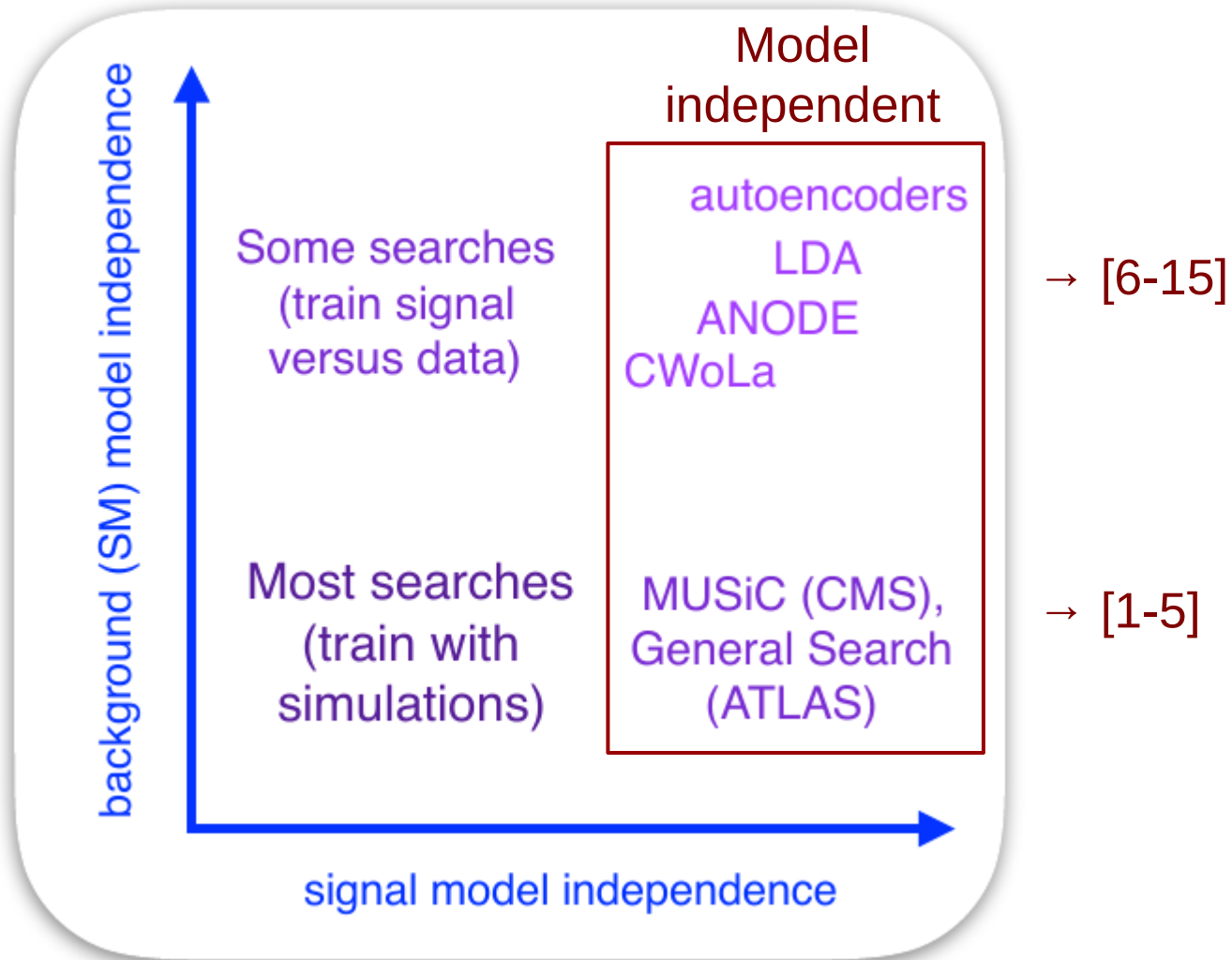


Search for New Physics using un-supervised ML techniques

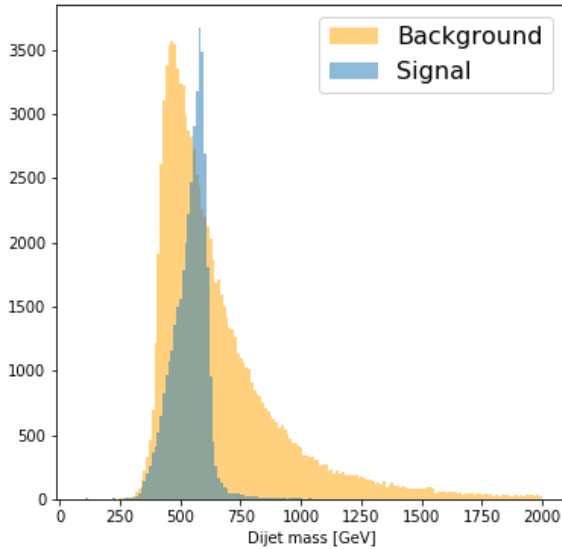
Ioan Dinu (IFIN-HH), Louis Vaslin (LPC)
Vincent Barra (LIMOS), Julien Donini (LPC)

Direct Searches for New Physics



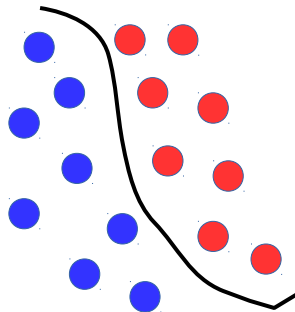
B. Nachman, D. Shih, [arxiv:2001.04990](https://arxiv.org/abs/2001.04990)

Bump hunt use-case



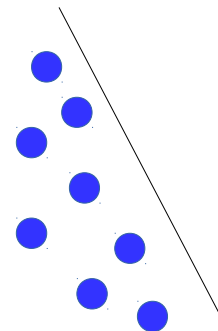
→ Search for resonance in a spectrum using ML

Supervised (labels)
