PASCOS 2025

25/07/2025

Exploring the C3HDM with ML

Unearthing large pseudoscalar Yukawa couplings

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based on: Souza et al,
arXiv:2505.10625, accepted in JHEP

Fundação para a Ciência e a Tecnologia
PDM-QUEST_2024.01362.CERN
PRR Plano de Recuperação e Resiliência
REPÚBLICA PORTUGUESA
Financiado pela União Europeia NextGenerationEU

Introduction

Standard Model

- Elementary particles
- Interactions

Higgs Field

- Discovered in 2012
- Explains particle masses

Multi-Higgs

- Found one, are there more?

$$\mathrm{SU}(3)_c \times \mathrm{SU}(2)_L \times \mathrm{U}(1)_Y$$

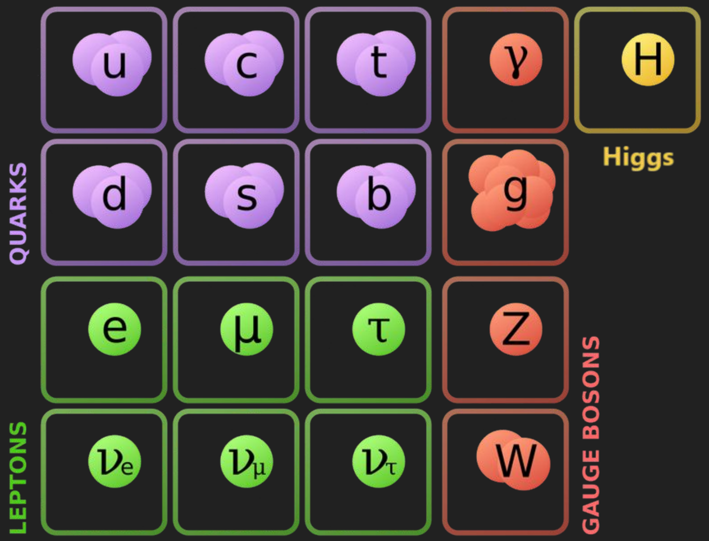


Fig 1: SM Gauge group and particle content.

Introduction

Multi-Higgs

- NHDM
- Additional Higgs doublets
- Motivated, studied and testable
- Dark Matter
- CP Violation for Baryogenesis
- Flavor
- Neutrino Masses
- (. . .)

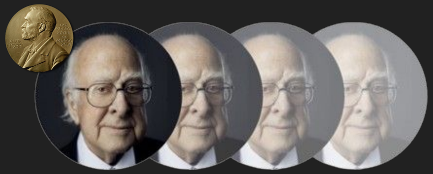


Fig 2: Peter Higgs(es). (Image: here)

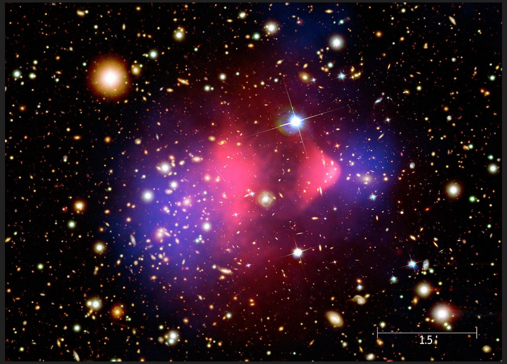


Fig 3: Bullet Cluster, from Chandra X-Ray Observatory. X-Ray, visible and Grav. Lensing. (Image: here)

Complex Three Higgs Doublet Model

C3HDM

- Three Higgs doublets
- Potential violates CP (explicitly)
- Reals vevs
- 5 Higgs neutral states
- 2 Charged Higgses

Boto, Lourenço et al,
JHEP 2024

$$\Phi_i = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} w_i^+ \\ v_i + x_i + i\ z_i \end{pmatrix}$$

