Machine Learning in search for New Physics: Looking for the Unexpected

Higgs Maxwell Workshop 2025
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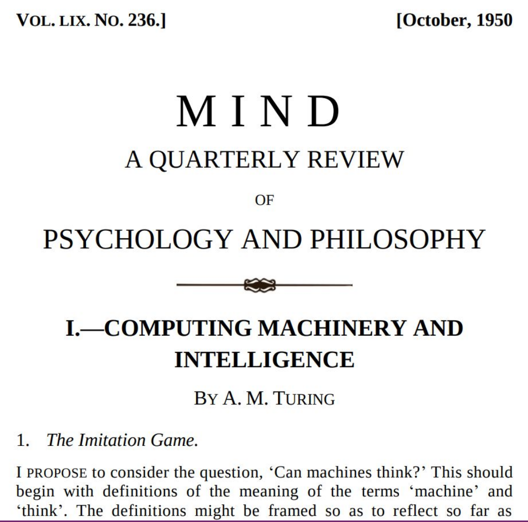
Celebrating the Meeting of Two Histories

400 BC	Mid XX Century	2024
Democritus’ Atomic Theory	Modern Day Particle Physics	Nobel Prize

700 BC	1950	2024
Homer and Hesiod Automata	Alan Turing Seminal Work	Nobel Prize

> *Artificial Intelligence is the quest of creating machines that think and act intelligently*



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MIND

A QUARTERLY REVIEW

OF

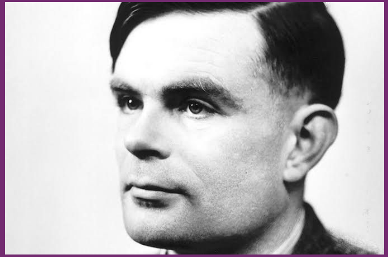
PSYCHOLOGY AND PHILOSOPHY

I.—COMPUTING MACHINERY AND INTELLIGENCE

BY A. M. TURING

1. *The Imitation Game.*

I PROPOSE to consider the question, ‘Can machines think?’ This should begin with definitions of the meaning of the terms ‘machine’ and ‘think’. The definitions might be framed so as to reflect so far as



An operational definition of Machine Learning by Tom M. Mitchell

> ***A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P if its performance at tasks in T, as measured by P, improves with experience E***

Machine Learning in HEP
A flourishing area of research

https://iml-wg.github.io/HEPML-LivingReview/

Machine Learning in HEP
@IPPP: Advancing AI in Phenomenology

Communicating Likelihoods with Normalising Flows #1
Jack Y. Araz (SUNY, Stony Brook), Anja Beck (MIT), Méril Reboud (IJCLab, Orsay), Michael Spannowsky (Durham U., IPPP), Danny van Dyk (Durham U., IPPP) (Feb 13, 2025)
e-Print: 2502.09494 [hep-ph]
pdf cite claim reference search 0 citations

Optimal Equivariant Architectures from the Symmetries of Matrix-Element Likelihoods #17
Daniel Maître (Durham U., IPPP), Vishal S. Ngairangbam (Durham U., IPPP), Michael Spannowsky (Durham U., IPPP) (Oct 24, 2024)
e-Print: 2410.18553 [hep-ph]
pdf cite claim reference search 3 citations

Collective variables of neural networks: empirical time evolution and scaling laws #22
Samuel Tovey, Sven Krippendorf, Michael Spannowsky, Konstantin Nikolaou, Christian Holm (Oct 9, 2024)
e-Print: 2410.07451 [cs.LG]
pdf cite claim reference search 0 citations

The role of data embedding in quantum autoencoders for improved anomaly detection #27
Jack Y. Araz (Jefferson Lab), Michael Spannowsky (Durham U., IPPP) (Sep 6, 2024)
e-Print: 2409.04519 [quant-ph]
pdf cite claim reference search 1 citation

Optimal Symmetries in Binary Classification #32
Vishal S. Ngairangbam, Michael Spannowsky (Aug 16, 2024)
e-Print: 2408.08823 [cs.LG]
pdf cite claim reference search 1 citation

Symbolic regression for beyond the standard model physics #58
Shehu AbdusSalam (Shahid Beheshti U.), Steven Abel (Durham U., IPPP), Miguel Crispim Romão (Durham U., IPPP) (May 28, 2024)
Published in: *Phys.Rev.D* 111 (2025) 1, 015022 • e-Print: 2405.18471 [hep-ph]
pdf DOI cite claim reference search 3 citations

Improving Neutrino Energy Reconstruction with Machine Learning #60
Joachim Kopp (CERN and Mainz U., Inst. Phys. and U. Mainz, PRISMA), Pedro Machado (Fermilab), Margot MacMahon (University Coll. London), Ivan Martinez-Soler (Durham U., IPPP) (May 24, 2024)
e-Print: 2405.15867 [hep-ph]
pdf links cite claim reference search 3 citations

Foundations of automatic feature extraction at LHC–point clouds and graphs #64
Akanksha Bhardwaj (Oklahoma State U.), Partha Konar (Ahmedabad, Phys. Res. Lab), Vishal S. Ngairangbam (Durham U., IPPP) (Apr 24, 2024)
Published in: *Eur.Phys.J.ST* 233 (2024) 15-16, 2619-2640, *Eur.Phys.J.ST* (2024) • e-Print: 2404.16207 [hep-ph]
pdf DOI cite claim reference search 1 citation

Outline

Looking for Unexpected New Physics

1. Semi-supervised Anomaly Detection (AD) to search for New Physics **-> Collider Physics**
2. Artificial Intelligence to Explore Beyond the Standard Model (BSM) Parameter Spaces **-> BSM Physics**
3. Machine Learning to Look for Exotic Dark Matter **-> Astroparticle Physics**

1) Semi-supervised Anomaly Detection to search for New Physics

AD for New Physics Searches
Why

Semi-supervised AD promises **generic New Physics** discriminants

- Semi-supervision: **Trained only on Standard Model background** events
- AD: A single discriminant that measures **how different from the Standard Model** a process is
- Many different semi-supervised AD models in the ML market
    - No free lunch theorem suggests that its likely that no single AD model will outperform the others

AD for New Physics Searches
Previous work

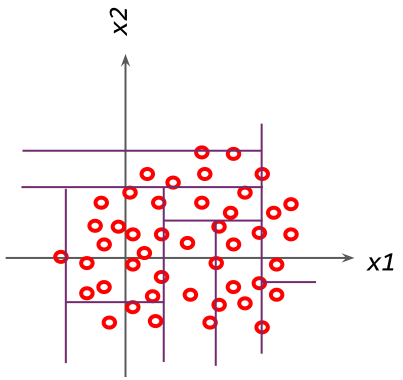
MCR, N. F. Castro, and R. Pedro. "Finding new physics without learning about it: anomaly detection as a tool for searches at colliders." *The European Physical Journal C* 81.1 (2021): 27. [2006.05432]