DNN, BDT, SVM

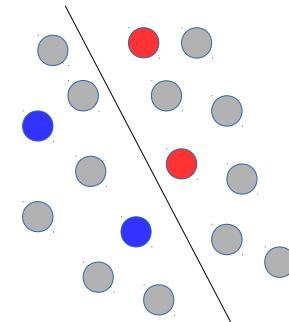


**Unsupervised
(no labels)**

SVM-1class, **AE**, VAE,
WAE, **GAN-AE**,...



**Semi-supervised
(some labels)**
triplet NN,...



Direct search for New Physics at the LHC using **Autoencoders**

Two use-cases with **dijet** simulated samples

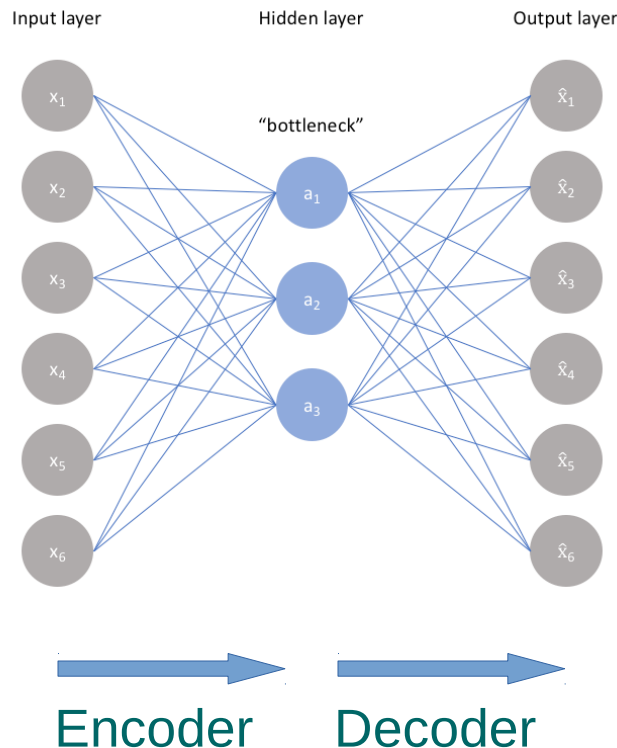
- **LHC Olympics challenge** → AE (jet substructure variables)
- Simulated **dijet data** → GAN-AE (Event variables)

Conclusion and outlook

Why Autoencoders ?