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ z_2 \\ z_3 \end{pmatrix} \to \begin{pmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \\ h_5 \end{pmatrix} \qquad \begin{pmatrix} w_2^+ \\ w_3^+ \end{pmatrix} \to \begin{pmatrix} H_1^+ \\ H_2^+ \end{pmatrix}$$

$\mathbb{Z}_2 \times \mathbb{Z}_2$ C3HDM

Potential

- Introduce $\mathbb{Z}_2 \times \mathbb{Z}_2'$ symmetry
- Soft-breaking terms

$$\mathbb{Z}_2 : \Phi_1 \to -\Phi_1 \,, \quad \ell_R \to -\ell_R$$
$$\mathbb{Z}_2' : \Phi_2 \to -\Phi_2 \,, \quad d_R \to -d_R$$

$$V = V_2 + V_4 = \mu_{ij}(\Phi_i^\dagger \Phi_j) + z_{ijkl}(\Phi_i^\dagger \Phi_j)(\Phi_k^\dagger \Phi_l)$$

$$V_2 \supset \mu_{12}(\Phi_1^\dagger \Phi_2) + \mu_{13}(\Phi_1^\dagger \Phi_3) + \mu_{23}(\Phi_2^\dagger \Phi_3) + \text{h.c.}$$

$\mathbb{Z}_2 \times \mathbb{Z}_2$ C3HDM

Yukawa

- Introduce $\mathbb{Z}_2 \times \mathbb{Z}_2'$ symmetry
- Avoid FCNCs
- Type-Z ➡ decoupled Yukawas

$$\mathbb{Z}_2 : \Phi_1 \to -\Phi_1\,, \quad \ell_R \to -\ell_R$$
$$\mathbb{Z}_2' : \Phi_2 \to -\Phi_2\,, \quad d_R \to -d_R$$

fermion type	type-I	type-II	type-X	type-Y	type-Z
up quarks (u)	Φ_3	Φ_3	Φ_3	Φ_3	Φ_3
down quarks (d)	Φ_3	Φ_2	Φ_3	Φ_2	Φ_2
charged leptons (ℓ)	Φ_3	Φ_2	Φ_2	Φ_3	Φ_1

Tab 1: 3HDM model types that describe how the scalars couple with the fermions.

$\mathbb{Z}_2 \times \mathbb{Z}_2$ C3HDM

Couplings

$$-\mathcal{L}_{\xi f f} = \sum_f \sum_{j=1}^{2N} \frac{m_f}{v} \bar{f} \left(c^e_{\xi_j f f} + i\gamma_5 c^o_{\xi_j f f} \right) f \xi_j$$

$$c^e_{\xi_j f f} + i\gamma_5 c^o_{\xi_j f f} = \frac{v}{v_f} \left(Q_{jf} \pm i\gamma_5 Q_{j,N+f} \right)$$

$$f = (1,2,3) \equiv (\ell, d, u)$$

$$R_{1i}(\vec{\alpha})$$

$$c^e_{ff} \equiv c^e_{h_{125} f f} = \frac{R_{11}}{c_{\beta_2} c_{\beta_1}}, \frac{R_{12}}{c_{\beta_2} s_{\beta_1}}, \frac{R_{13}}{s_{\beta_2}}$$

$$c^o_{ff} \equiv c^o_{h_{125} f f} = \frac{-R_{14} s_{\beta_1} - R_{15} c_{\beta_1} s_{\beta_2}}{c_{\beta_2} c_{\beta_1}}, \frac{R_{14} c_{\beta_1} - R_{15} s_{\beta_1} s_{\beta_2}}{c_{\beta_2} s_{\beta_1}}, -\frac{R_{15} c_{\beta_2}}{s_{\beta_2}}$$

$\mathbb{Z}_2 \times \mathbb{Z}_2$ C3HDM

Couplings $$-\mathcal{L}_{\xi f f} = \sum_f \sum_{j=1}^{2N} \frac{m_f}{v} \bar{f} \left(c^e_{\xi_j f f} + i \gamma_5 c^o_{\xi_j f f} \right) f \xi_j$$

