LABORATÓRIO DE INSTRUMENTAÇÃO E FÍSICA EXPERIMENTAL DE PARTÍCULAS
partículas e tecnologia

FCT Fundação para a Ciência e a Tecnologia
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E ENSINO SUPERIOR

Universidade do Minho
Escola de Ciências

Using Machine Learning to Scan Beyond Standard Model Parameter Spaces

In collaboration with Miguel Crispim Romão, Nuno Filipe Castro, Mehraveh Nikjoo, Werner Porod

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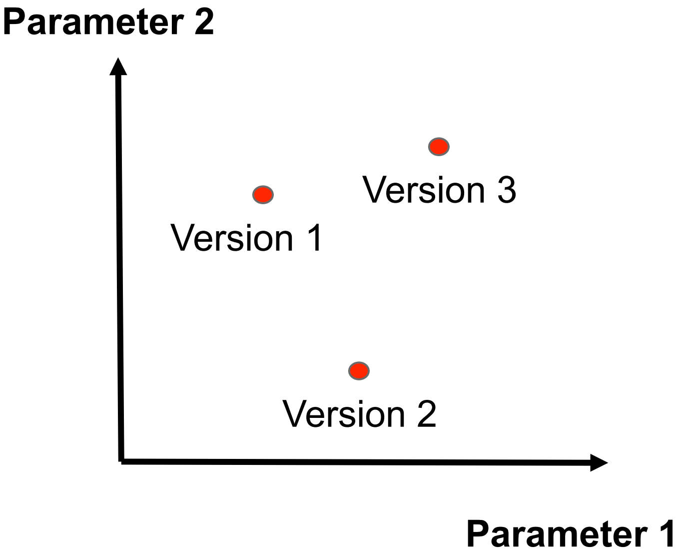
Introduction
Beyond Standard Model Parameter Spaces



- BSM models typically have many free parameters.
  These parameter form a **parameter space**

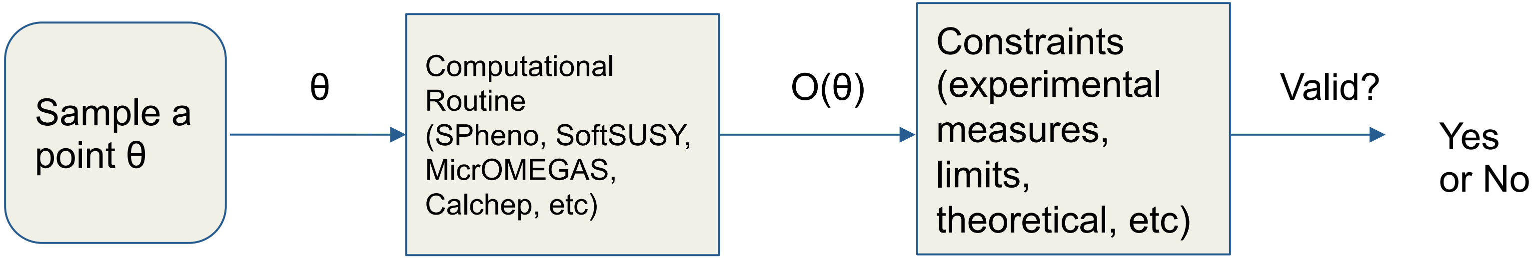
- **Each point** in the **parameter space** corresponds to a **unique version** of the **theoretical model**

- Which versions agree with **experimental data**?

