Looking for the Unexpected at the LHC with Semi-Supervised Anomaly Detection

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Anomaly Detection for New Physics Searches

Why

How do we look for New Physics at Colliders:

1. Choose BSM signal you are looking for
2. Study favourable kinematic region for the final state topology
3. Collect the data in such regime
4. Perform statistical tests on the data on the hypothesis of BSM being present
5. And put bounds until we find something

Anomaly Detection for New Physics Searches

Why

An event is characterised by a collection of kinematic variables used in **Multivariate Analyses**

- What are the best discriminating variables?
- What if the signal region on these variables change as we change the parameters of New Physics?

An **explicit New Physics hypothesis** is tested

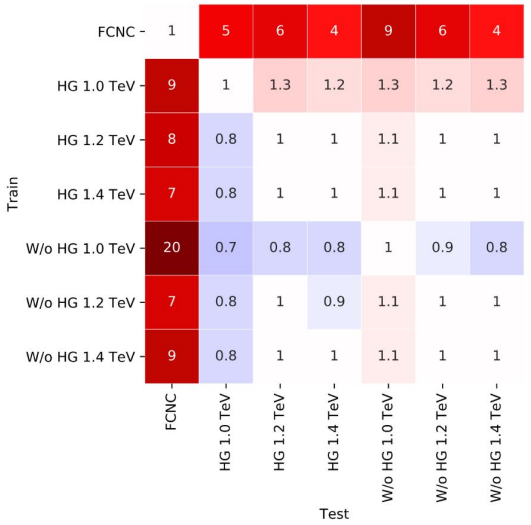
- What if another New Physics signal is presented instead?
- What if we are forgetting to consider a realised New Physics case (for example something more exotic that is not covered in standard analyses)

Anomaly Detection for New Physics Searches

Previous work

In an early work [MCR, et al Phys.Rev.D 101 (2020) 3, 035042], a **machine learning discriminant** trained on one signal was shown to **be sensitive to signals that was not trained on.**

- Especially sensitive to signals which are similar
- Motivated work by others on parametric classifiers
- **Still not signal agnostic**



Anomaly Detection for New Physics Searches
Previous work

Semi-supervised Anomaly Detection (AD) holds the promise for **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

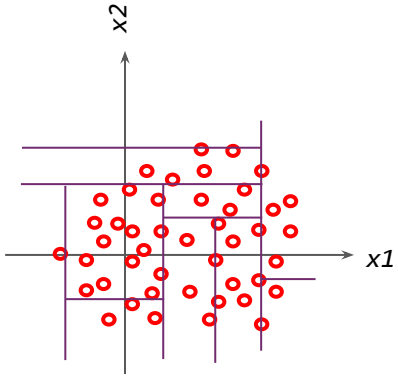
MCR, N. F. Castro, and R. Pedro. "Finding new physics without learning about it: anomaly detection as a tool for searches at colliders." *The European Physical Journal C* 81.1 (2021): 27. [2006.05432]

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 ($- \Sigma_i \log(h\_i)$) ~ 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



$$\text{iForest}(\mathbf{x}) = 2^{-\frac{\mathbb{E}[h(\mathbf{x})]}{d}}$$

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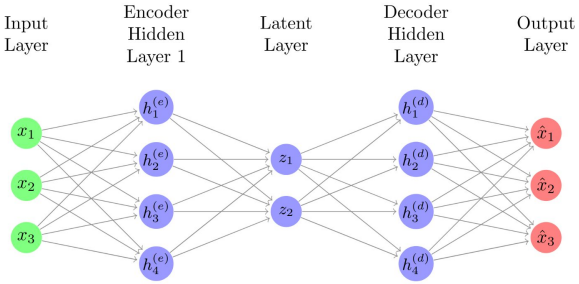
Auto-Encoder

- Reconstruction Error-based (~manifold embedding)

$$L = \mathbb{E}_{\mathbf{x}\sim \mathrm{SM}}[||\mathrm{AE}(\mathbf{x}, \mathcal{W}) - \mathbf{x}||^2]$$