An **Autoencoder** is a network trained to copy its input to its output

$$x \rightarrow h = f(x) \rightarrow \hat{x} = g(h)$$



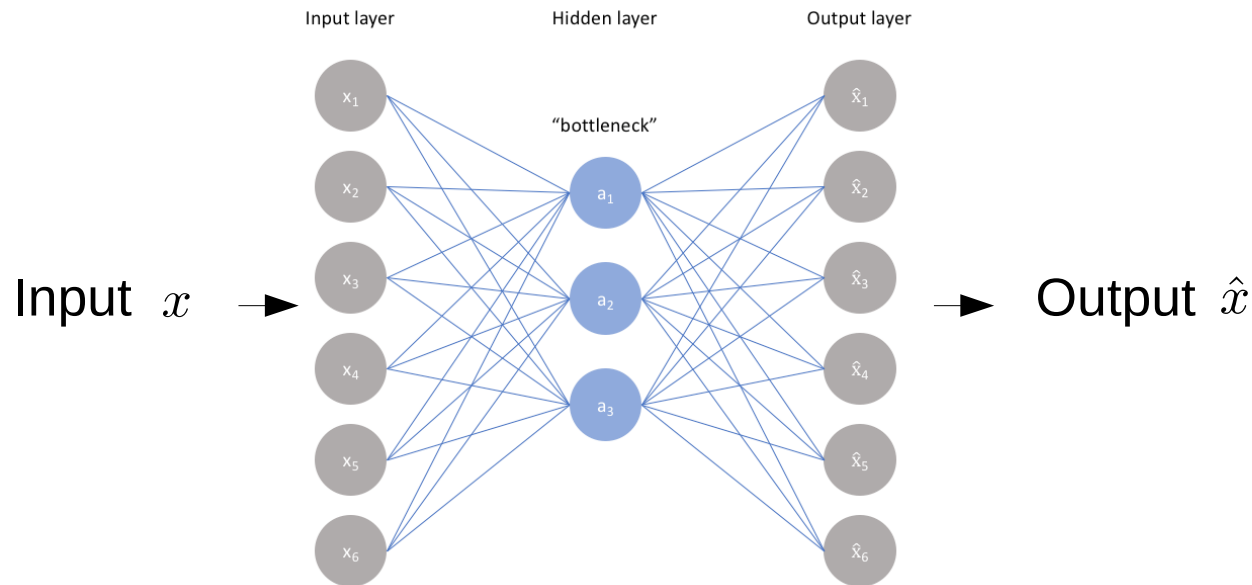
Reproducing the **identity** is not useful
→ Restricted to **copy imperfectly**:
forces the AE to **prioritize** information
to **learn useful features**



Undercomplete or regularized AE

Usage: dimensionality reduction, representation learning, manifold learning, generative network, **anomaly detection**, ...

Train AE on **background** samples: **reconstructed error** $\ell = ||x - \hat{x}||^2$



The idea being that the network will **learn** to main background features and **fail** to reconstruct **anomalous** sample → **larger reconstruction error**

Anomaly detection challenge for **ML4Jets2020** conference (15-17/01/20)

- **Simulated Background** (dijet data) + Signal
 - **Benchmark** samples to develop method
 - Three LHCO 2020 **Black Boxes** “data” with unknown signal
- **Datasets**
 - Event selection: ≥ 1 anti-kT $R = 1.0$ jet, $|\eta| < 2.5$ and $p_T > 1.2$ TeV.
 - Data consists of [pt,eta,phi] for of up to 700 hadrons
- **What was asked**
 - **p-value** of dataset (for null hypothesis)
 - As complete as possible **description** of NP process
 - **Number** of signal events in the data (with uncertainties)
- Challenge ran until Jan 12th, **10 team** submitted their results