In the plane of the couplings, $\sqrt{|c^e_{ff}|^2 + |c^o_{ff}|^2} \lesssim 1$

In the SM, $c^e_{ff} = 1$ and $c^o_{ff} = 0$

Constraints

Theoretical

Potential Stability

- Bounded from Below sufficient conditions

Perturbativity

- Yukawa couplings

Unitarity

Experimental

Oblique Parameters STU

Flavor Searches

- 1-loop $b \to s\gamma$

LHC signal strengths

electron EDM

- More stringent than other EDMs

HiggsTools 1.1.3

- Searches for new particles
- $\Delta\chi^2$ at 3σ

Machine Learning

Romão and Romão
PRD 2024

In the $\mathbb{Z}_2 \times \mathbb{Z}_2$ C3HDM

Found 1 point p/ 10^13

Adopt “trick”

- Sample in real limit, near alignment
- Enlarge pseudoscalar component progressively

In the $\mathbb{Z}_3$ 3HDM

Parameter space exploration

- Inefficient
- Time-consuming

Evolutionary Strategy

- Biological evolution
- Variation and Selection by fitness
- Population evolves toward fitter individuals

Machine Learning

C Function Properties

Observable or parameter

- Upper Bound
- Lower Bound

Returns zero if in bounds otherwise

Returns “distance”

- *How far* from valid?
- Ruled out points are useful!

- Constraint Function

$$C(\mathcal{O}) = \max(0, -\mathcal{O} + \mathcal{O}_{LB}, \mathcal{O} - \mathcal{O}_{UB})$$

- Constraints Loss Function

$$L(\theta) = \sum_{i=1}^{N_c} C(\mathcal{O}_i(\theta))$$

Machine Learning

CMAES

Powerful optimizer

Limited discovery

Final Loss Function

$\tilde{L}(\theta) = 1 + L(\theta) \text{ if } L(\theta) > 0, \text{ 0 otherwise}$

$$L_T(\theta) = \tilde{L}(\theta) + \frac{1}{2}\left(\frac{1}{N_p^{\mathcal{P}}}\sum_{i=1}^{N_p^{\mathcal{P}}} p_i^{\mathcal{P}}(\theta^i) + \frac{1}{N_p^{\mathcal{O}}}\sum_{i=1}^{N_p^{\mathcal{O}}} p_i^{\mathcal{O}}[\mathcal{O}^i(\theta)]\right)$$

HBOS

Anomaly detection

Penalizes dense regions

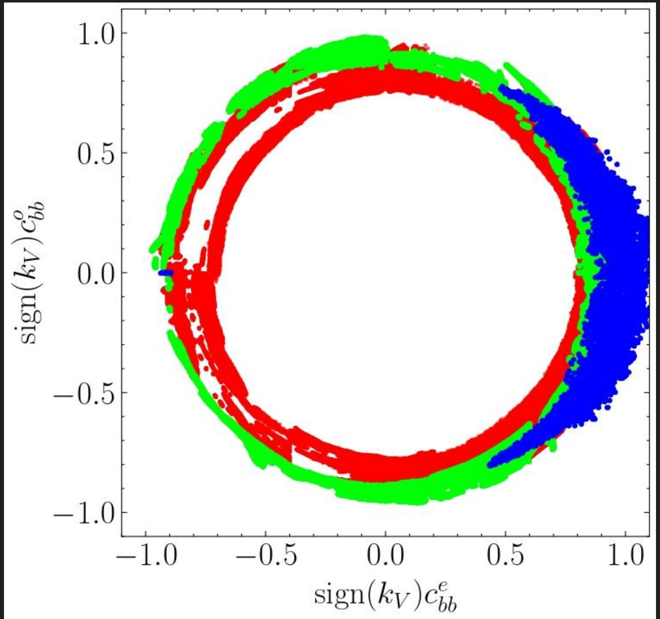
Focused Scans and *Seeds*

Incentivises exploration!

