Measuring the trilinear Higgs boson self-coupling at the 100 TeV hadron collider via multivariate analysis

Jubin Park\textsuperscript{1,2}, Jung Chang\textsuperscript{2}, Kingman Cheung\textsuperscript{3,4,5}, and Jae Sik Lee\textsuperscript{2,1}

\textsuperscript{1}IUEP, Chonnam National University, Gwangju 61186, Korea
\textsuperscript{2}Department of Physics, Chonnam National University, Gwangju 61186, Korea
\textsuperscript{3}Physics Division, National Center for Theoretical Sciences, Hsinchu, Taiwan
\textsuperscript{4}Division of Quantum Phases and Devices, School of Physics, Konkuk University, Seoul 143-701, Republic of Korea
\textsuperscript{5}Department of Physics, National Tsing Hua University, Hsinchu 300, Taiwan

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Abstract

We perform a multivariate analysis of Higgs-pair production via the decay channel $HH \to b\bar{b}\gamma\gamma$ at the future 100 TeV $pp$ collider to determine the trilinear Higgs self-coupling (THSC) $\lambda_{3H}$, which takes the value of 1 in the standard model. We consider all known background processes. For the signal we adopt the most recent event generator of POWHEG-BOX-V2 to exploit the NLO distributions for Toolkit for Multivariate Data Analysis (TMVA). Through the technique of Boosted Decision Tree (BDT) analysis trained for $\lambda_{3H} = 1$, compared to the conventional cut-and-count approach, the signal-to-background ratio improves tremendously from about 1/10 to 1 and the significance can reach up to 20.5 with a luminosity of 3 ab\textsuperscript{-1}. In addition, by implementing a likelihood fitting of the signal-plus-background $M_{\gamma\gamma bb}$ distribution with optimized bin sizes, the THSC can be determined with the precision of 7.5% at 68% CL with 3 ab\textsuperscript{-1}.
I. INTRODUCTION

Since the discovery of the 125 GeV Higgs boson in 2012 at the LHC [1], we have been looking for a clear signal or even a hint of new physics beyond the Standard Model (SM) but without much success. Moreover, after completing the Runs I and II at the LHC, it turns out that the 125 GeV Higgs boson is best described as the SM Higgs boson [2], although there is an upward trend in the overall signal strength [3]. Under this situation, one of the most solid avenues to explore for new physics is to measure the Higgs potential which could be significantly different from that of the SM.

Higgs-boson pair production at the high-luminosity and/or high-energy hadron colliders provides a very useful way to probe the Higgs potential via the investigation of the trilinear Higgs self-coupling (THSC) [4–6]. The specific decay modes considered are: $b\bar{b}b\bar{b}$ [7], $b\bar{b}\gamma\gamma$ [8, 9], $b\bar{b}\tau^+\tau^−$ [10], $b\bar{b}W^+W^−$ [11], and some combinations of these channels [12, 13]. Higgs-boson pair production also has been vastly studied in models beyond the SM [14].

The current limits on the THSC in units of $\lambda_{3H}$, which takes the value of 1 in the SM, are $−5.0 < \lambda_{3H} < 12$ from ATLAS [15] and $−11.8 < \lambda_{3H} < 18.8$ from CMS [16] at 95% confidence level (CL). At the high-luminosity option of the LHC running at 14 TeV (HL-LHC) with an integrated luminosity of 3 ab$^{-1}$, a combined ATLAS and CMS projection of the 68% CL interval is $0.57 < \lambda_{3H} < 1.5$ without including systematic uncertainties [17]. On the other hand, at the International Linear Collider (ILC) operated at 1 TeV can reach the precision of 10% at 68% CL with an integrated luminosity of 8 ab$^{-1}$ [18, 19].