Pre-processing was necessary to extract jet features from raw data

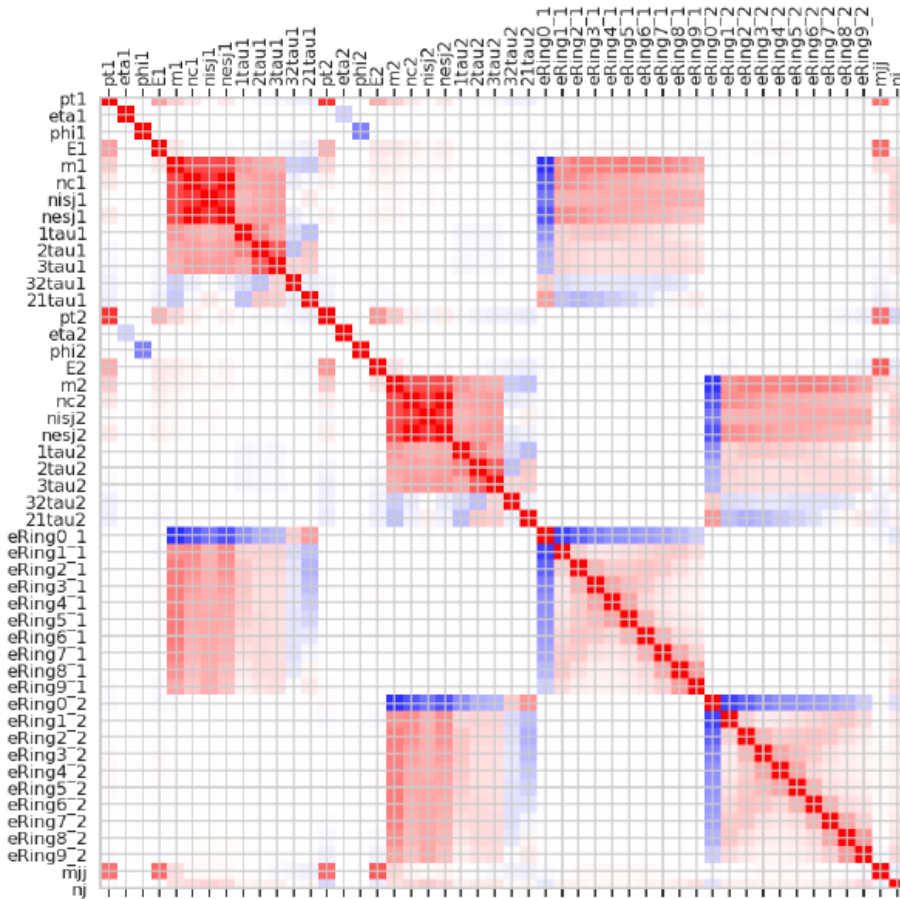
Jet Features (\times two jets)

- $(p_T, \eta, \phi, m), E$
- $nsj_{inclusive}, nsj_{exclusive}$ (based on d_{cut}), $n_{constit}$
- $\tau_1, \tau_2, \tau_3, \tau_3/\tau_2, \tau_2/\tau_1$ (subjettinesses)
- Energy rings $E_i = (\sum E_{constit})/E_{jet}$, where $\Delta R(jet, constit) \in [R_{jet}(i/n); R_{jet}((i+1)/n)]$, $n=10$