Results - Plot Legend Key

- Red points:
  Pass all constraints
  Agreement with 125 GeV μ_i^f at 2σ
  Pass Higgs searches
  May have high $\Delta\chi^2$
- Green points: $\Delta\chi^2$ at 3σ
  Red points with in agreement
  Points generated with ML constraint
- Blue points:
  Imported from previous paper
  No requirements on $\Delta\chi^2$
  Serve as comparison
- Sidebar colour code:
  Difference to $\Delta\chi^2$
  Mass difference between 125 GeV higgs and lightest scalar

Results - *hbb*



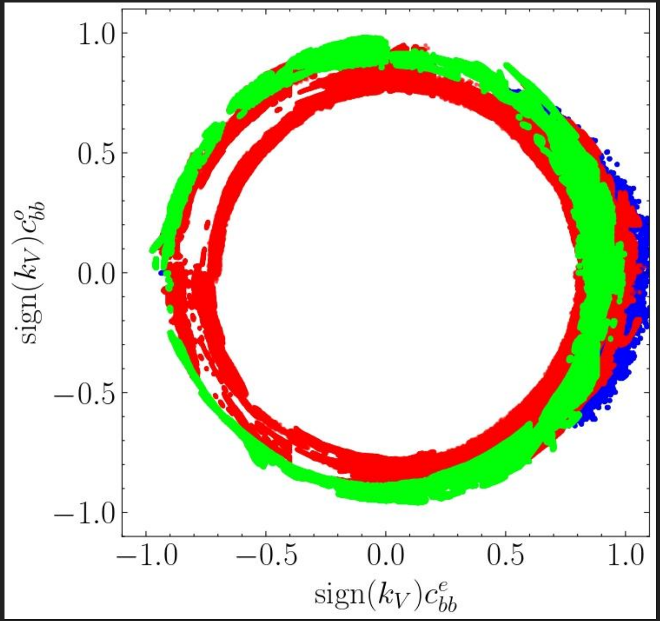
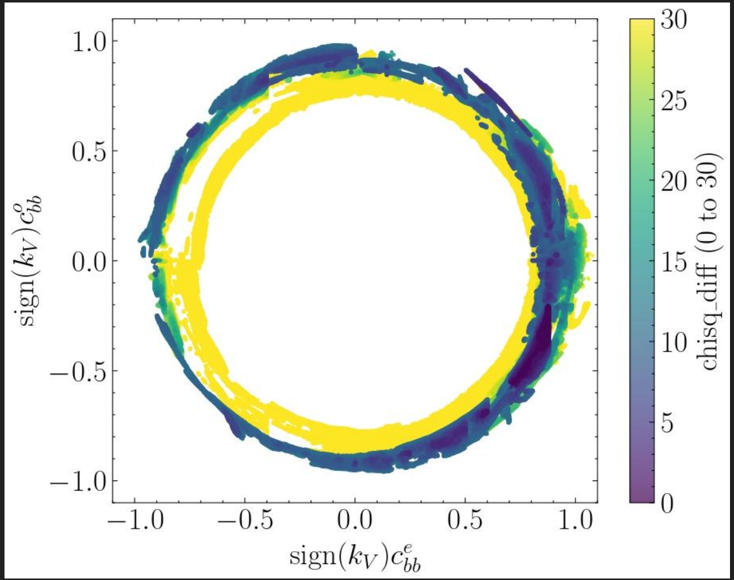


Fig 4: Couplings to bb, achieving maximal pseudoscalar values, completing circle with Chi2 agreement.

