Probing the trilinear Higgs boson self-coupling at the high-luminosity LHC via multivariate analysis

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We perform a multivariate analysis of Higgs-pair production in $HH \rightarrow b\bar{b}\gamma\gamma$ channel at the HL-LHC to probe the trilinear Higgs self-coupling (THSC) λ_{3H} , which takes the value of 1 in the standard model (SM). We consider all known background processes. For the signal we are the first to adopt the most recent event generator of POWHEG-BOX-V2 to exploit the next-to-leading order (NLO) distributions for the toolkit for multivariate data analysis (TMVA), taking account of the full top-quark mass dependence. Through boosted decision tree (BDT) analysis trained for $\lambda_{3H} = 1$, we find that the significance can reach up to 1.95 with about 9 signal and 18 background events. In addition, the THSC can be constrained to $1.00 < \lambda_{3H} < 6.22$ at 95% confidence level (CL). We also perform a likelihood fitting of $M_{\gamma\gamma bb}$ distribution and find the 1σ confidence interval (CI) of $0.1 < \lambda_{3H} < 2.2 \cup 5.4 < \lambda_{3H} < 6.6$ for the $\lambda_{3H} = 1$ nominal set. On the other hand, using BDTs trained for each value of λ_{3H} , we find a bulk region of $0.5 \lesssim \lambda_{3H} \lesssim 4.5$, for which it is hard to pin down the THSC.

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I. INTRODUCTION

Since the discovery of the Higgs boson in 2012 [1], the most pressing question is to understand the underlying mechanism for electroweak symmetry breaking (EWSB). There is no particular reason why the EWSB sector only consists of a single Higgs doublet. Indeed, the simplest version suffers from the so-called gauge hierarchy problem. After completing Run I and II at the LHC, the identity of the Higgs boson has been established. It is best described as the standard model (SM) Higgs boson [2], although there is an upward trend in the overall signal strength [3]. All current measurements of the Higgs boson properties confine to the couplings of the Higgs boson to the SM particles, like gauge bosons and fermions. However, the self-couplings of the Higgs boson are not established at all, which depends on the dynamics of the EWSB sector. The self-couplings of the Higgs boson can be very different

between the SM and other extensions of the EWSB sector, like the two-Higgs doublet models (2HDM), and minimal supersymmetric extension of the standard model. Higgs boson pair production at the LHC provides a very useful avenue to investigate the THSC [4–6]. There is a vast literature on Higgs-pair production in the SM [7], in model-independent formalism [8], in models beyond the SM [9], and in supersymmetry (SUSY) [10].

Furthermore, the high luminosity option of the LHC running at 14 TeV (HL-LHC) was approved. It is a legitimate machine to investigate the EWSB sector. In a previous work [11], we showed that even with the high-luminosity LHC one cannot establish the THSC λ_{3H} at the SM value using the most promising decay mode $HH \rightarrow (b\bar{b})(\gamma\gamma)$. Indeed, one can only constrain the THSC to be within $-1.0 \lesssim \lambda_{3H} \lesssim 7.6$ at 95% CL [11]. These results were based on a conventional cut-based analysis. In this paper, we show that with the use of BDT method, the significance of the signal can be substantially improved by 80%.

II. EVENT GENERATION

The Higgs bosons in the signal event samples are generated on-shell with zero width by POWHEG-BOX-V2 [12,13] with the damping factor `hdamp` set to the default value of 250 to limit the amount of hard radiation.

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TABLE I. Sequence of event preselection criteria applied in this analysis.