HBOS: Histogram-Based Outlier System

- Fit a histogram to all features
- Inline score = the sum of the heights of the bins where an event lies ~ binned likelihood

iForest: Isolation Forest

- Recursively random partition the feature space with trees of fixed depth
- Inline score = the amount of nodes an event traverses in an ensemble of trees



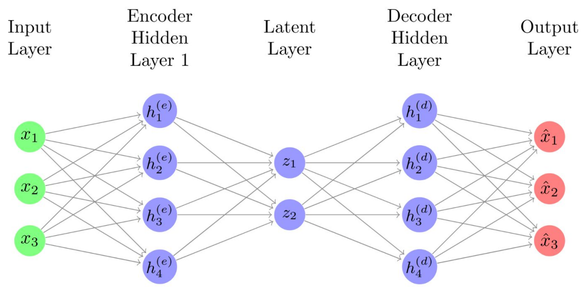
MCR, N. F. Castro, and R. Pedro. "Finding new physics without learning about it: anomaly detection as a tool for searches at colliders." *The European Physical Journal C* 81.1 (2021): 27. [2006.05432]

AD for New Physics Searches
Previous work

Auto-Encoder

- Reconstruction Error-based (~manifold embedding)

$$L = \frac{1}{N}\sum_{i=1}^{N} |x_i - \mathrm{AE}(x_i)|^2$$



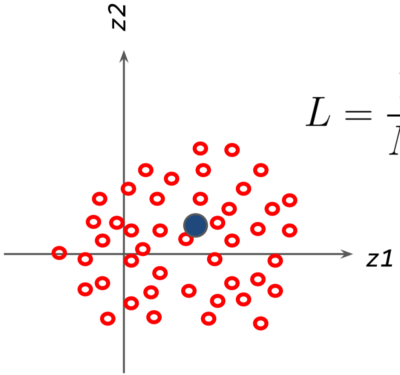
- Discriminant: Reconstruction error
  - BSM events should have higher reconstruction error (“more different”)

MCR, N. F. Castro, and R. Pedro. "Finding new physics without learning about it: anomaly detection as a tool for searches at colliders." *The European Physical Journal C* 81.1 (2021): 27. [2006.05432]

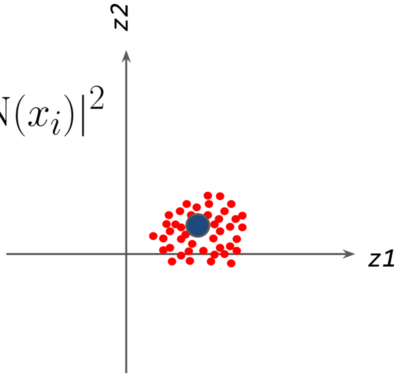
AD for New Physics Searches
Previous work

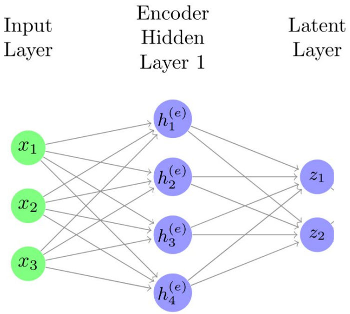
Deep Support Vector Data Description

- Distance to mean-based (but also manifold embedding)



$$L = \frac{1}{N}\sum_{i=1}^{N} |c - \mathrm{NN}(x_i)|^2$$



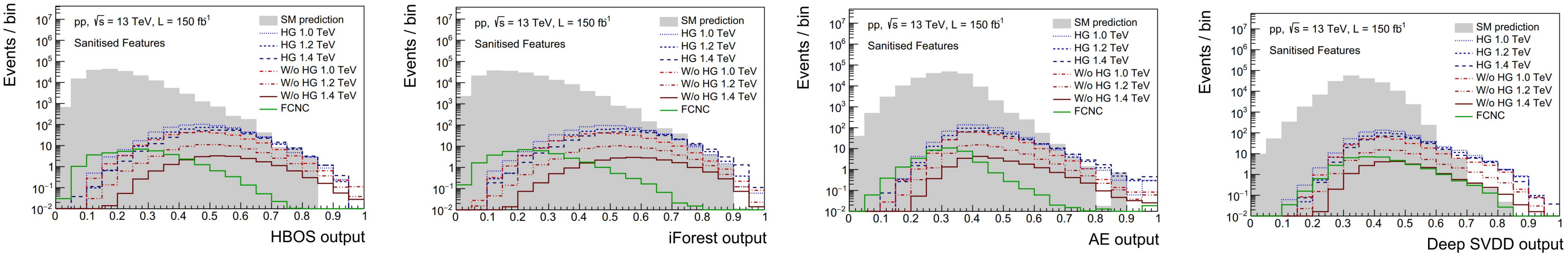


- Discriminant: Distance to mean
  - BSM events should be further away from centre

AD for New Physics Searches
Previous work

MCR, N. F. Castro, and R. Pedro. "Finding new physics without learning about it: anomaly detection as a tool for searches at colliders." *The European Physical Journal C* 81.1 (2021): 27. [2006.05432]

When applied to a collection of different BSM candidates: all models provided sensitivity while capturing different notions of anomaly



AD for New Physics Searches
Previous work

MCR, N. F. Castro, and R. Pedro. "Finding new physics without learning about it: anomaly detection as a tool for searches at colliders." *The European Physical Journal C* 81.1 (2021): 27. [2006.05432]

AD shows promise for generic New Physics searches. However:

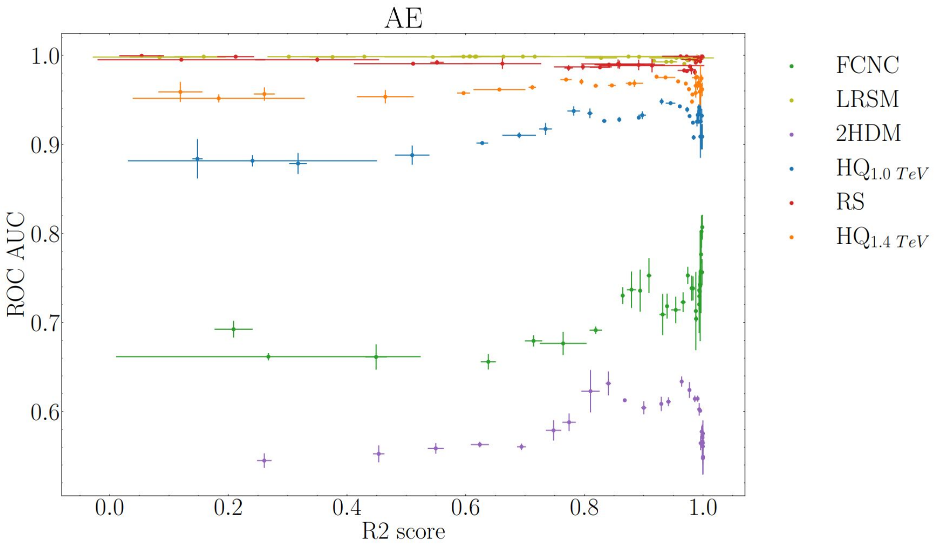
- The **discriminant** for Auto-Encoders is a **reconstruction error**
  - Is the lore "the better the reconstruction the better the discrimination" correct?
- Some **hyperparameters** of the models have **no semi-supervised metric** to use for tuning (the "untunables")
  - How does this affect the sensitivity?
- All **measurements of sensitivity** used are fundamentally **supervised**
  - How can we communicate semi-supervised limits on New Physics?