Results - *hbb*



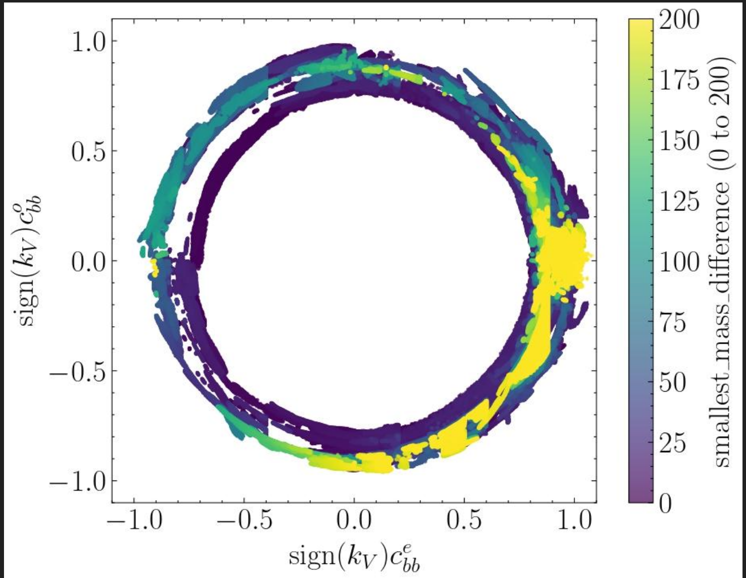


Fig 5: Couplings to bb, showing Chi2 and mass difference between the 125 GeV Higgs and next lightest scalar.

Results - $h\tau\tau$

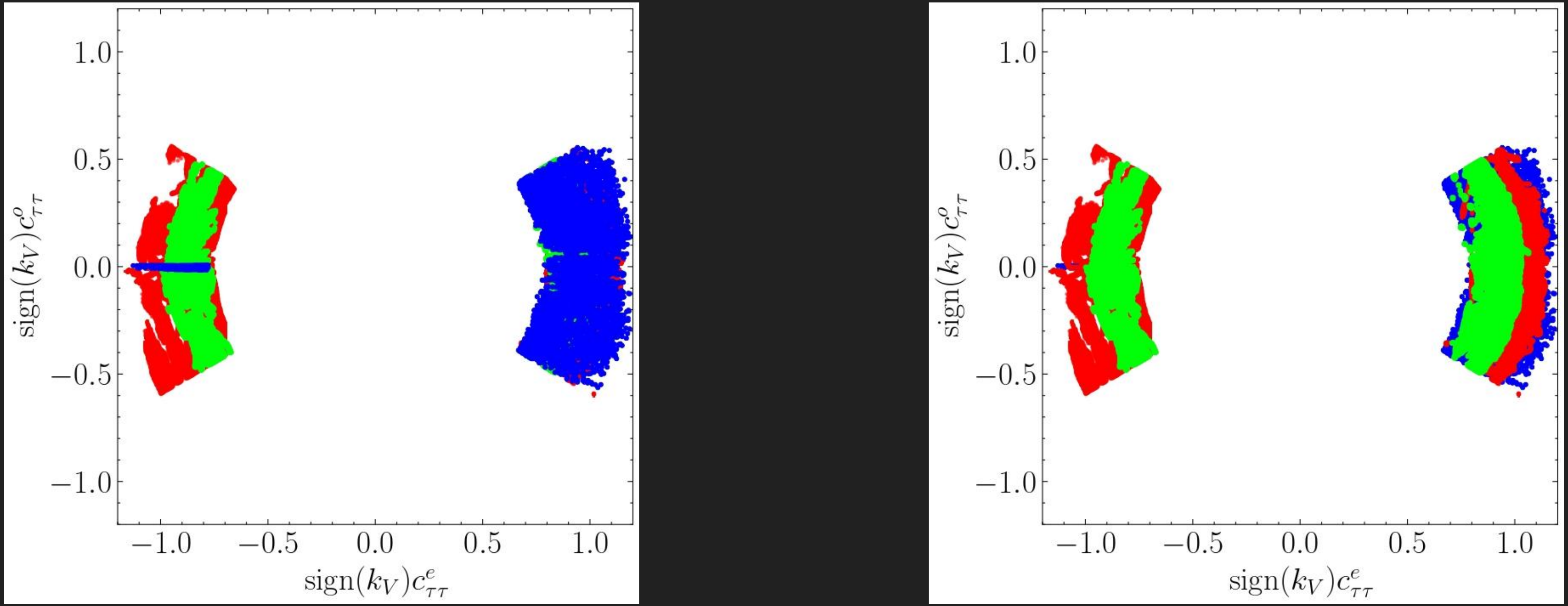


Fig 6: Couplings to $\tau\tau$, achieving maximal pseudoscalar couplings in wrong sign, within exp. bounds.