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

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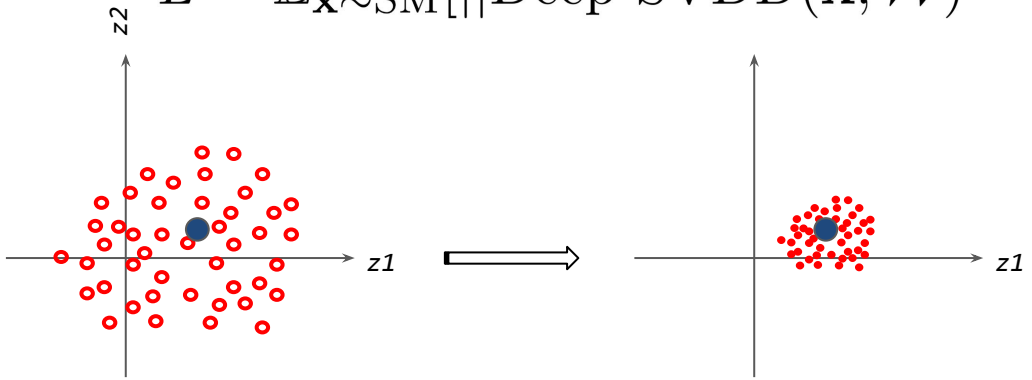
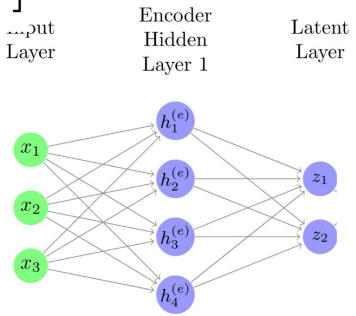
Deep Support Vector Data Description

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

$$L = \mathbb{E}_{\mathbf{x}\sim \mathrm{SM}}[||\text{Deep-SVDD}(\mathbf{x}, \mathcal{W}) - \mathbf{c}||^2]$$





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

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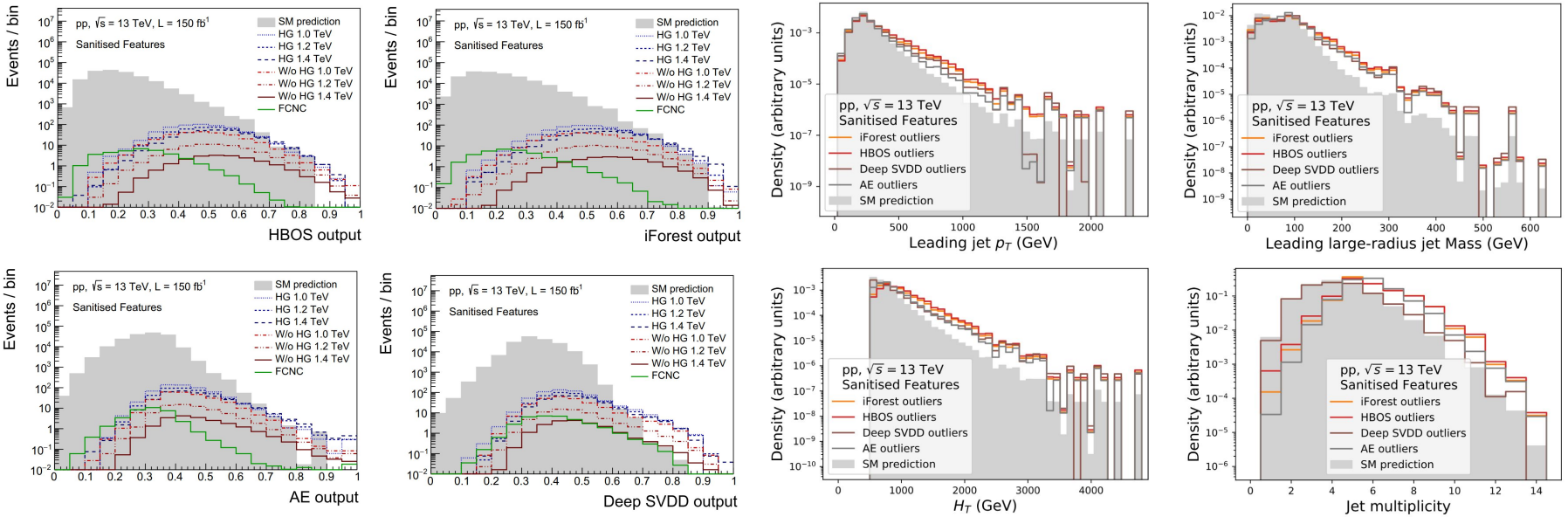
When applied to a collection of different BSM candidates: all models provided sensitivity while capturing different notions of anomaly