[WIP] Fernando Abreu de Souza, Maura Barros, Céu Neiva, MCR., N. F. Castro, and R. Pedro. [2502/03.ABCDE]

Also MSc Thesis by Ms. Patrícia Ferreira

AD for New Physics Searches
Ongoing work [PRELIMINARY]

The reconstruction quality of the Auto-Encoder is not a good proxy for its discrimination

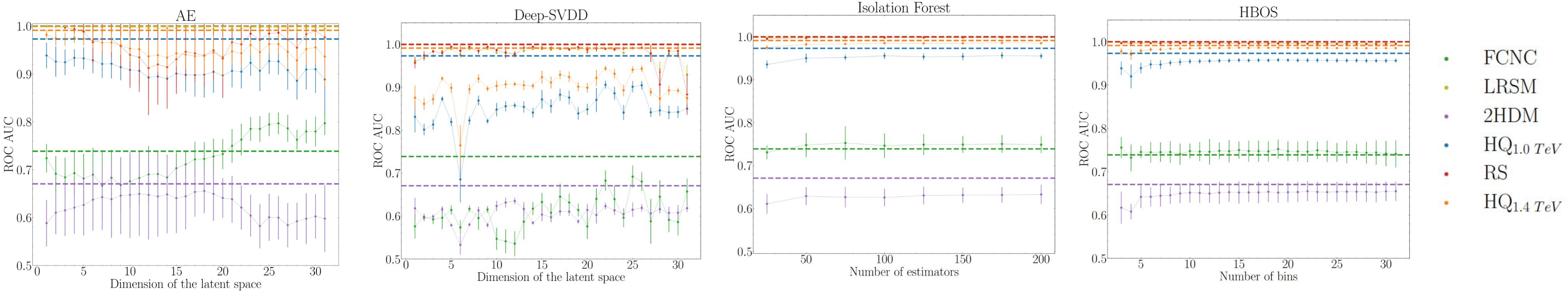


[WIP] Fernando Abreu de Souza, Maura Barros, Céu Neiva, MCR., N. F. Castro, and R. Pedro. [2502/03.ABCDE]

Also MSc Thesis by Ms. Patrícia Ferreira

AD for New Physics Searches
Ongoing work [PRELIMINARY]

Sensitivity to New Physics is ***largely*** independent of the untunable hyperparameters, and the sensitivity is ***capped*** by the sensitivity of the best feature



[WIP] Fernando Abreu de Souza, Maura Barros, Céu Neiva, MCR., N. F. Castro, and R. Pedro. [2502/03.ABCDE]

Also MSc Thesis by Ms. Patrícia Ferreira

AD for New Physics Searches
Ongoing work [PRELIMINARY]

Proposal for a semi-supervised statistical test based on permutation tests

- Prepare a “control” test set with only Standard Model events
- Prepare an “analysis” test set which can be contaminated with BSM
- Measure how the distributions differ using the Cramér–von Mises test

$$CvM = \int_{-\infty}^{\infty} |F(x) - G(x)|^2 dx$$

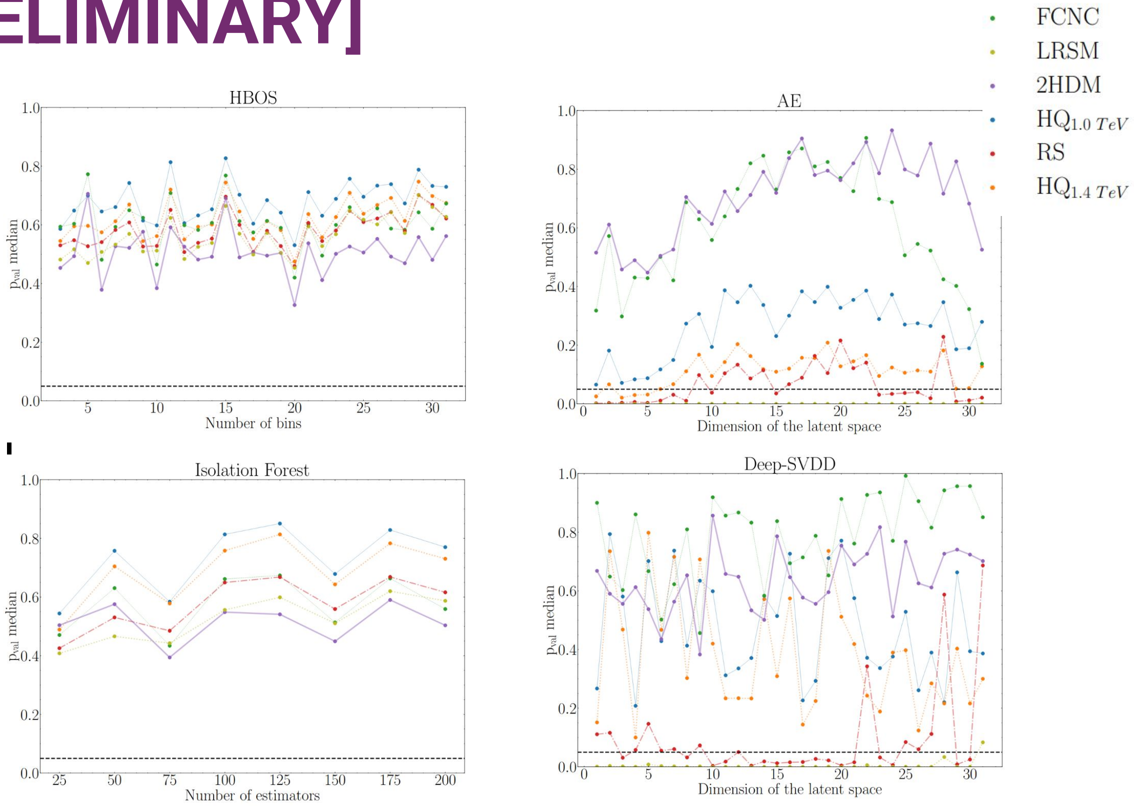
- Prepare P(CvM | H_0) with permutations
- Compute p-value of observed CvM

[WIP] Fernando Abreu de Souza, Maura Barros, Céu Neiva, MCR., N. F. Castro, and R. Pedro. [2502/03.ABCDE]

Also MSc Thesis by Ms. Patrícia Ferreira

AD for New Physics Searches
Ongoing work [PRELIMINARY]

