Note

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1 Signal

We consider a simple extension of the standard model (SM) [1], which includes a vectorlike dark fermion ($\overline{\chi}, \chi$) and a complex singlet scalar S. A signature of CP violation could come from the Higgs-to-Higgs decays, $h_3 \to h_2 h_1$, where $h_3/h_2/h_1$ are the heaviest scalar, second heaviest scalar, and the SM-like 125 GeV Higgs, respectively.

The signal process is the triple production of 125 GeV Higgs bosons via the gluon fusion:

$$gg \rightarrow h_3 \rightarrow h_2 h_1 \rightarrow h_1 h_1 h_1$$

The Higgs boson h_1 would further decay to the $b\bar{b}$ pair. We consider the banchmark point 1 (BP1), where $m_{h_3}=450$ GeV, $m_{h_2}=280$ GeV, $m_{h_1}=125$ GeV. This process is generated at $\sqrt{s}=13$ TeV. Following are the MadGraph scripts for generating signal samples:

```
import model cxSM_VLF_EFT
generate g g > h h h
output MG5/gghhh_bsm
launch MG5/gghhh_bsm
shower=Pythia8
detector=Delphes
analysis=OFF
madspin=ON
done
```

```
set param_card mh1 125
set param_card mh2 280
set param_card mh3 420
set param_card theta12 0.73
```

```
set param card theta13 1.67079632679
set param_card theta23 -0.73
set param card vs 200
set param card delta2 0
set param card Rdelta3 0
set param card Idelta3 -3.5
set param card b2 0
set param_card Rc1 0
set param_card Ic1 0
set param_card Rc2 0
set param card Ic2 0
set param card Rd3 0
set param card Id3 0
set param card msq -5033.406281907266
set param card lam 0.13850082540690806
set param card Rdelta1 -47.561525227572744
set param card Idelta1 853.05384671134
set param card Rb1 -70476.6380004269
set param_card Ib1 -30486.140015405872
set param card Rd1 -2.562109886826132
set param card Id1 2.257859679994403
set param_card d2 6.340799300844676
set param_card gh1ggr -0.00005478952893059635
set param_card gh1gagar -0.00003270447254456052
set param_card gh1Zgar -0.00005871986046374793
set param card gh2ggr -1.4279972541632635e-7
set param_card gh2gagar -8.237715486808595e-8
set param card gh2Zgar -1.3984990232267825e-7
set param card gh3ggr -6.031835872118092e-6
set param card gh3gagar -1.1377279177203616e-6
set param card gh3Zgar -2.2999597941282603e-6
set param_card decay 102 auto
set param_card decay 103 auto
set run card nevents 100000
```

```
set run_card ebeam1 6500.0
set run_card ebeam2 6500.0
set run_card ptb 24
set run_card etab 2.6
set spinmode none
decay h > b b~
```

done

2 SPANet pairing

We employ the novel neural network structure SPA-NET [2, 3, 4] to identify the correct pairings among the jets in the final states.

2.1 Training dataset preparation

Preselection: ≥ 6 jets with transverse momentum $p_{\rm T} \geq 25$ GeV in range $|\eta| < 2.5$.

The input features for the SPA-NET are a list of jets, each represented by its 4-component vector (p_T, η, ϕ, m) as well as a boolean b-tag. We only keep each event's 15 highest p_T jets. For each event, we define the correct jet assignments by matching the jets to the simulated truth quarks within an angular distance of $\Delta R < 0.4$. If a simulated truth quark is matched to more than one jet, such an event will be dropped. Furthermore, some simulated truth quarks may not be matched to any jet, in which case the event will not be used in training either.

After the selection and matching, we could obtain the following results from 1M events:

• Total sample size: 522,899

• 1h sample size: 184,769

• 2h sample size: 161,476

• 3h sample size: 94,464

Here, the 1h sample is the event where we could define the correct jet assignments for 1 Higgs boson.

2.2 Training results

• Training sample:

- Total sample size: 470,609

- 1h sample size: 166,490

- 2h sample size: 145,309

- 3h sample size: 84,913

- 5% used on validation

• Testing sample:

- Total sample size: 52,290

- 1h sample size: 18,279

- 2h sample size: 16,167

- 3h sample size: 9,551

Some useful definitions for evaluating jet assignment performance:

• Event Efficiency

$$\epsilon^{\text{event}} \equiv \frac{\text{number of events with and all Higgs are correctly identified}}{\text{number of events}}$$
(1)

• Higgs Efficiency

$$\epsilon^{\rm h} \equiv \frac{\text{number of correctly identified Higgs}}{\text{number of identifiable Higgs}}$$
(2)

The training results are shown in Table 1.

Table 1: Spa-Net pairing efficiencies on 3h events.

$N_{ m Jet}$	Event Fraction	Event Efficiency	Higgs Efficiency
= 6	0.077	0.532	0.650
=7	0.057	0.345	0.536
≥ 8	0.052	0.237	0.452
Total	0.186	0.375	0.548

3 χ^2 pairing

 χ^2 method considers all possible combinations of final jets and selects the configuration that minimizes the mass difference between Higgs candidates and SM Higgs, i.e., minimizes this:

$$\chi^2 = [m(j_1 j_2) - m_h]^2 + [m(j_3 j_4) - m_h]^2 + [m(j_5 j_6) - m_h]^2$$
(3)

where $m(j_i j_j)$ is the invariant mass of jet i, j and $m_h = 125$ GeV.

Table 2 is the performance of the χ^2 method.

Table 2: χ^2 pairing efficiencies on 3h events.

$N_{ m Jet}$	Event Fraction	Event Efficiency	Higgs Efficiency
= 6	0.077	0.403	0.450
=7	0.057	0.158	0.281
≥ 8	0.052	0.000	0.077
Total	0.186	0.215	0.294

References

- [1] Ting-Kuo Chen, Cheng-Wei Chiang, and Ian Low. Simple model of dark matter and CP violation. *Phys. Rev. D*, 105(7):075025, 2022.
- [2] Michael James Fenton, Alexander Shmakov, Ta-Wei Ho, Shih-Chieh Hsu, Daniel Whiteson, and Pierre Baldi. Permutationless many-jet event reconstruction with symmetry preserving attention networks. *Phys. Rev. D*, 105:112008, Jun 2022.
- [3] Michael James Fenton, Alexander Shmakov, Hideki Okawa, Yuji Li, Ko-Yang Hsiao, Shih-Chieh Hsu, Daniel Whiteson, and Pierre Baldi. Extended Symmetry Preserving Attention Networks for LHC Analysis. 9 2023.
- [4] Alexander Shmakov, Michael James Fenton, Ta-Wei Ho, Shih-Chieh Hsu, Daniel Whiteson, and Pierre Baldi. SPANet: Generalized permutationless set assignment for particle physics using symmetry preserving attention. *SciPost Phys.*, 12:178, 2022.