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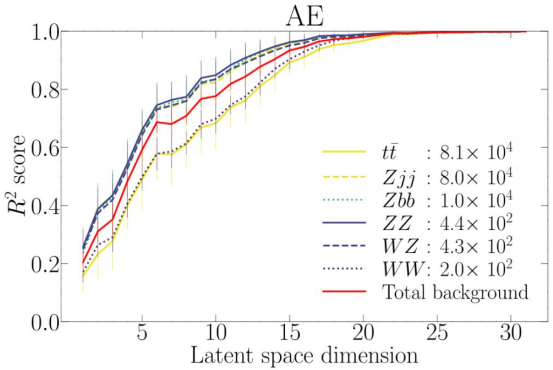
AD shows promise for generic New Physics searches. However:

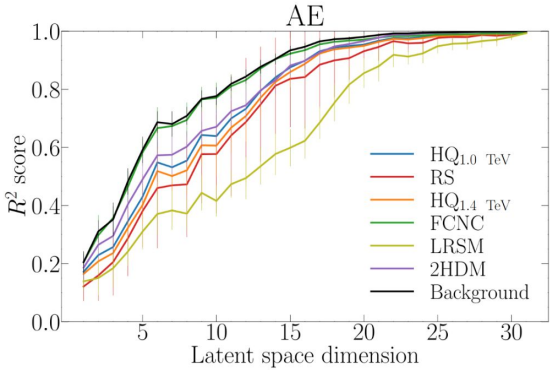
- The **discriminant** for Auto-Encoders is a **reconstruction error**
  - Is the lore “the better the reconstruction the better the discrimination” correct?
- Some **hyperparameters** of the models have **no semi-supervised metric** to use for tuning (the “untunables”)
  - How does this affect the sensitivity?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

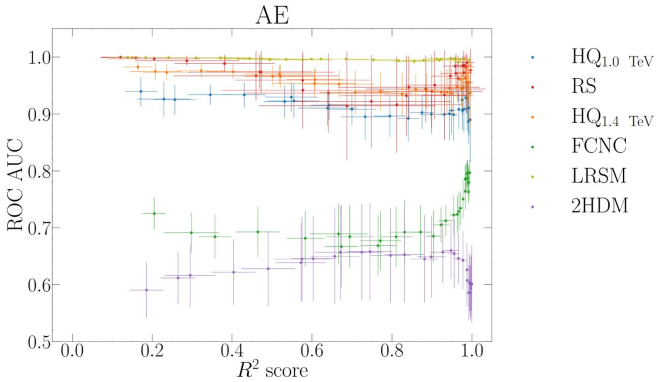
AD for New Physics Searches
Latest Work

Fernando Abreu de Souza, Maura Barros , N. F. Castro, MCR, R. Pedro, and Céu Neiva. “Sensitivity to New Physics Phenomena in Anomaly Detection: A Study of Untunable Hyperparameters” [2505.13228]

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







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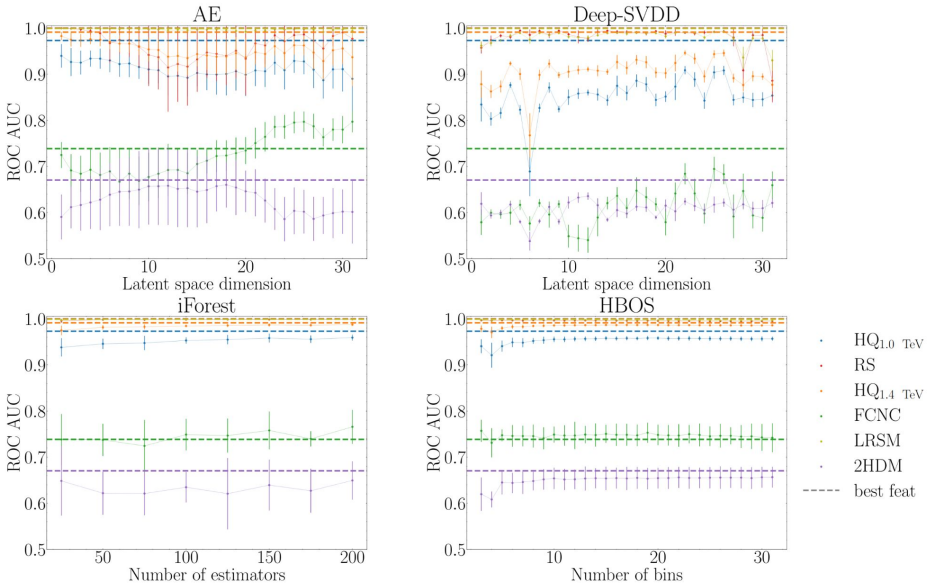
Sensitivity to New Physics is ***largely*** independent of the untunable hyperparameters, and the sensitivity is ***capped*** by the sensitivity of the best feature