- No strong relation between ROC AUC and p-values
- Deep learning models exhibit higher sensitivity, but not for al' hyperparameters
- Not shown: a similar study with the test $$\max_x |F(x) - G(x)|$$ produced no sensitivity

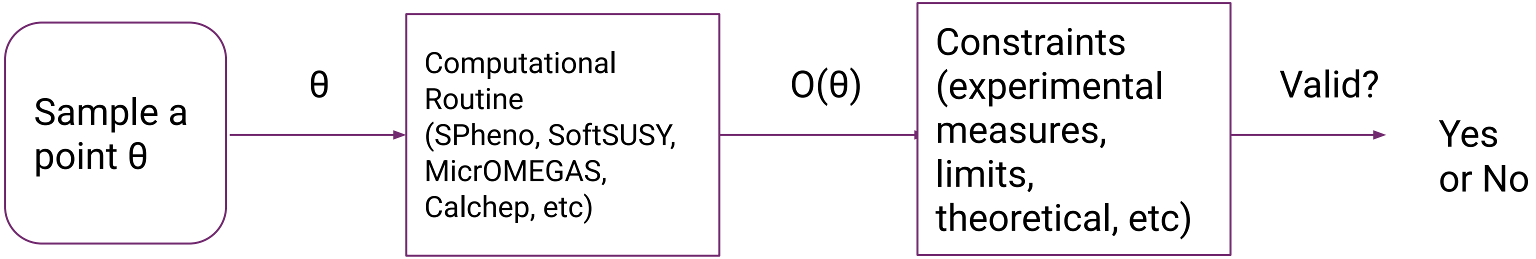


At s/√b=2 contamination

2) Artificial Intelligence to Explore Beyond the Standard Model Parameter Spaces

AI for BSM
Why

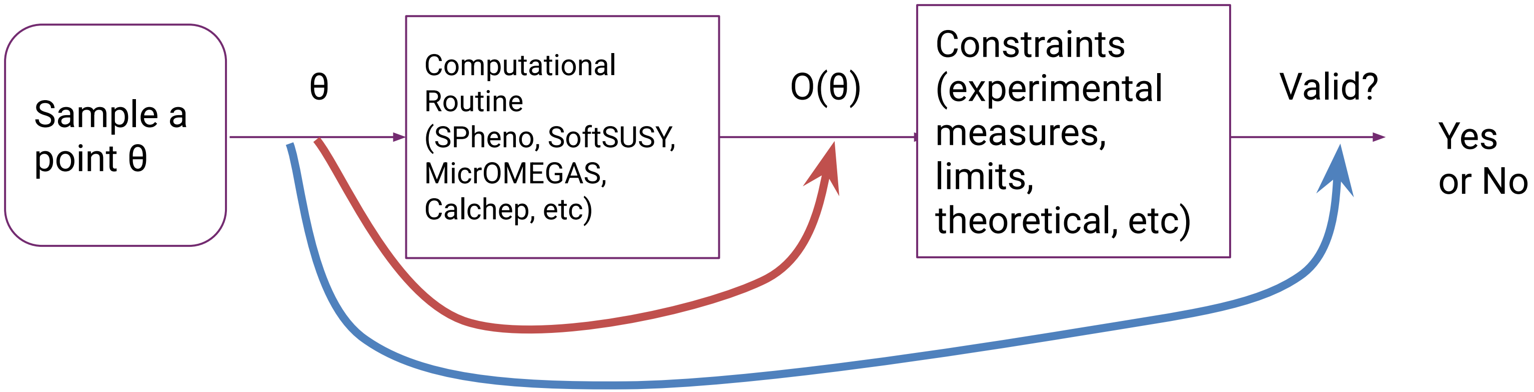
Studying **highly constrained** and **multidimensional** BSM parameter spaces is becoming a **bottleneck** for phenomenological studies purely due to **practical reasons**



Studies often **simplify the problem**, **reducing** their **generalisation** and phenomenological **scope**

AI for BSM
Why

Considering that the **observable computation** is the heavy step, early AI/ML attempts tried to **replace it**, either by **predicting the observables (regression)** or **predicting if a point is valid (classification)**



AI for BSM
Why

- These methodologies require **large amounts of training data** to **cover the whole parameter space**
- Predicting the observables using a **regressor**:
  - If training data do not cover the whole parameter space: **might map the parameter to observables incorrectly**
- Predicting whether a point is valid using a **classifier**:
  - If training data do not cover the whole parameter space: **wrong guess**

For **highly constrained** and **realistic scans**, it is **computationally prohibitive** to get enough valid points to use some of these methods

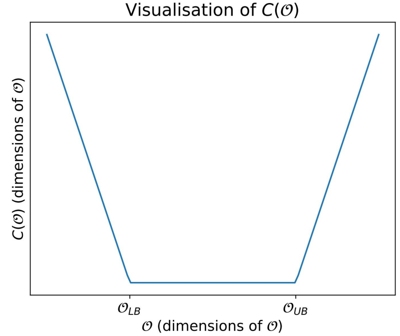
AI for BSM
Previous work

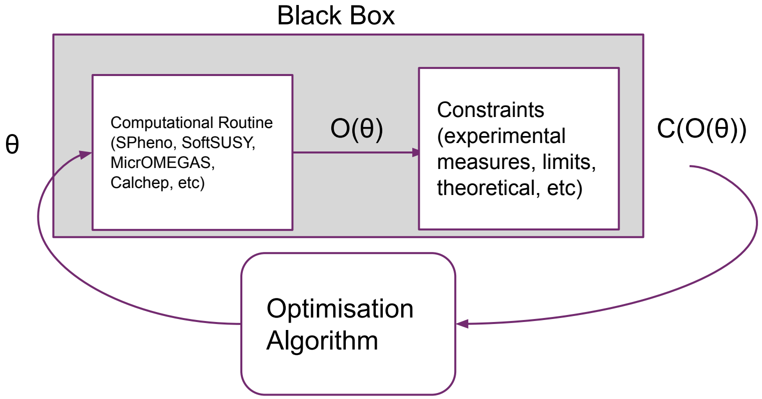
Reframed the problem: **black box optimisation**

- **How far** is a point from being **valid**
  $$C(\mathcal{O}) = max(0, -\mathcal{O} + \mathcal{O}_{LB}, \mathcal{O} - \mathcal{O}_{UB})$$
- Such that the set of valid points
  $$\mathcal{V} = \{\theta^* : \theta \in \mathcal{P} \text{ s.t. } C(\theta) = 0\}$$
- or, equivalently
  $$\mathcal{V} = \{\theta^* : \theta \in \mathcal{P} \text{ s.t. } \theta^* = \text{argmin } C(\theta)\}$$

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

de Souza, Fernando Abreu, et al. "Exploring parameter spaces with artificial intelligence and machine learning black-box optimisation algorithms." *Physical Review D* 107 (2023) 3, 035004. [2206.09223]