Results - *htt*

- With conventional scans,

$$c_{tt}^{o} \sim 0$$

Was effectively excluded

- With ML, top couplings recovered
- The “best one can do” is misleading
- Narrow viable regions can misrepresent the full model phenomenology

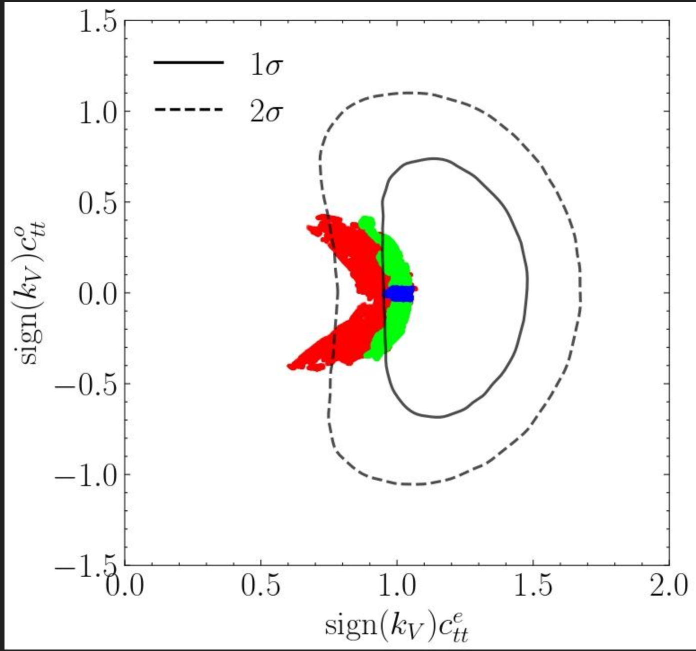


Fig 7: Top couplings with experimental contour lines.

Results - *htt*

- With conventional scans,

$$c_{tt}^{o} \sim 0$$

$$\Rightarrow \frac{c_{\tau\tau}^{o}}{c_{bb}^{o}} = -\frac{v_2}{v_1} = -\tan^2\beta_1$$

- Thought to hold, yet disproved by ML
- Restores Type-Z decouples Yukawa sectors

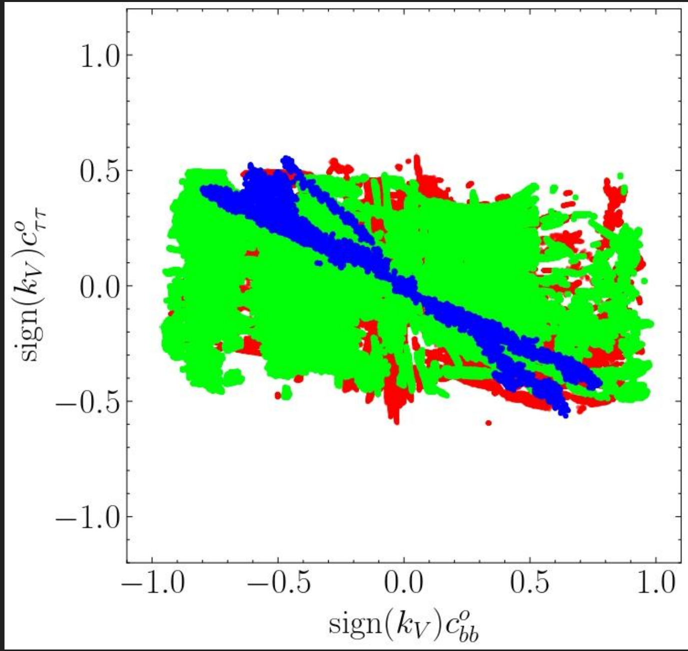


Fig 8: bb and $\tau\tau$ are now larger and uncorrelated.