In this work, we perform a multivariate analysis of Higgs-pair production in $HH → b\bar{b}\gamma\gamma$ channel at the 100 TeV hadron collider. In our previous work, based on the conventional cut-and-count analysis, it was shown that the THSC can be measured with about 20% accuracy at the SM value with a luminosity of 3 ab$^{-1}$ [20]. In this Letter, with the use of the BDT method closely following Ref. [21], we show that the THSC can be measured with a precision of 7.5% at 68% CL at the 100 TeV hadron collider assuming 3 ab$^{-1}$ luminosity, which is superior to the accuracy expected at the 1 TeV ILC even with 8 ab$^{-1}$. 
II. EVENT GENERATION AND TMVA ANALYSIS

The Higgs bosons in the signal event samples are generated on-shell with a zero width by 
\texttt{POWHEG-BOX-V2} \cite{22,23} with the damping factor \(hdamp\) set to the default value of 250 to limit 
the amount of hard radiation. This code provides NLO distributions matched to a parton 
shower taking account of the full top-quark mass dependence. The signal cross section at 
NNLO order in QCD is calculated according to 
\[ \sigma_{\text{NNLO}}(\lambda_3 H) = K_{\text{NNLO}/\text{NLO}}^{\text{NNLO}/\text{NLO}} \sigma_{\text{NLO}}(\lambda_3 H) \]
using \(\sigma_{\text{NLO}}(\lambda_3 H)\) from \texttt{POWHEG-BOX-V2} and \(K_{\text{NNLO}/\text{NLO}} = 1.067\) \cite{24} in the FT approximation in 
which the full top-quark mass dependence is considered only in the real radiation while the 
Born improved Higgs Effective Field Theory is taken in the virtual part. And then, the 
\texttt{MadSpin} code \cite{25} is used for the decay of both Higgs bosons into two bottom quarks and 
two photons.

For generation and simulation of backgrounds, we closely follow Ref. \cite{20}, except for the 
use of the post-LHC PDF set of \texttt{CT14LO} \cite{26} for non-resonant backgrounds. Furthermore, 
for the two main non-resonant backgrounds of \(b\bar{b}\gamma\gamma\) and \(c\bar{c}\gamma\gamma\), we use the merged cross 
sections and distributions by MLM matching \cite{27,28} with \(xqcut\) and \(Q_{\text{cut}}\) set to 20 GeV 
and 30 GeV, respectively. For the remaining non-resonant backgrounds, we are using the 
cross sections and distributions obtained by applying the generator-level cuts as adopted 
in Ref. \cite{9,13} which might provide more reliable and conservative estimation of the non-
resonant backgrounds containing light jets \cite{20}.

For parton showering and hadronization, \texttt{PYTHIA8} \cite{29} is used both for signal and back-
grounds. Finally, fast-detector simulation and analysis are performed using \texttt{Delphes3} \cite{30} 
with the \texttt{Delphes-FCC} template.

All the signal and backgrounds are summarized in Table I together with information of 
the corresponding event generator, the cross section times the branching ratio and the order 
in QCD, and the Parton Distribution Function (PDF) used.

A multivariate analysis is performed using TMVA \cite{31} with \texttt{ROOTv6.18} \cite{32}. After applying a sequence of event selections as in Table II we choose the following 8 kinematic 
variables for TMVA:

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

The judicious choice of the two photons or two \(b\) quarks for the above TMVA variables has 
been made as in \cite{21}. We also refer to Ref. \cite{21} for the details of our TMVA setup and
TABLE I. Monte Carlo samples used in Higgs-pair production analysis $H(\rightarrow b\bar{b})H(\rightarrow \gamma\gamma)$, and the corresponding codes for the matrix-element generation. PYTHIA8 is used for parton showering and hadronization.

| Signal process | Generator       | $\sigma \cdot BR$ [fb] | Order | PDF used               |
|----------------|-----------------|------------------------|-------|------------------------|
| $gg \rightarrow HH \rightarrow b\bar{b}\gamma\gamma$ | POWHEG-BOX-V2   | 3.25                   | NNLO  | PDF4LHC15_nlo          |