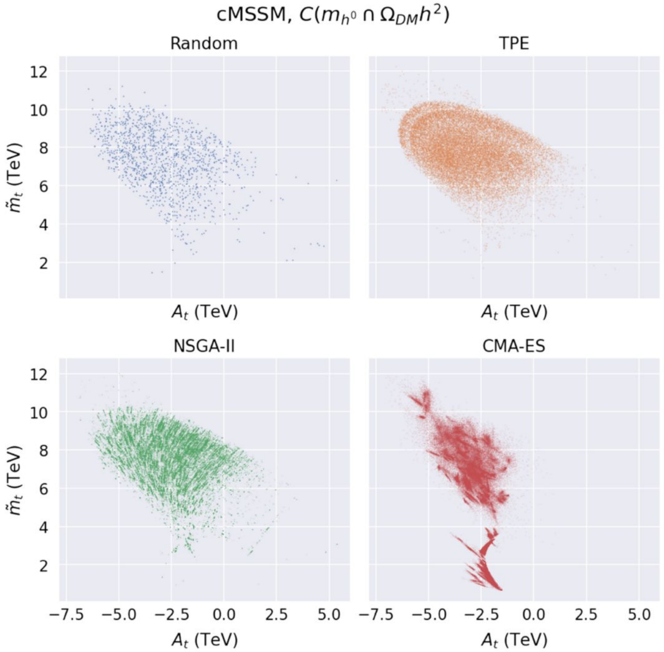
AI for BSM
Previous work

de Souza, Fernando Abreu, et al. "Exploring parameter spaces with artificial intelligence and machine learning black-box optimisation algorithms." *Physical Review D* 107 (2023) 3, 035004. [2206.09223]

Studied three different classes of algorithms, each embodying different **exploration exploitation** trade-offs

- **Bayesian Optimisation**: Tree-Parzen Estimator (TPE)
- **Genetic Algorithm**: Non-dominated Sorting Genetic Algorithm II (NSGA-II)
- **Evolutionary Strategy**: Covariant Matrix Approximation Evolution Strategy (CMAES)

They do not require data prior to the run as they **adapt dynamically** to the search

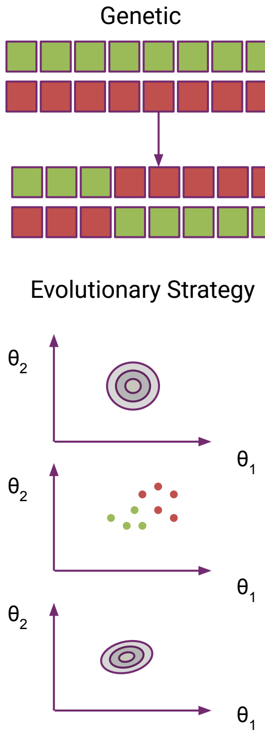


AI for BSM
Previous work

de Souza, Fernando Abreu, et al. "Exploring parameter spaces with artificial intelligence and machine learning black-box optimisation algorithms." *Physical Review D* 107 (2023) 3, 035004. [2206.09223]

Both evolutionary algorithms work similarly and show the greatest promise

- Initial population created randomly
- Sort population by fitness (i.e. by C(O))
- Generate an offspring population
- Repeat until stopping criteria



For a symbolic regression application using genetic programming see S. AbdusSalam, S. Abel, MCR “Symbolic Regression for Beyond the Standard Model Physics” *Physical Review* D 111 (2025) 1, 015022 [2405.18471]

AI for BSM
First Realistic Scan

Crispim Romão, Jorge, and MCR. "Combining evolutionary strategies and novelty detection to go beyond the alignment limit of the Z 3 3HDM." *Physical Review D* 109.9 (2024): 095040. [2402.07661]

First realistic scan on the(Real) Z_3 3 Higgs Doublet Model parameter space

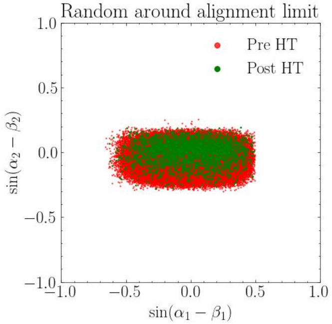
- **Multidimensional**: 16 real parameters
- **Highly Constrained**: 61 experimental and theoretical constraints
  - STU, Boundedness from Below, Perturbative Unitarity, LHC Higgs Couplings, LHC New Scalar Bounds, B->S Gamma
- Less than 1:10 billion random search efficiency (1 week on 16 cores produces O(1) points)
- Hitherto studies **restricted** to alignment limits
- CMAES seems to fail to explore at all

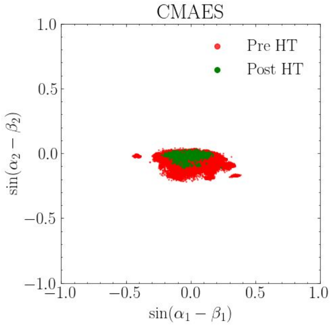
$$\alpha_1,\, \alpha_2,\, \alpha_3,\, \gamma_1,\, \gamma_2 \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]; \qquad \tan\beta_1,\, \tan\beta_2 \in [0, 10]\,;$$

$$m_{H_1} \equiv m_{h_2},\, m_{H_2} \equiv m_{h_3} \in [125, 1000]\ \text{GeV};$$

$$m_{A_1},\, m_{A_2}\, m_{H_1^\pm},\, m_{H_2^\pm} \in [100, 1000]\ \text{GeV};$$

$$m_{12}^2, m_{13}^2, m_{23}^2 \in \left[\pm 10^{-1}, \pm 10^{7}\right]\ \text{GeV}^2\,,$$

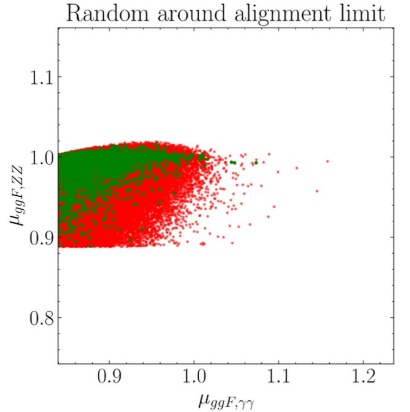


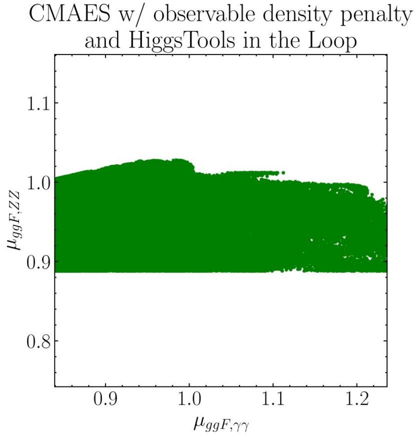


Crispim Romão, Jorge, and MCR. "Combining evolutionary strategies and novelty detection to go beyond the alignment limit of the Z 3 3HDM." *Physical Review D* 109.9 (2024): 095040. [2402.07661]