Sequence	Event preselection criteria
1	Diphoton trigger condition, ≥ 2 isolated photons with $P_T > 25$ GeV, $ \eta < 2.5$
2	≥ 2 isolated photons with $P_T > 30$ GeV, $ \eta < 1.37$ or $1.52 < \eta < 2.37$, $\Delta R_{\gamma\gamma,j\gamma} > 0.4$
3	≥ 2 jets identified as b-jets with leading(subleading) $P_T > 40(30)$ GeV, $ \eta < 2.4$, $\Delta R_{bb} > 0.4$
4	Events are required to contain ≤ 5 jets with $P_T > 30$ GeV within $ \eta < 2.5$
5	No isolated leptons with $P_T > 25$ GeV, $ \eta < 2.5$

This code provides NLO distributions matched to a parton shower taking account of the full top-quark mass dependence. The variation of the THSC, λ_{3H} , is also allowed in this code. The MadSpin code [14] is used after generating a pair of Higgs bosons in order to decay both Higgs bosons into two bottom quarks and two photons. For parton showering and hadronization, PYTHIA8 [15] is used. Here an appropriate setup provided by POWHEG-BOX-V2 is used to correctly perform a matching of POWHEG-BOX-V2 with PYTHIA8. Finally, fast detector simulation and analysis at the HL-LHC are performed using Delphes3 [16] with the ATLAS template. The parameters in the template are tuned as in Ref. [11]. The signal cross section at NNLO order in QCD is calculated according to $\sigma^{\text{NNLO}}(\lambda_{3H}) = K_{\text{SM}}^{\text{NNLO/NLO}} \sigma^{\text{NLO}}(\lambda_{3H})$, where λ_{3H} -dependent NLO cross section of $\sigma^{\text{NLO}}(\lambda_{3H})$ is computed by the use of POWHEG-BOX-V2 and we take $K_{\text{SM}}^{\text{NNLO/NLO}} = 1.116$ [17]. For generation and simulation of backgrounds, we closely follow Ref. [11], except for the use of the post-LHC PDF set of CT14LO [18] and merged cross sections for nonresonant backgrounds. More precisely, for the two main nonresonant backgrounds of $b\bar{b}\gamma\gamma$ and $c\bar{c}\gamma\gamma$, we use the merged cross sections and distributions by MLM matching [19,20] with xqcut and Q_{cut} set to 20 GeV and 30 GeV, respectively. For the remaining nonresonant backgrounds, we are using the cross sections and distributions obtained by applying the generator-level cuts as adopted in Ref. [21] which might provide more reliable and conservative estimation of the nonresonant backgrounds containing light jets [11].

III. TMVA ANALYSIS

Before performing a multivariate analysis using TMVA [22] with ROOTv6.18 [23], a sequence of event selections is applied to the signal and background samples, see Table I. We choose these 8 kinematic variables for TMVA:

$$M_{bb}, P_T^{bb}, \Delta R_{bb}; M_{\gamma\gamma}, P_T^{\gamma\gamma}, \Delta R_{\gamma\gamma}; M_{\gamma\gamma bb}, \Delta R_{\gamma b}.$$

We observe that significance can be meaningfully improved by judiciously choosing the two photons or two b quarks for the above TMVA variables. For $M_{bb,\gamma\gamma}$ and $P_T^{bb,\gamma\gamma}$, in terms of P_T , we choose the least energetic two photons or two b quarks while the most energetic ones are

chosen for $\Delta R_{bb,\gamma\gamma}$ and $M_{\gamma\gamma bb}$. For $\Delta R_{\gamma b}$, on the other hand, we choose the least energetic b and the next-to-the-least energetic photon.

We have scrutinized the normalized distributions of these 8 variables for signal with $\lambda_{3H} = 1$ and backgrounds after applying the pre-selection cuts in Table I. We observe the broad peak around 125 GeV in the M_{bb} distribution of the signal while the peak in the $M_{\gamma\gamma}$ distribution of the signal is very sharp. The signal tends to give larger transverse momenta of $P_T^{bb,\gamma\gamma}$ while it populates more in the region of smaller $\Delta R_{bb,\gamma\gamma}$, implying a strong negative correlation between P_T and ΔR . Furthermore, the signal has larger $M_{\gamma\gamma bb}$ and its distribution is peaked around 400 GeV, and $\Delta R_{\gamma b}$ provides another good discriminant observable.