| Background(BG) | Process | Generator       | $\sigma \cdot BR$ [fb] | Order | PDF used         |
|----------------|---------|-----------------|------------------------|-------|-----------------|
| Single-Higgs   | $ggH(\rightarrow \gamma\gamma)$ | POWHEG - BOX        | $1.82 \times 10^3$     | NNNLO | CT10            |
|                | $t\bar{t}H(\rightarrow \gamma\gamma)$ | PYTHIA8              | $7.29 \times 10^1$     | NLO   |                 |
|                | $ZH(\rightarrow \gamma\gamma)$ | PYTHIA8              | $2.54 \times 10^1$     | NNLO  |                 |
| Non-resonant BG | $b\bar{b}\gamma\gamma$ | MG5_aMC@NLO         | $2.28 \times 10^3$     | LO    | CT14LO          |
|                | $c\bar{c}\gamma\gamma$ | MG5_aMC@NLO         | $1.92 \times 10^4$     | LO    | MLM [27, 28]    |
|                | $jj\gamma$  | MG5_aMC@NLO       | $4.20 \times 10^5$     | LO    |                 |
|                | $b\bar{b}jj$ | MG5_aMC@NLO       | $0.96 \times 10^7$     | LO    |                 |
|                | $c\bar{c}jj$ | MG5_aMC@NLO       | $3.19 \times 10^7$     | LO    | CT14LO          |
|                | $Z(\rightarrow b\bar{b})\gamma\gamma$ | MG5_aMC@NLO     | $1.00 \times 10^{10}$  | LO    | Refs. [9, 13, 20] |
| $t\bar{t}$ and $t\bar{t}\gamma$ BG ($\geq 1$ lepton) | $t\bar{t}$ | MG5_aMC@NLO     | $1.76 \times 10^7$     | NLO   | CT10            |
|                | $t\bar{t}\gamma$ | MG5_aMC@NLO       | $4.18 \times 10^4$     | NLO   | CTEQ6L1         |

analysis. And we choose BDT for our analysis since the BDT-related methods show higher performance with better signal efficiency and stronger background rejection.

III. RESULTS

In the left panel of Fig. [1] we show the BDT responses obtained using BDT trained for $\lambda_{3H} = 1$ which is dubbed as BDTSM. By validating the BDT distributions for
TABLE II. Sequence of event selection criteria applied in this analysis.

| Sequence | Event Selection Criteria at the 100 TeV hadron collider |
|----------|--------------------------------------------------------|
| 1        | Di-photon trigger condition, ≥ 2 isolated photons with $P_T > 30$ GeV, $|\eta| < 5$ |
| 2        | ≥ 2 isolated photons with $P_T > 40$ GeV, $|\eta| < 3$, $\Delta R_{jj,\gamma\gamma} > 0.4$ |
| 3        | ≥ 2 jets identified as b-jets with leading(subleading) $P_T > 50(40)$ GeV, $|\eta| < 3$, $\Delta R_{bb} > 0.4$ |
| 4        | Events are required to contain ≤ 5 jets with $P_T > 40$ GeV within $|\eta| < 5$ |
| 5        | No isolated leptons with $P_T > 40$ GeV, $|\eta| < 3$ |
| 6        | TMVA analysis |

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, which mostly populate in the regions with positive and negative BDT response, respectively. (Right) Signal and background efficiencies (inset) and significance $Z = \sqrt{2 \cdot [(s + b) \cdot \ln(1 + s/b) - s]}$ with $s$ and $b$ being the numbers of signal and background events.
TABLE III. Expected number of signal and background events at the 100 TeV hadron collider assuming 3 ab$^{-1}$ using BDT$_{SM}$ with the BDT response cut of 0.216. See text for explanation.