AI for BSM
First Realistic Scan

- Fixed the lack of exploration by endowing CMAES with **novelty detection reward** (based on **HBOS**)
- Found **new phenomenological realisations** that have so far been overlooked
- Overall obtained **orders of magnitude** in sampling efficiency
  - **Up to eight orders of magnitude** (~ 1 second:3 years) compared to random sampling
  - **Up to four orders of magnitude** compared to alignment limit sampling





[WIP]: Extending to C3HDM with DM constraints

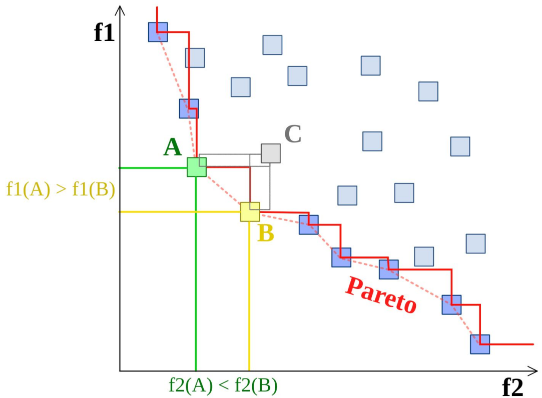
[WIP] Fernando Abreu de Souza, MCR., N. F. Castro, Andreas Karle, Werner Porod
[2502/03.ABCDE]

AI for BSM
Ongoing work [PRELIMINARY]

Now working on a T1-2-A Scotogenic that accommodates g-2 A. Alvarez, et al 2023

- Expanded the parameter space beyond simplifications made in previous study
    - With Casas-Ibarra parameterisation
        - 25 + 12 = 37 parameters
        - 26 + 6 = 32 constraints
    - And without
        - 25 + 18 = 43 parameters
        - 26 + 6 = 32 constraints
- Introducing a novel approach: **multi-objective optimisation** using NSGA-3

	Fermions				Scalars	
	Ψ_1	Ψ_2	F_1	F_2	η	S
$SU(2)_L$	**2**	**2**	**1**	**1**	**2**	**1**
$U(1)_Y$	-1	1	0	0	1	0

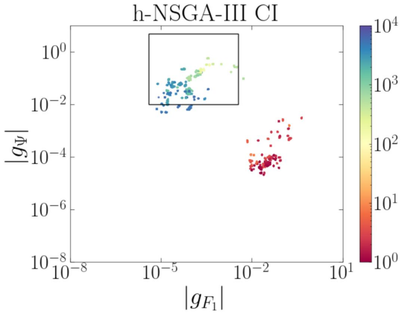


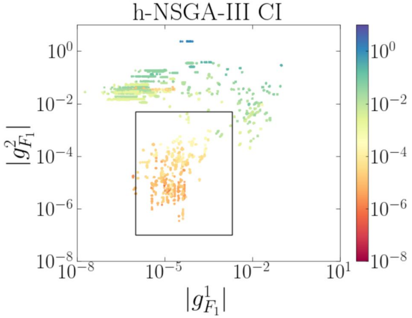
Wikipedia

[WIP] Fernando Abreu de Souza, MCR., N. F. Castro, Andreas Karle, Werner Porod [2502/03.ABCDE]

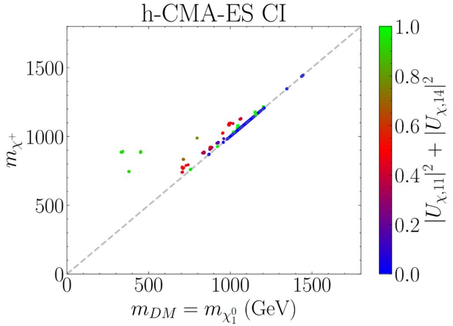
AI for BSM
Ongoing work [PRELIMINARY]

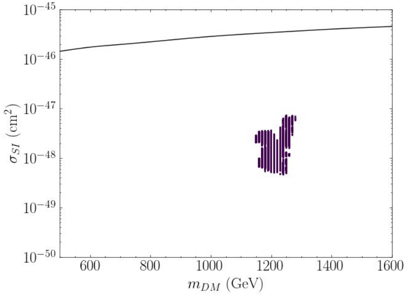
- Drastically improved coverage of the parameter space





- New phenomenological realisations and potential signatures



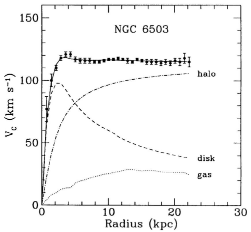


3) Machine Learning to Look for Exotic Dark Matter

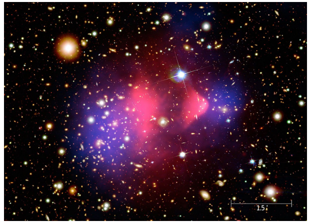
ML for Microlensing

Why

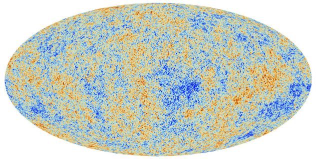
- **All evidence** for Dark Matter is **gravitational**. Nonetheless, the dominant paradigm has been field theoretical
- With no direct (or indirect) detection of particle Dark Matter, **alternatives gain traction**
- One such alternative is that (at least a portion of) Dark Matter is composed by **celestial dark objects**



