 30820817; the Ministry of Education, Youth and Sports (MEYS) of the Czech Republic; the Lendület ("Momentum") Programme and the János Bolyai Research Scholarship of the Hungarian Academy of Sciences, the New National Excellence Program ÚNKP, the NKFI research grants 123842, 123959, 124845, 124850 and 125105 (Hungary); the Council of Science and Industrial Research, India; the HOMING PLUS programme of the Foundation for Polish Science, cofinanced from European Union, Regional Development Fund, the Mobility Plus programme of the Ministry of Science and Higher Education, the National Science Center (Poland), contracts Harmonia 2014/14/M/ST2/00428, Opus 2014/13/B/ST2/02543, 2014/15/B/ST2/03998, and 2015/19/B/ST2/02861, Sonata-bis 2012/07/E/ST2/01406; the National Priorities Research Program by Qatar National Research Fund; the Programa Estatal de Fomento de la Investigación Científica y Técnica de Excelencia María de Maeztu, grant MDM-2015-0509 and the Programa Severo Ochoa del Principado de Asturias; the Thalís and Aristeia programmes cofinanced by EU-ESF and the Greek NSRF; the Rachadapisek Sompot Fund for Postdoctoral Fellowship, Chulalongkorn University and the Chulalongkorn Academic into Its 2nd Century Project Advancement Project (Thailand); the Welch Foundation, contract C-1845; and the Weston Havens Foundation (USA).

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A Supplemental material

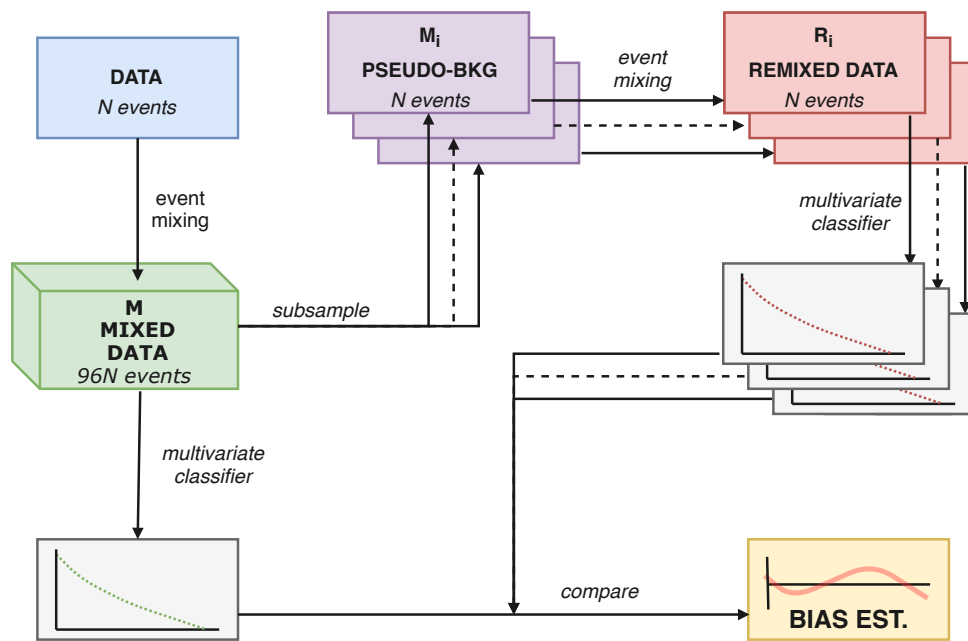


Figure 11: Diagram describing the procedure used to estimate the background bias correction. All possible combinations of mixed hemispheres except those used for training are added together to create a large sample M of $96N$ events from which we repeatedly subsample without replacement 200 replicas M_i of N events. The hemisphere mixing procedure is then carried out again for each of this replicas to produce a set of re-mixed data replicas R_i . The trained multivariate classifier trained is then evaluated over all the events of M and each R_i . and the histograms of the classifier output are compared to obtain the differences for each of the replicas. The median difference is taken as bias correction.

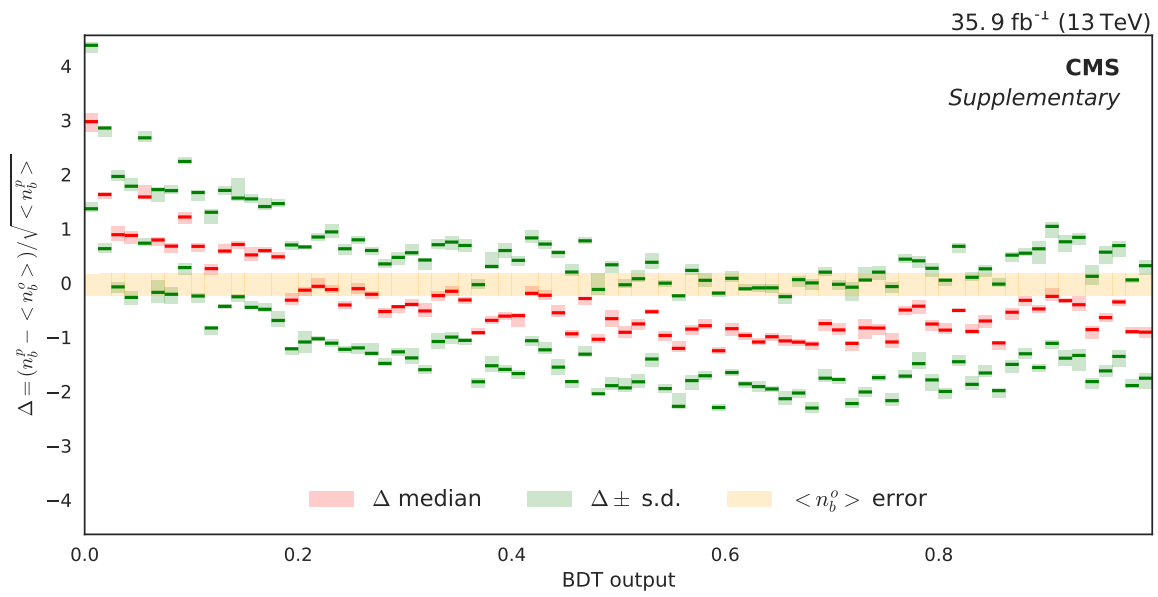


Figure 12: Bias estimation by resampling, in relative units of the statistical uncertainty of the predicted background, used to correct the background estimation. The median (red line) and the upper and lower one s.d. quantiles (green lines) have been computed from 200 subsamples of the re-mixed data comparing the predicted background n_b^p with the observed n_b^o . The variability due to the limited number of subsamples is estimated by bootstrap and it is shown for each estimation using a coloured shadow around the quantile estimation. The light yellow shadow represents the uncertainty due to the limited statistics of the reference observed sample. The separation between the one s.d. quantiles is compatible with the expected variance if the estimation was Poisson or Gaussian distributed.

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- 66: Also at Utah Valley University, Orem, USA
- 67: Also at Purdue University, West Lafayette, USA

68: Also at Beykent University, Istanbul, Turkey

69: Also at Bingol University, Bingol, Turkey

70: Also at Sinop University, Sinop, Turkey

71: Also at Mimar Sinan University, Istanbul, Istanbul, Turkey

72: Also at Texas A&M University at Qatar, Doha, Qatar

73: Also at Kyungpook National University, Daegu, Korea