| Signal and Backgrounds | Pre-Selection | BDT$_{SM}$ | Cut-and-Count | Eff. Lumi. (ab$^{-1}$) |
|------------------------|--------------|------------|---------------|----------------------|
| $H(b\bar{b}) H(\gamma \gamma)$, $\lambda_{3H} = -3$ | 7253.98 | 2408.37 | 3400.08 | 10.7 |
| $H(b\bar{b}) H(\gamma \gamma)$, $\lambda_{3H} = 0$ | 2072.09 | 902.49 | 1146.21 | 44.5 |
| $H(b\bar{b}) H(\gamma \gamma)$, $\lambda_{3H} = 1$ | **1124.48** | **548.02** | **673.29** | **615** |
| $H(b\bar{b}) H(\gamma \gamma)$, $\lambda_{3H} = 5$ | 1480.24 | 251.13 | 439.29 | 40.9 |
| $ggH(\gamma \gamma)$ | 5827.41 | 255.86 | 875.71 | 17.0 |
| $t\bar{t}H(\gamma \gamma)$ | 11371.21 | 145.88 | 868.73 | 13.2 |
| $ZH(\gamma \gamma)$ | 593.29 | 38.88 | 168.86 | 39.4 |
| $b\bar{b}H(\gamma \gamma)$ | 205.45 | 2.59 | 9.82 | 51.0 |
| $b\bar{b}\gamma\gamma$ | 183493.56 | 55.01 | 336.49 | 19.2 |
| $c\bar{c}\gamma\gamma$ | 66600.78 | 0.00 | 54.66 | 0.11 |
| $jj\gamma\gamma$ | 14182.56 | 2.52 | 25.20 | 2.38 |
| $b\bar{b}jj$ | 1228956.91 | 38.53 | 1176.93 | 3.74 |
| $c\bar{c}jj$ | 208285.83 | 0.00 | 187.92 | 0.26 |
| $b\bar{b}jj$ | 1622778.23 | 0.00 | 2231.08 | 0.19 |
| $Z(b\bar{b})\gamma\gamma$ | 4540.20 | 4.72 | 45.33 | 12.7 |
| $tt$ ($\geq 1$ leptons) | 78490.03 | 0.00 | 56.93 | 11.5 + 3.68 |
| $tt\gamma$ ($\geq 1$ leptons) | 74885.54 | 9.09 | 105.16 | 8.69 + 2.07 |
| Total Background | 3500211.00 | 553.09 | 6142.83 |
| Significance $Z$, $\lambda_{3H} = 1$ | **20.50** | **8.44** |

Events as functions of the cut value on BDT response. The significance can reach up to 20.50 when the BDT response is cut at 0.216, at which, the signal and background efficiencies are 0.48 and $1.58 \times 10^{-4}$, respectively. We denote by vertical lines the positions of the optimal cut on the BDT response which maximizes the significance.
In Table III, we present the expected number of signal and background events at the 100 TeV hadron collider assuming 3 ab$^{-1}$ using BDT$_{SM}$ with the BDT response cut of 0.216. We show the four representative values of $\lambda_{3H}$ for signal and the backgrounds are separated into three categories. For comparisons, we also show the results obtained using the cut-and-count analysis [20]. In the last column, we additionally present the effective luminosity (Eff. Lumi.) for each of signal and background samples. In the $t\bar{t}$ and $t\bar{t}\gamma$ backgrounds, the first (second) number is the effective luminosity when the two top quarks decay fully (semi-) leptonically. We find about 550 signal and 550 background events for $\lambda_{3H} = 1$. Comparing to the results using the cut-and-count analysis [20], the number of signal events decreases by only 19% while the number of backgrounds by almost 90%, resulting in an increase in significance from 8.44 to 20.50. Note that the composition of backgrounds changes drastically by the use of BDT. In the cut-and-count analysis, the non-resonant background is about two times larger than the single-Higgs associated background. While, in the BDT analysis, the single-Higgs associated background is more than four times larger than the non-resonant one and $t\bar{t}$ associated background becomes negligible. Note that we generate relatively smaller number of events for the $c\bar{c}\gamma\gamma$, $c\bar{c}j\gamma$, and $b\bar{b}jj$ backgrounds since we observe that they quickly decrease when the BDT response cut approaches to the point $Z_{\text{max}}$ of 0.216. Specifically, the $b\bar{b}jj$ background vanishes for the BDT response cut larger than 0.2. Otherwise, we generate enough number of events considering the assumed luminosity of 3 ab$^{-1}$.

First, we try to determine the THSC considering the total number of events. As shown in the left panel of Fig. 2, we find that the THSC can be measured with about 11% accuracy at the SM value which is about two times better than the result based on the conventional cut-and-count analysis [20]. However, there is a second solution around $\lambda_{3H} = 6.5$. To lift up the two-fold ambiguity, we implement a likelihood fitting of the signal-plus-background $M_{\gamma\gamma bb}$ distribution and find the second solution is ruled out by more than 8$\sigma$ confidence, see the right panel of Fig. 2.