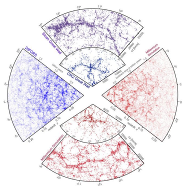
dx.doi.org/10.1093/mnras/249.3.523



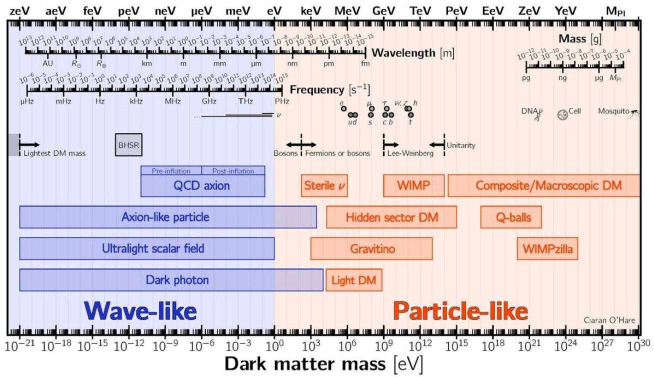
dx.doi.org/10.1093/mnras/249.3.523



ESA

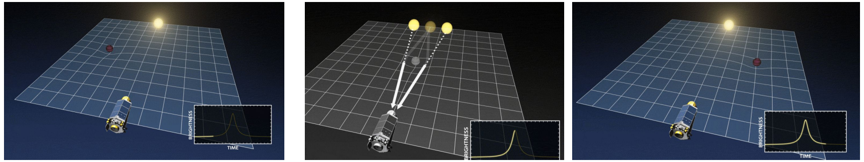


astro-ph/0604561, doi:10.1038/nature04805

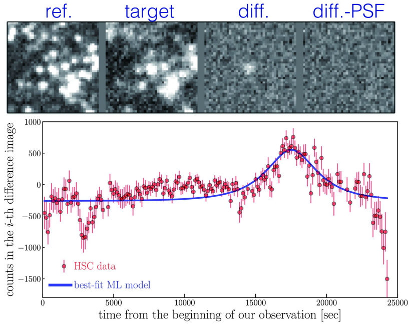


ML for Microlensing
Why

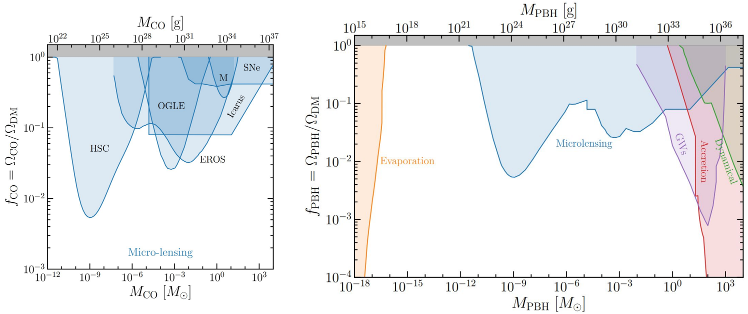
- A famous example of these would be **primordial black holes**
- These objects could be detected via **gravitational microlensing**, but efforts in this direction have **only focused on point-like microlensing events**
  - What if more exotic celestial dark objects compose the bulk of Dark Matter?



Wikipedia



Niikura, H, et al - Subaru/HSC observation

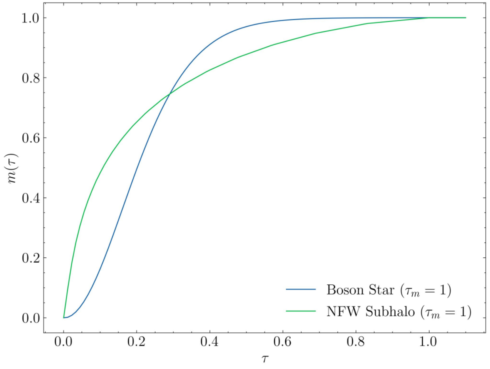


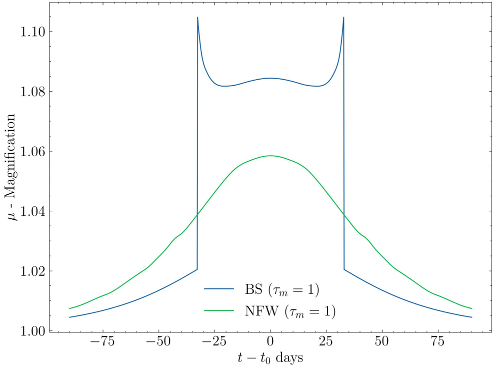
Green, Kavanagh 2020

ML for Microlensing
Previous work

MCR, and Djuna Croon. "Microlensing signatures of extended dark objects using machine learning." *Physical Review D* 109.12 (2024): 123004. [2402.00107]

- Croon, McKeen, Raj 2020 proposed that **extended dark objects** such as **Boson Stars** and **Navarro-Frenk-White** (NFW) subhalos could be detected through microlensing
- In particular, **Boson Stars** are expected to exhibit **unique light curve profiles** due to the appearance of symmetric **caustics**



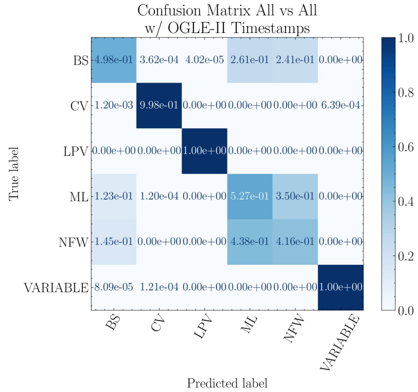


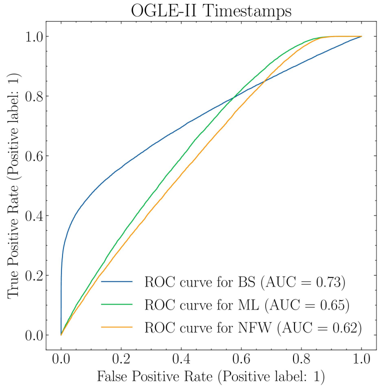
ML for Microlensing
Previous work

MCR, and Djuna Croon. "Microlensing signatures of extended dark objects using machine learning." *Physical Review D* 109.12 (2024): 123004. [2402.00107]

Tested the sensitivity to different objects of Optical Gravitational Lensing Experiment (OGLE)

- Boson Stars
- NFW subhalos
- Point-like Microlensing
- Variable sources
  - Cataclysmic Variables (CV)
  - RR Lyrae & Cepheid Variables (VARIABLE)
  - Mira long-period variables (LPV)



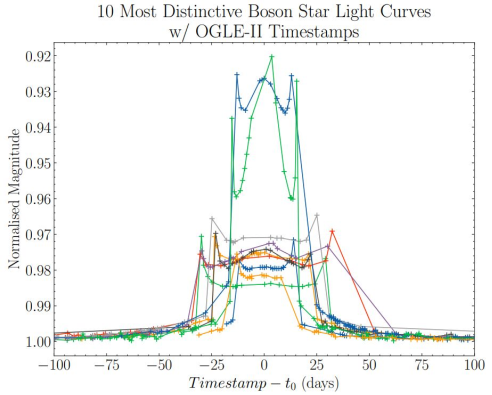


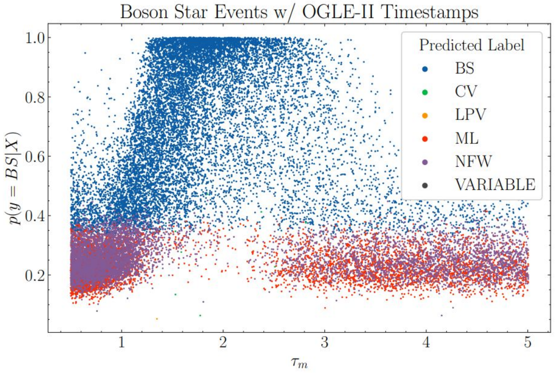
MCR, and Djuna Croon. "Microlensing signatures of extended dark objects using machine learning." *Physical Review D* 109.12 (2024): 123004. [2402.00107]

ML for Microlensing
Previous work

More importantly:

- Microlensing surveys should be especially sensitive to **Boson Stars**, with the potential to have a **positive discovery** with the possibility of constraining their parameter space
- NFW subhalos, are also detectable, but would likely pass as point-like lensing phenomena