First, we try various multivariate analysis (MVA) methods provided by TMVA with the default setup for each method. After examining the receiver operating characteristic (ROC) curves for various methods, we find that the BDT-related methods show higher performance with better signal efficiency and stronger background rejection. We choose the best method of BDT for our analysis. Let us first describe our setup for BDT briefly. For each event sample of signal and backgrounds, we randomly divide it into two halves with a default split seed. The first half is used for training and the second one for testing. We use 800 trees and node splitting is allowed only when the number of events in a node is larger than 2.5% of total number of events of the training sample in order to improve the BDT performance. Maximum tree depth is set to 4. Training is carried out using adaptive boost with learning rate $\beta = 0.5$. One half of the training sample is randomly chosen at the end of each boosting iteration. The cut value on the variable in a node is optimized by comparing the separation index (we choose Gini Index) of the parent node and the sum of the indices of the two daughter ones. Finally, the whole range of the variable is equally gridded into 20 cells.

IV. RESULTS

In the left panel of Fig. 1, we show the BDT responses obtained using BDT trained for $\lambda_{3H} = 1$ which is to be called BDT_{SM} shortly. By validating the BDT distributions for the training sample (dots with error bars) with those for the test sample (histogram), we check that BDT_{SM} is not overtrained. In the right panel of Fig. 1, we compare the

FIG. 1. (Left) Normalized SM BDT responses for test (histogram) and training (dots with error bars) samples. BDT responses for signal (blue) and background (red) samples mostly populates in the regions with positive and negative BDT response, respectively. (Right) Normalized BDT responses for test sample obtained by using NLO (solid) and LO (dashed) distributions of the 8 TMVA input variables. The vertical lines show the position of the optimal cut on the BDT response which maximizes the significance.

BDT responses for the test sample obtained using NLO (solid) and LO (dashed) distributions of the 8 kinematic variables for TMVA. We observe that the NLO BDT distributions provide a bit better separation between signal and background. We denote by vertical lines the positions of the optimal cut on the BDT response which maximizes the significance $Z = \sqrt{2 \cdot [(s + b) \cdot \ln(1 + s/b) - s]}$,

where s and b represent the numbers of signal and background events, respectively.

In Fig. 2, using BDT_{SM} we show the behavior of signal and background efficiencies and significance Z versus the cut value on BDT response. The significance can reach up

FIG. 2. Signal and background efficiencies (inset) and significance Z as functions of BDT response cut. BDT_{SM} is used.

TABLE II. Expected number of signal and background events at the HL-LHC assuming 3000 fb^{-1} using BDT_{SM} with the BDT response cut of 0.145. We consider the four representative values of λ_{3H} for signal and the backgrounds are separated into three categories. For comparisons, we also show the results obtained using the cut-and-count analysis [11].

Signal and backgrounds	Expected yields (3000 fb^{-1})		
	Preselection	BDT_{SM}	Cut-and-Count
$H(b\bar{b})H(\gamma\gamma)$, $\lambda_{3H} = -5$	223.22	72.73	90.19
$H(b\bar{b})H(\gamma\gamma)$, $\lambda_{3H} = 0$	33.69	14.63	16.70
$H(b\bar{b})H(\gamma\gamma)$, $\lambda_{3H} = 1$	17.77	8.85	9.63
$H(b\bar{b})H(\gamma\gamma)$, $\lambda_{3H} = 5$	26.37	4.04	6.77
$ggH(\gamma\gamma)$	70.72	3.94	7.04
$t\bar{t}H(\gamma\gamma)$	157.20	3.64	13.14
$ZH(\gamma\gamma)$	23.60	2.27	3.60
$b\bar{b}H(\gamma\gamma)$	2.65	0.08	0.13
$b\bar{b}\gamma\gamma$	4676.36	3.72	10.92
$c\bar{c}\gamma\gamma$	3787.00	1.20	5.41
$j\bar{j}\gamma\gamma$	1015.48	0.39	2.89
$b\bar{b}j\gamma$	10017.91	0.82	13.91
$c\bar{c}j\gamma$	4679.36	0.55	4.78
$b\bar{b}j\gamma$	2517.71	0.05	3.83
$Z(b\bar{b})\gamma\gamma$	184.07	0.32	0.88
$t\bar{t} (\geq 1 \text{ leptons})$	7338.84	0.35	5.09
$t\bar{t}\gamma (\geq 1 \text{ leptons})$	2369.11	0.62	3.69
Total Background	36839.99	17.94	75.31
Significance Z, $\lambda_{3H} = 1$		1.95	1.09