Need to **scan** the parameter space in search for valid points

Introduction
Scanning Parameter Spaces

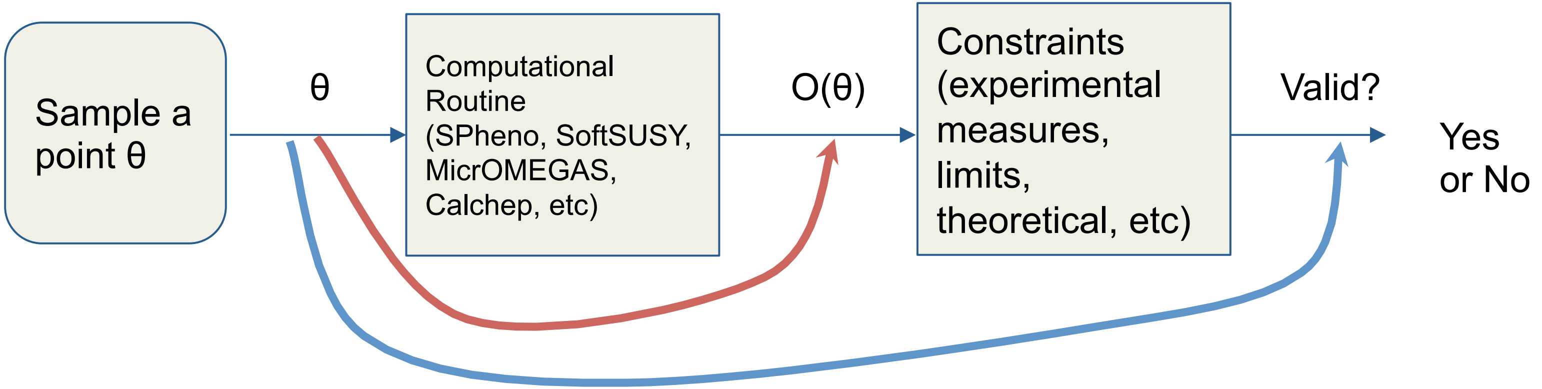
- Parameter space scanning is usually **computationally** and **time consuming**
- Difficulty increases for highly constrained cases: **low parameter sampling efficiency**



For more difficult scans one usually adapts for simplicity (e.g. known alignment limits, a priori choice of parameter space corners, less constraints, etc)

Introduction
Scanning Parameter Spaces

- Considering that the **observable computation** is the heavy step, try to **replace it**, either by **predicting the observables (regression)** or **predicting if a point is valid (classification)**
- **Problem**: Vast amount of data required for training



Kronheim, et al [2007.04506]

Caron, et al [1605.02797]; Ren, et al [1708.06615]; Staub [1906.03277]

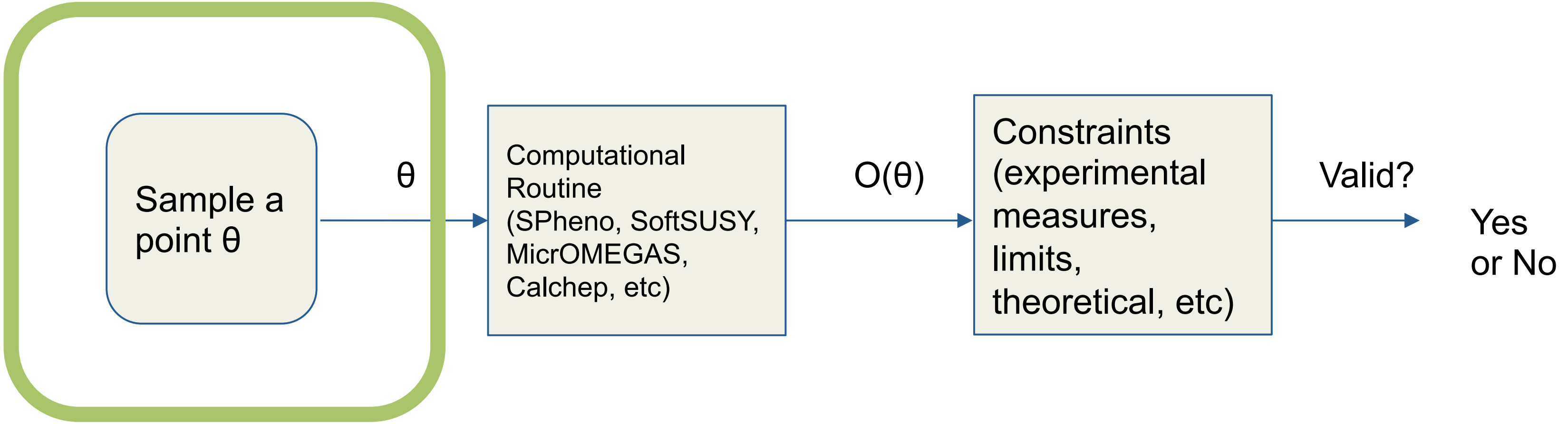
Exploring Parameter Spaces with ML/AI Search Algorithms