MCR, and Djuna Croon. "Microlensing signatures of extended dark objects using machine learning." *Physical Review D* 109.12 (2024): 123004. [2402.00107]

ML for Microlensing
Previous work

While exciting, some shortcomings and questions stand out

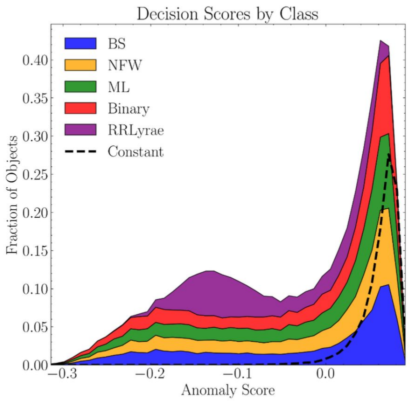
- Dataset does not include possible sources of misclassification, such as **binary lenses**
- Did not include **signal-less light curves**
- Simulation made use of a **simplistic noise model**
- OGLE does not have **public raw datasets**
- How does the methodology apply to the upcoming **Legacy Survey of Space and Time** (LSST) conducted at the Vera Rubin observatory?
- Analysis is **purely offline**, could it be adapted as an **alert system for brokers**?

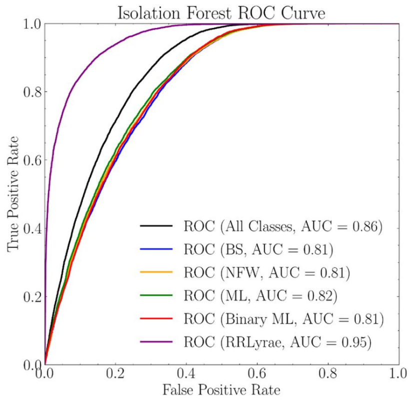
[WIP]MCR, Djuna Croon, and Daniel Godines [2502/03.ABCDE]

ML for Microlensing
Ongoing work [PRELIMINARY]

Now analysing the sensitivity for the upcoming LSST

- Vera Rubin observations simulated using rubin-sim
- Included **Binary** lenses and **Constant** light curves
- Developed an **AD** methodology based on **iForest** trained on **Constant** to find signal-full candidates

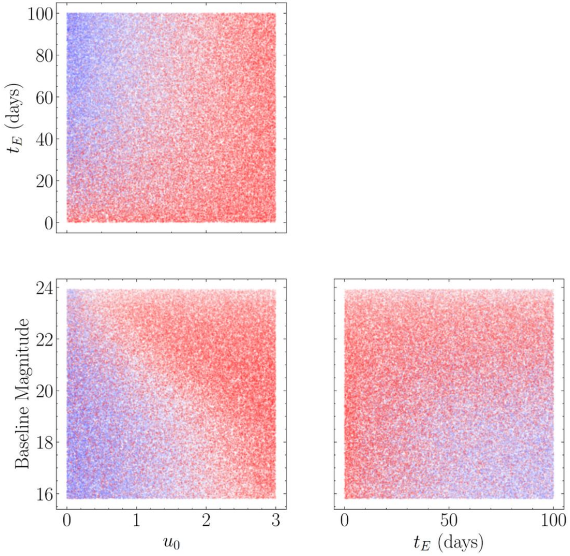


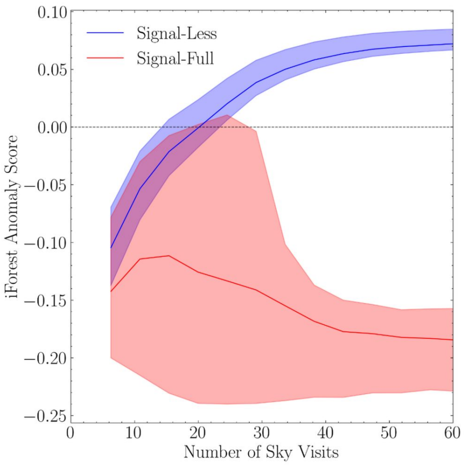


[WIP]MCR, Djuna Croon, and Daniel Godines
[2502/03.ABCDE]

ML for Microlensing
Ongoing work [PRELIMINARY]

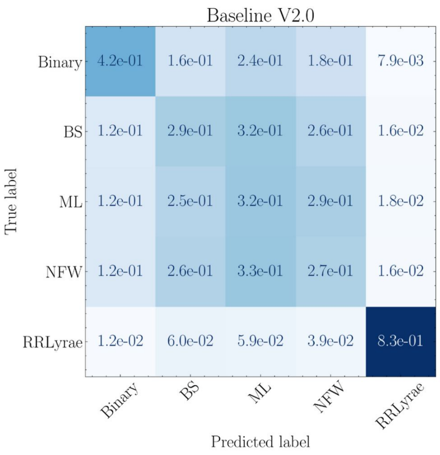
- Showed **how to use the AD** for **online alerts**
- The cut is especially sensitive to certain regions of the astrophysical parameters

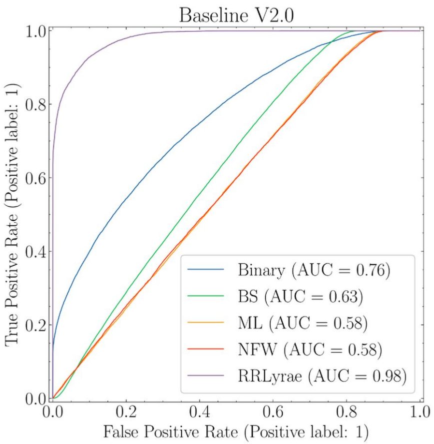


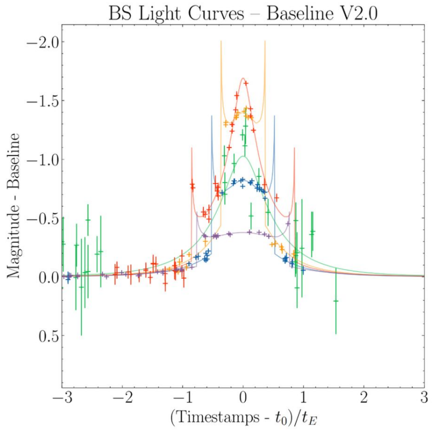


ML for Microlensing
Ongoing work [PRELIMINARY]

- Conducted an **offline analysis** on the light curves that **survive the cut**
- **More difficult** to isolate different microlensing classes than OGLE
- However, **the prospect of positive Boson Star detection remains**







Conclusions

Conclusions

- AI and ML are **here to stay** and represent a **new era in computational Physics**
- They offer **unique** approaches to **search for New Physics**
- More importantly they provide **novel ways** of looking for the **unexpected**
    - **Semi-supervised methods** can search for **model agnostic signals**
    - **Search algorithms** can quickly map viable parameter space regions and find **novel phenomenological possibilities**

And stay tuned for more progress in **searching for New Physics by looking for the unexpected**!

Thank you!

Get in touch!
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