Results - Parameters

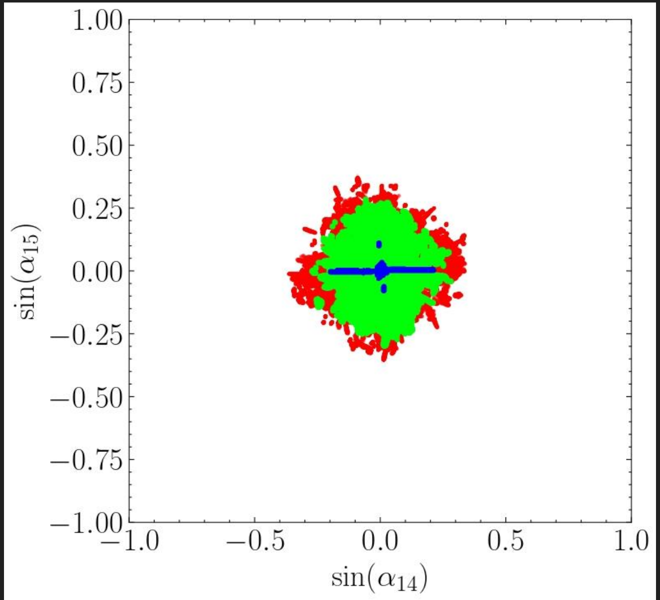


Fig 9: Angles restricted due to eEDM. No *focused scans* were performed for these angles, only for the couplings.

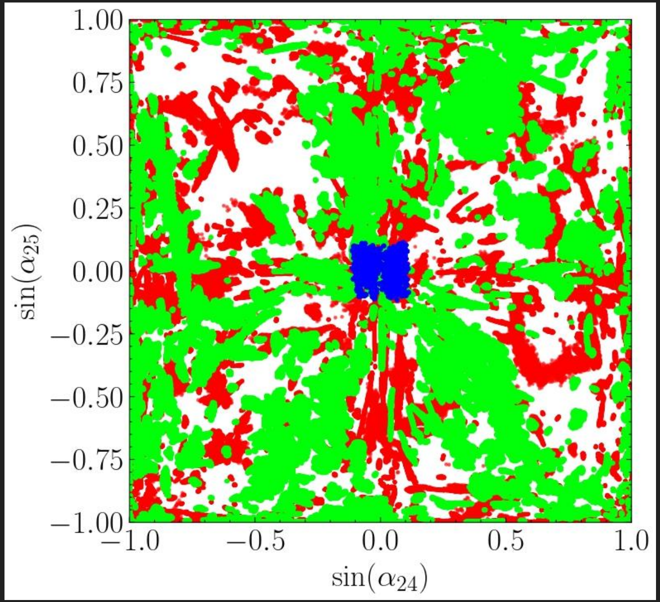


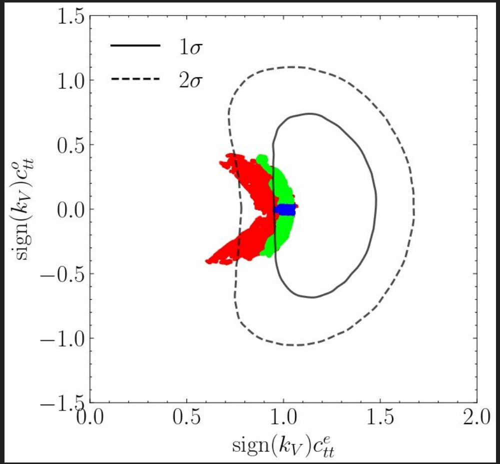
Fig 10: Angles responsible for CPV in heavier scalars. No *focused scans* were performed for these angles, only for the couplings.