Exploring Parameter Spaces with Artificial Intelligence and Machine Learning Black-Box Optimisation Algorithms
FAS, Miguel Crispim Romão, Nuno Filipe Castro, Mehraveh Nikjoo, Werner Porod
https://arxiv.org/abs/2206.09223
code: https://gitlab.com/lip_ml/blackboxbsm

Exploring Parameter Spaces with AI/ML[2206.09223]

Problem (re)framing: face the sampling

- The “ah-ah” moment of this work was to consider: **what if we change the sampling itself**



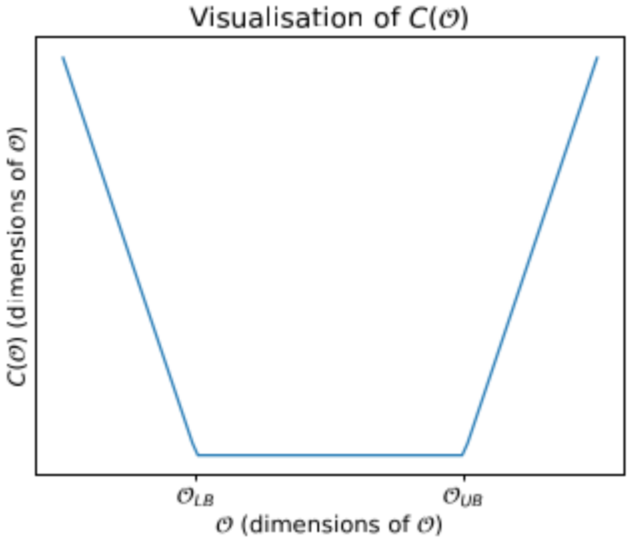
Exploring Parameter Spaces with AI/ML 2206.09223

Problem (re)framing: BSM as a black-box

- We do not look at if a point is valid or try to predict observables
- Instead, we look at **how far a point is from being valid**
- Let **C(O)** be a function of a observable

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

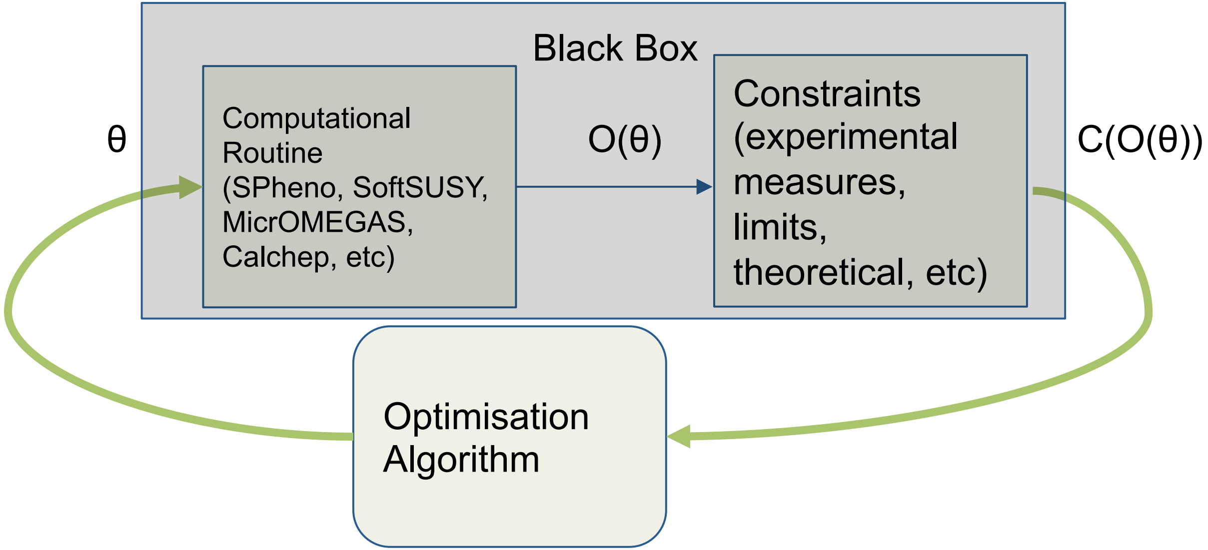
Finding the valid points is the same as minimising C(O)