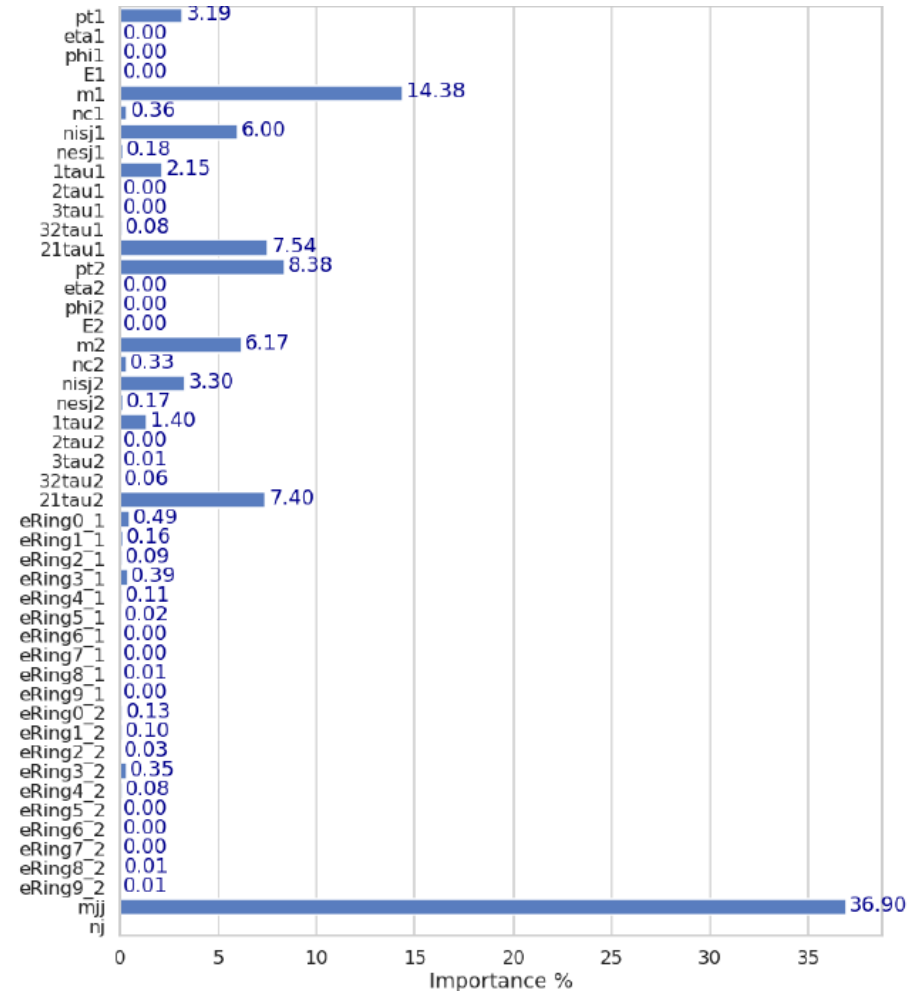
Event Features

- $m_{jj}, n_{jets}(p_T \geq 20 GeV)$

Correlation



Importance (ranked with Gradient BDT)

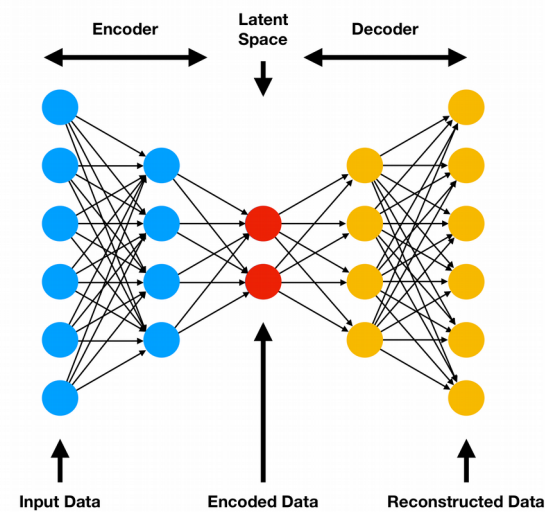


HLF-AE: High Level Feature AE

I. Dinu

Hyperparameter space scan

- Learning rate: 0.01, 0.005, 0.001, 0.0005, 0.0001
- Features used: 44
- 1st hidden layer nodes: 30, 25
- 2nd hidden layer nodes: 20, 15
- Encoding dimension: 10, 7, 5
- Activations: ReLU, Leaky ReLU, ELU
- Batch size: 32, 64, 128, 256, 512, 1024