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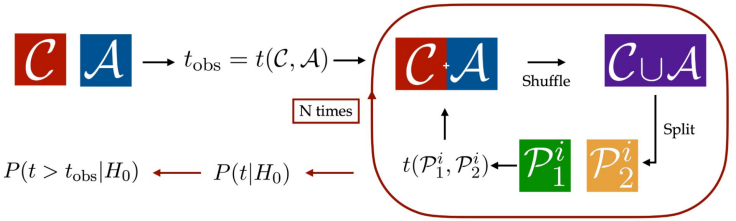
Proposal for a semi-supervised statistical test based on permutation tests

- Prepare a “control” test set of Standard Model events
- Prepare an “analysis” test set which can be contaminated with BSM
- Measure how the distributions differ

$$\mathrm{Cr}_{A,B} = \int_{-\infty}^{\infty} |\mathrm{eCDF}_A(x) - \mathrm{eCDF}_B(x)|^2 dx$$

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



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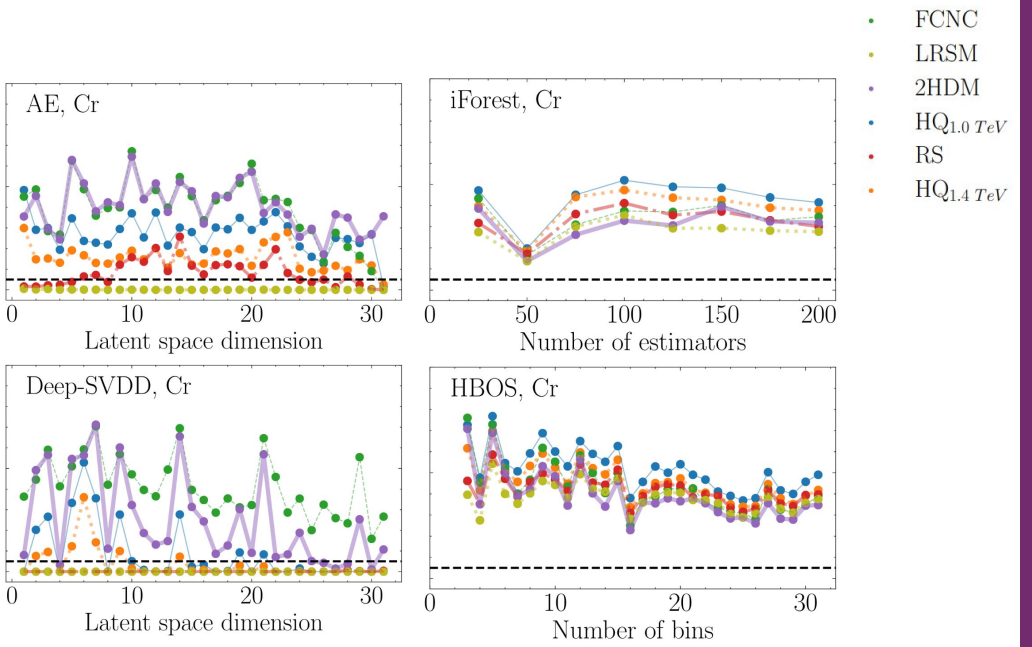
- No strong relation between ROC AUC and p-values
- Deep learning models exhibit higher sensitivity, but not for all hyperparameters
- Not shown: a similar study with the test

$$\mathrm{M}\Delta_{A,B} = \max_x |\mathrm{eCDF}_A(x) - \mathrm{eCDF}_B(x)|$$

produced no sensitivity



At s/√b=2 contamination

Conclusions and Outlook

Conclusions and Outlook

- **Semi-supervised AD methods** can search for **model agnostic signals** and set a statistical interpretation on the SM-only hypothesis
- Still room for improvement
  - High variance across ML AD discriminant (no free lunch theorem)
  - p-value aggregation
  - High dependence on the choice of the test statistics
- Nonetheless: as semi-supervised AD and resulting statistical interpretation mature, we can **expect signal agnostic analysis to be conducted alongside dedicated analysis**
- Stay tuned for more progress in searching for BSM Physics by looking for the unexpected!

Thank you!

Get in touch!
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