Exploring Parameter Spaces with AI/ML[2206.09223]

Problem (re)framing: BSM as a black-box

- Since **O=O(θ)** we can **close the loop** and **optimise in order to the parameters C(O)=C(O(θ)).** From the outside, **C(O(θ))** is a **Black-Box => Black-Box Optimisation Problem**



Exploring Parameter Spaces with AI/ML [2206.09223]

The physics models and computational routine

- We used the same physics cases as Hollingsworth, et al [2103.06957]
  - **cMSSM**: 4 parameters
  - **pMSSM**: 19 parameters
- We performed two studies:
  - **Higgs mass** constraint

$$Loss(\theta) = C(m_{h^0}(\theta))$$

  - **Higgs mass** and **Dark Matter Relic Density** constraints by adding them up

$$Loss(\theta) = C(m_{h^0}(\theta)) + C(\Omega_{DM}h^2(\theta))$$

Constraint	$\mathcal{O}_{LB}$	$\mathcal{O}_{UB}$
m_h	122 GeV	128 GeV
$\Omega_{DM}h^2$	0.08	0.14

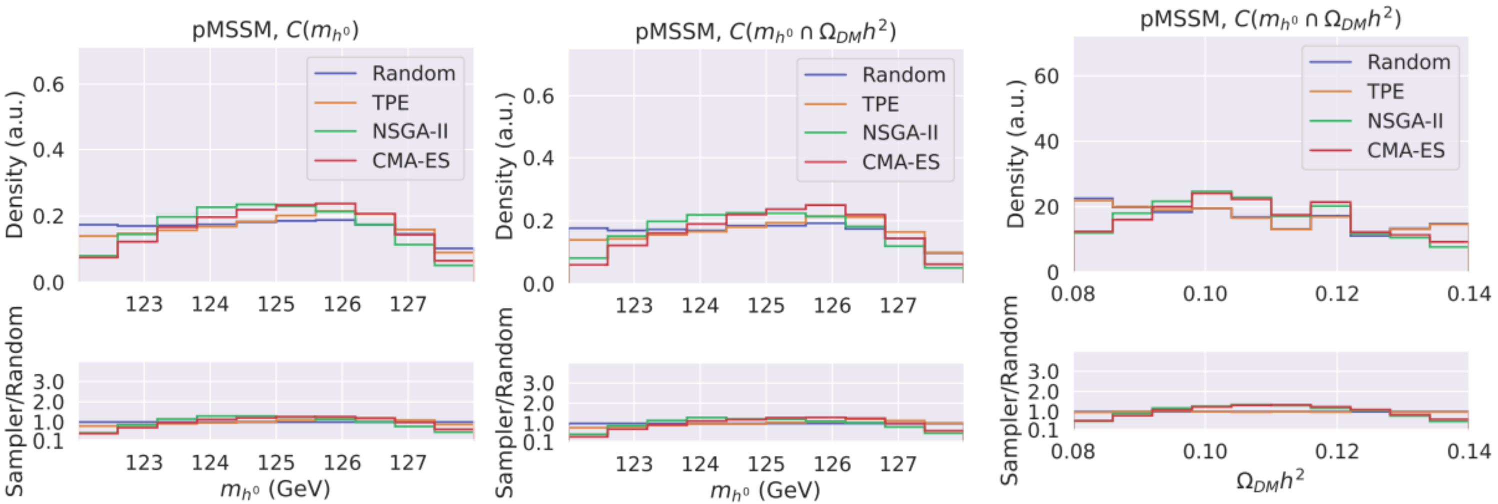
Exploring Parameter Spaces with AI/ML[2206.09223]