To improve the sensitivity of the THSC around the SM value and to tame the statistical fluctuation due to the limited size of the MC samples, we repeat the likelihood fitting of $M_{\gamma\gamma bb}$ distribution by optimizing the bin size between 1/20 GeV and 1/60 GeV. Finally, we find that the THSC can be determined with a precision of 7.5% at 68% CL as shown in the left panel of Fig. 3. In the right panel of Fig. 3, $M_{\gamma\gamma bb}$ distributions are shown for the THSC at the SM value and for the two values deviated by 1$\sigma$. 

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FIG. 2. (Left) The total number $N = s + b$ of signal ($s$) and background ($b$) events versus $\lambda_{3H}$ with 3 ab$^{-1}$. The horizontal solid line denotes the total number of events obtained using the SM value of $\lambda_{3H} = 1$ and the dashed lines for the statistical 1-σ error. (Right) The relative log likelihood distribution for the nominal value of $\lambda_{3H} = 1$ at the 100 TeV hadron collider assuming 3 ab$^{-1}$ and using BDT$_{\text{SM}}$ with the BDT response cut of 0.216. The distribution has been obtained by likelihood fitting of $M_{\gamma\gamma bb}$ distribution for each value of $\lambda_{3H}$. The black solid line shows the result of a polynomial fitting and the horizontal solid (red) line at $-\ln(L_{\lambda_{3H}}/L_{\lambda_{3H}=1}) = 32$ indicates the value corresponding to the 8σ level.

Before we end this section, in Table IV we show the relative importance of the variables that we employed in this BDT analysis. We observe that the two most important variables are $\Delta R_{bb}$ and $\Delta R_{\gamma\gamma}$, which is consistent with our previous cut-and-count analysis [20].

| Variable | Importance |
|----------|------------|
| $\Delta R_{bb}$ | 0.163 |
| $\Delta R_{\gamma\gamma}$ | 0.152 |
| $M_{\gamma\gamma}$ | 0.150 |
| $\Delta R_{\gamma b}$ | 0.133 |
| $P_T^{\gamma\gamma}$ | 0.110 |
| $M_{\gamma\gamma bb}$ | 0.102 |
| $P_T^{bb}$ | 0.096 |
| $M_{bb}$ | 0.095 |

IV. CONCLUSIONS:

Higgs-pair production is one of the most useful avenue to probe the EWSB sector. We have studied in great details, with the help of machine learning, the sensitivity of measuring
FIG. 3. (Left) The relative log likelihood distribution for the nominal value of $\lambda_{3H} = 1$ at the 100 TeV hadron collider with 3 ab$^{-1}$. The black circles are the values obtained by likelihood fitting of $M_{\gamma\gamma bb}$ distributions using BDT$_{\text{SM}}$ with the BDT response cut of 0.216. The black solid line shows the result of a polynomial fitting and the thin dashed line at 0.5 (2.0) indicates the value corresponding to a 1$\sigma$ (2$\sigma$) CI. The shaded region shows the 1$\sigma$ CI expected at the ILC at 1 TeV with 8 ab$^{-1}$. (Right) The SM $M_{\gamma\gamma bb}$ distribution (solid line with dots with 1$\sigma$ error bars) and those for $\lambda_{3H} = 0.92$ and 1.08 (dashed lines).

the THSC $\lambda_{3H}$ that one can expect at the 100 TeV $pp$ collider with an integrated luminosity 3 ab$^{-1}$. With TMVA one can improve the signal-to-background ratio for $\lambda_{3H} = 1$ to 1 : 1 compared with the ratio 1 : 10 obtained in the conventional cut-and-count approach. Furthermore, the significance of such a signal jumps to 20.

Other than determining the THSC by measuring the total number of events, one can also improve the sensitivity and lift the two-fold degeneracy by implementing a likelihood fitting of the signal-plus-background $M_{\gamma\gamma bb}$ distribution with optimized bin sizes. The THSC can be determined with a precision of 7.5% at 68% CL with 3 ab$^{-1}$, which is indeed better than the ILC running at 1 TeV with 8 ab$^{-1}$. Extrapolating our result conservatively, we expect that one can achieve the precision better than $\sim$ 2% with 30 ab$^{-1}$.

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