FIG. 3. (Left) $M_{\gamma\gamma b\bar{b}}$ distributions at HL-LHC for the signal and background combined, assuming 3000 fb⁻¹ and using BDT_{SM} with the BDT response cut of 0.145. (Right) The relative log likelihood distribution for the nominal value of $\lambda_{3H} = 1$. The dashed line at 0.5(2.0) indicate the values corresponding to a 1σ(2σ) confidence interval.

to 1.95 when the BDT response is cut at 0.145, at which, the signal and background efficiencies are 0.50 and 4.9×10^{-4} , respectively.

In Table II, we present expected number of signal and background events at the HL-LHC assuming 3000 fb⁻¹ using BDT_{SM} with the BDT response cut of 0.145. We find 9 signal and 18 background events for $\lambda_{3H} = 1$. Comparing to the results using the cut-and-count analysis [11], the number of signal events decreases by only 10% while the number of backgrounds by almost 80%, resulting in an increase in significance from 1.09 to 1.95. Note that the composition of backgrounds changes drastically by the use of BDT. In the cut-and-count analysis, the nonresonant background is about two times larger than the single-Higgs associated background. While, in the BDT analysis, the single-Higgs associated background is larger than the nonresonant one and $t\bar{t}$ associated background becomes negligible. Also, the sensitivity to the THSC can be improved to $1.00 < \lambda_{3H} < 6.22$ at 95% CL, which removes the region of negative λ_{3H} in contrast to the results based on the cut-and-count analysis.

Nevertheless, the significance standing at 1.95 may not be high enough to make a precise measurement of the THSC at the HL-LHC. We implement a likelihood fitting of $M_{\gamma\gamma b\bar{b}}$ distribution to quantify the uncertainty in the determination of λ_{3H} and to see how much the two-fold ambiguity in the determination could be lifted up. In the left frame of Fig. 3, we show $M_{\gamma\gamma b\bar{b}}$ distributions for the signal and combined background (shaded histograms) taking four representative values of λ_{3H} . In the right frame of Fig. 3, we show the log likelihood distribution obtained by fitting the signal-plus-background $M_{\gamma\gamma b\bar{b}}$ distributions with the nominal value of $\lambda_{3H} = 1$. The solid line shows the result of a polynomial fitting and we find the 1σ CI of $0.1 < \lambda_{3H} < 2.2 \cup 5.4 < \lambda_{3H} < 6.6$. We observe that the two-fold ambiguity is slightly lifted up by the amount of $\Delta[-\ln(L_{\lambda_{3H}}/L_{\lambda_{3H}=1})] \simeq 0.4$.