Meet the algorithms

- The fields of Artificial Intelligence and Machine Learning have a multitude of **search algorithms** for **black-box optimisation**
- We explore **three different classes of algorithms** to see their differences
  - A **Bayesian** Optimisation Algorithm: Tree-Parzen Estimator (TPE)
  - A **Genetic** Algorithm: Nondominated Sorting Genetic Algorithm II (NSGA-II)
  - An (non-genetic) **Evolutionary** Algorithm: Covariant Matrix Approximation Evolution Strategy (CMA-ES)

Exploring Parameter Spaces with AI/ML[2206.09223]

Results: pMSSM observables



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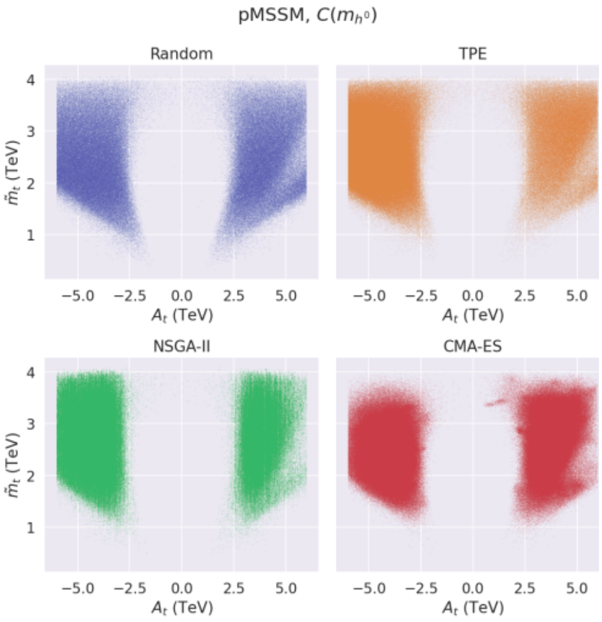
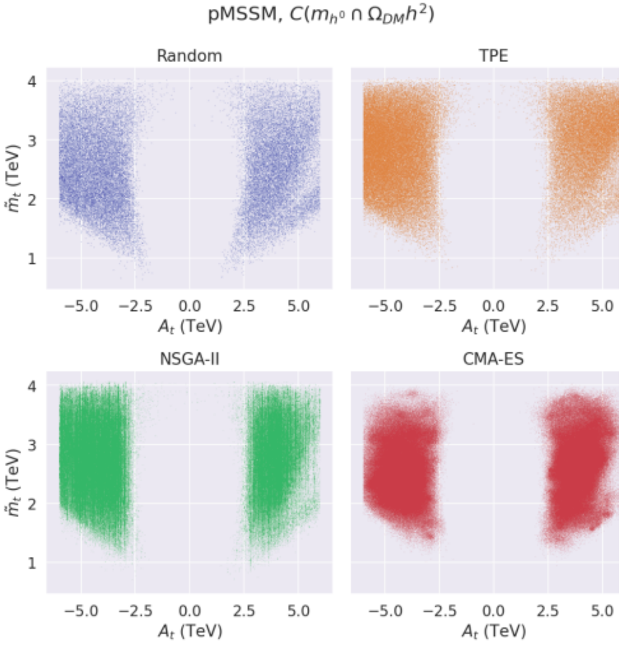
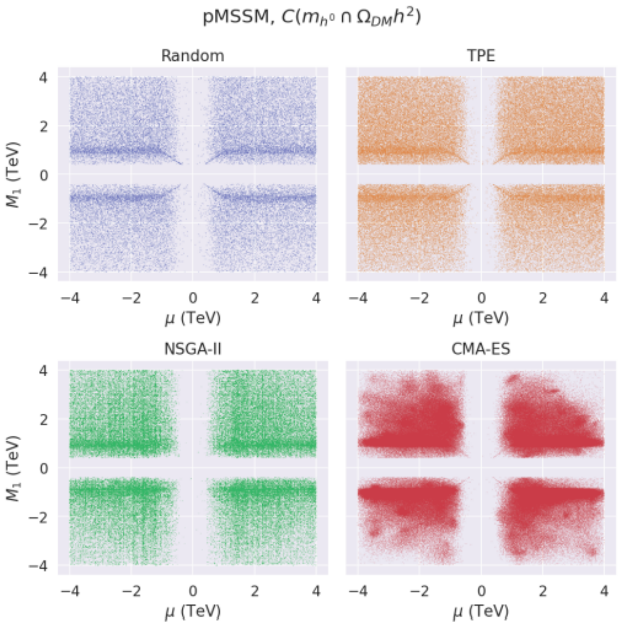
Results: pMSSM parameter scatters