Conclusion

- Explore the CP violating C3HDM
- Employ state of the art ML algorithm
- Uncover phenomenology
  - Enlarge pseudoscalar Yukawas
  - Recover top couplings
  - Restore Type-Z decoupled Yukawas
- Applicable to any BSM physics

Information

- arXiv:2505.10625, accepted in JHEP
- pedro.m.figueiredo@tecnico.ulisboa.pt



Backup slides

Optimisation with an CMAES

- CMAES
  - Covariant Matrix Adaptation Evolutionary Strategy
  - Stochastic
  - Derivative-free
  - Non-linear or non-convex
  - Localized Multivariate Gaussian
  - Approaches steepest descent
  - Limited exploration!

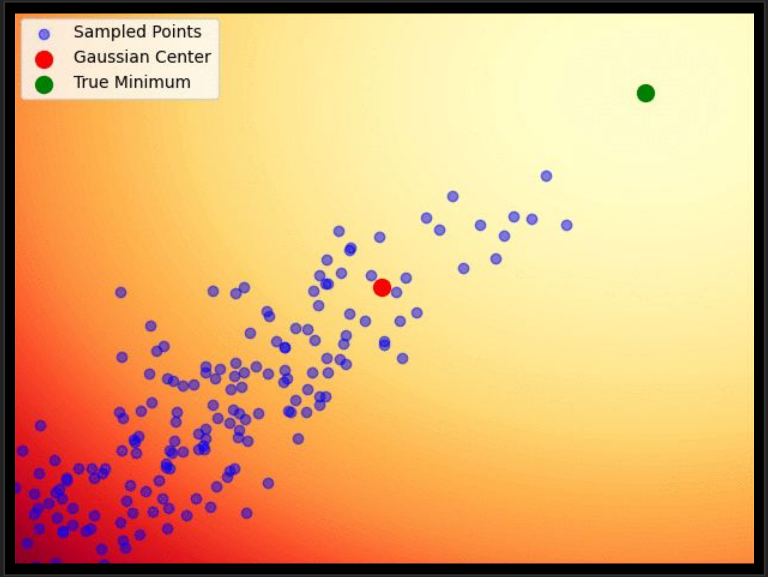


Fig A: CMAES converging to function minimum.

Novelty Reward

- <u>Anomaly Detection</u>
  - CMAES converges quickly
  - Limited discovery

➡ Introduce Novelty Reward to Loss
  - Penalize discovered regions
  - HBOS Density estimation
  - Fits Histogram with *N* bins, for each dimension (parameter)
  - Lower density? Outlier!

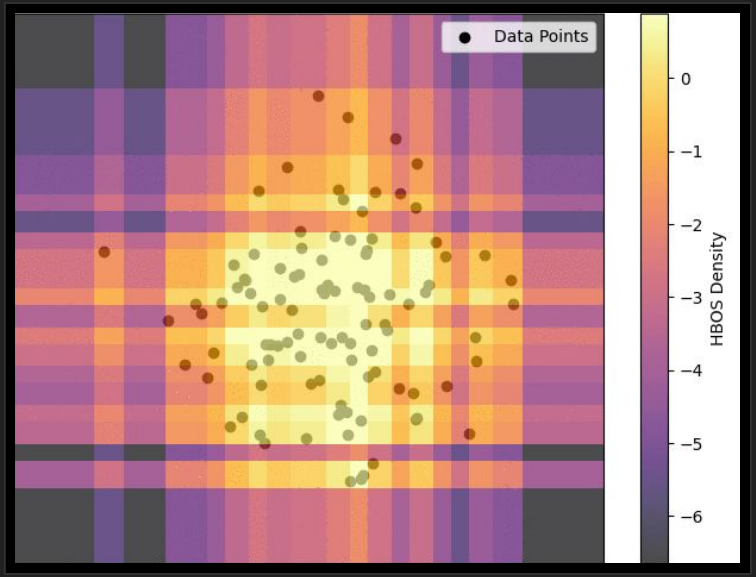


Fig B: Density estimation by HBOS.