So far we have used the BDT trained for $\lambda_{3H} = 1$ or BDT_{SM} independently of the input value of λ_{3H} . Without knowing the value of λ_{3H} *a priori*, it would be more desirable to use separate BDTs trained for specific values of λ_{3H} , which we call BDT _{λ_{3H}} in short. In Fig. 4, we show the contour plot showing the 1σ and 2σ CI regions obtained by likelihood fitting of $M_{\gamma\gamma b\bar{b}}$ distributions. For each value of λ_{3H}^{in} , we use the corresponding BDT _{λ_{3H}} together with $\lambda_{3H} = \lambda_{3H}^{\text{in}}$ nominal set and the BDT response cut is set to

FIG. 4. The 1- and 2-σ CI regions versus the input values of λ_{3H}^{in} at the HL-LHC assuming 3 ab⁻¹. The CI regions are obtained by likelihood fitting of $M_{\gamma\gamma b\bar{b}}$ distributions using BDT _{λ_{3H}} . The solid and dashed lines delimit the 1- and 2-σ CI regions, respectively. And the diagonal red dotted line denotes $\lambda_{3H}^{\text{out}} = \lambda_{3H}^{\text{in}}$ and the vertical blue line at $\lambda_{3H}^{\text{in}} = 1$ indicates the case shown in the lower frame of Fig. 3 with BDT_{SM}.

TABLE III. NLO and LO results obtained using BDT_{SM} and comparison with the recent ATLAS result [24]. Z_{max} , $s|_{Z_{\text{max}}}$, and $b|_{Z_{\text{max}}}$ denote the significance, the number of signal events, and the number of background events, respectively, obtained after applying the BDT cut which maximizes the significance. Also compared are the 95% CL and 1σ CI ranges of λ_{3H} .

	BDT_{SM}		ATLAS_2018 [24]
	MLM $\oplus$ NLO _{dist}	MLM $\oplus$ LO _{dist}	Ref. [21] $\oplus$ LO _{dist}
Z_{max}	1.95	1.79	2.1
$s _{Z_{\text{max}}}$	8.85	8.61	6.46
$b _{Z_{\text{max}}}$	17.94	20.44	6.8
95% CL	(1.00, 6.22)	(0.87, 6.55)	(1.3, 6.2)
1σ CI	(0.1, 2.2) $\cup$ (5.4, 6.6)	(0.1, 2.3) $\cup$ (5.3, 6.7)	(−0.1, 2.4)

maximize significance. Using $\text{BDT}_{\lambda_{3H}}$, the 95% CL region is narrowed into $1.01 < \lambda_{3H} < 5.42$ at 95% CL. Compared to that obtained using BDT_{SM} , we observe the noticeable changes of Z for $\lambda_{3H} \gtrsim 4$. We also find there exists a bulk region of $0.5 \lesssim \lambda_{3H} \lesssim 4.5$ in which it is hard to pin down the THSC, see the 1σ error region delimited by solid lines in Fig. 4.

In Fig. 1, we show that using the NLO distributions of signal for TMVA may lead to better results. For quantitative comparisons we use the LO distributions for TMVA and find that the significance can reach up to 1.79 with about 9 signal and 20 background events. The details of the NLO and LO results based on BDT_{SM} are presented in Table III where we also make comparison with the recent ATLAS result without systematic uncertainties [24] in which the LO distributions of signal and the generator-level cuts adopted in Ref. [21] are used for TMVA.¹

¹A similar approach using BDTs was explored in Ref. [25] previously. But they consider only a part of the background processes considered in this work and, being different from the case of ATLAS, it is difficult to make a direct comparison of our results with theirs.

V. CONCLUSIONS

Higgs-pair production is the most useful avenue to probe the EWSB sector. We have studied in great detail, with the help of machine learning, the sensitivity of measuring the THSC λ_{3H} that one can expect at the HL-LHC with 3000 fb^{-1} . With TMVA one can improve upon the signal-to-background significance over the traditional cut-based analysis. In this work, we have shown that the significance is improved by about 80% and found a narrower range of λ_{3H} below the sensitivity. With BDTs trained for each value of λ_{3H} , we found the bulk region further down to $0.5 \lesssim \lambda_{3H} \lesssim 4.5$ in which one cannot pin down the THSC. For the Supplemental Material, we refer to Ref. [26].

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