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Results: Performance metrics

- **Efficiency** (bigger is better) → ***exploitation***

$$\text{Efficiency} = \frac{\#\ \text{valid trials}}{\#\ \text{total trials}}$$

		Sampler			
Model	Constraint	Random	TPE	NSGA-II	CMA-ES
cMSSM	m_h	0.401 ± 0.010	0.668 ± 0.012	0.715 ± 0.014	$\mathbf{0.924 \pm 0.023}$
	$m_{h_0} \cap \Omega_{DM}h^2$	0.006 ± 0.001	0.127 ± 0.008	0.281 ± 0.041	$\mathbf{0.687 \pm 0.084}$
pMSSM	m_h	0.309 ± 0.010	0.557 ± 0.038	0.862 ± 0.015	$\mathbf{0.899 \pm 0.034}$
	$m_h \cap \Omega_{DM}h^2$	0.038 ± 0.004	0.099 ± 0.013	$\mathbf{0.663 \pm 0.036}$	0.576 ± 0.073

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Results: Performance metrics

- **Wasserstein Distance** (smaller is better) → ***exploration***

$$WD(f,g) = \int_U |F(u) - G(u)| du$$

		Sampler			
Model	Constraint	Random	TPE	NSGA-II	CMA-ES
cMSSM	m_{h_0}	0.229 ± 0.014	$\mathbf{0.276 \pm 0.020}$	0.364 ± 0.039	0.627 ± 0.099
	$m_{h_0} \cap \Omega_{DM}h^2$	0.797 ± 0.113	$\mathbf{1.101 \pm 0.062}$	1.150 ± 0.090	1.186 ± 0.117
pMSSM	m_{h_0}	0.495 ± 0.030	$\mathbf{1.270 \pm 0.137}$	2.028 ± 0.188	3.997 ± 0.449
	$m_{h_0} \cap \Omega_{DM}h^2$	0.939 ± 0.079	$\mathbf{2.369 \pm 0.274}$	2.800 ± 0.278	4.932 ± 0.331

Conclusions

- We presented a new approach to parameter space scanning: **black-box optimisation**
- The dynamic samplers introduced produced **up to 2 orders of magnitude increased sampling efficiency without the need of a prior training dataset**
- Different samplers have different **exploration-exploitation trade-off**
  - **Bayesian** (TPE) → best **coverage**
  - **Evolutionary** (CMA-ES) → best **efficiency**
  - **Genetic** (NSGA-II) → somewhere **in between**

Future work

- Develop **custom** samplers that can maximise **coverage** and **efficiency**
- Explore **multi-objective** optimisation algorithms
- Go **beyond proof-of-concept** and apply methodology to more difficult and realistic scans