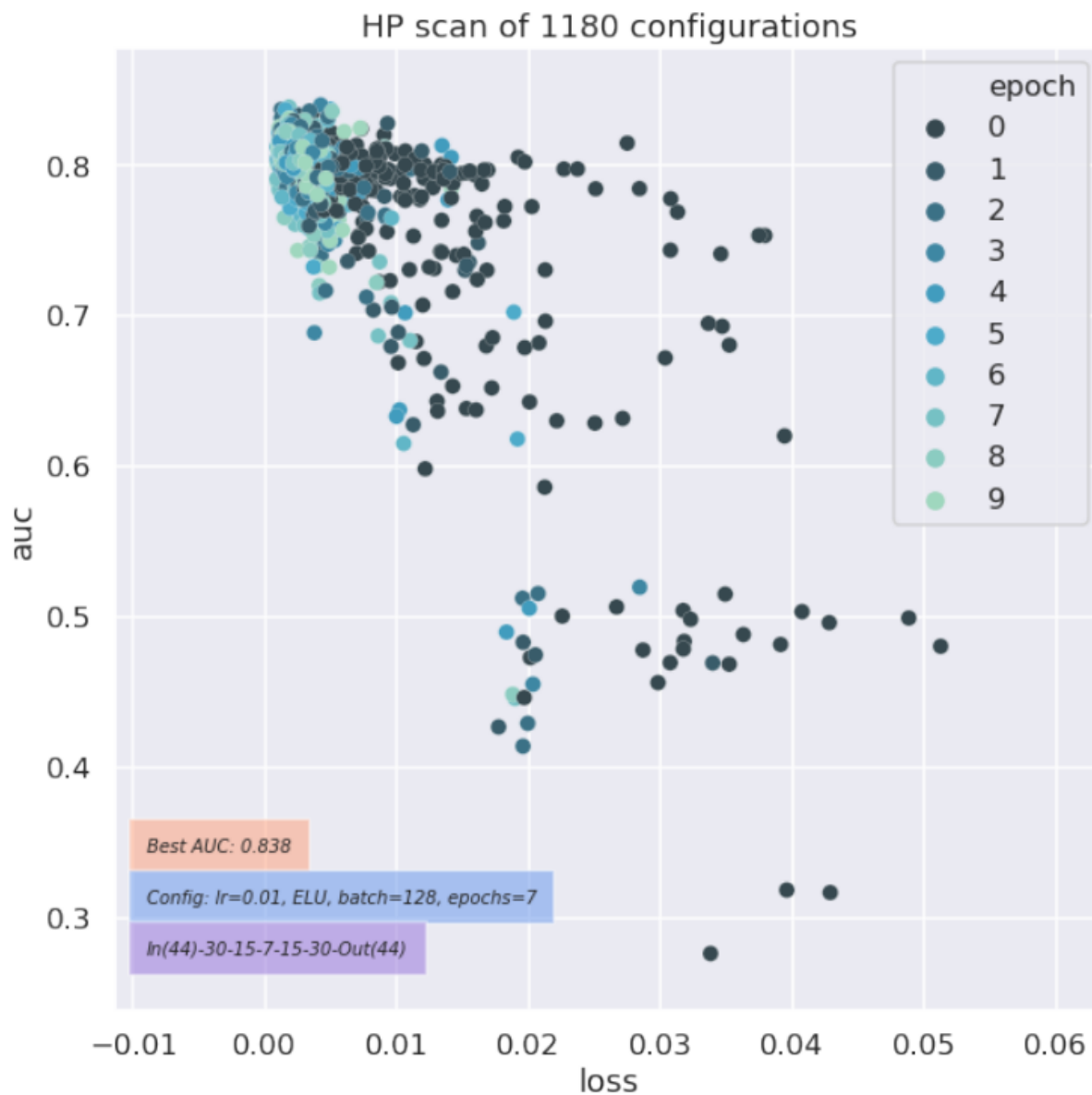


Grid Task on Manchester GPU Test Site

- 1180 configurations spread among 10 jobs
- custom Docker container for this architecture
→ [gitlab link](#) to code

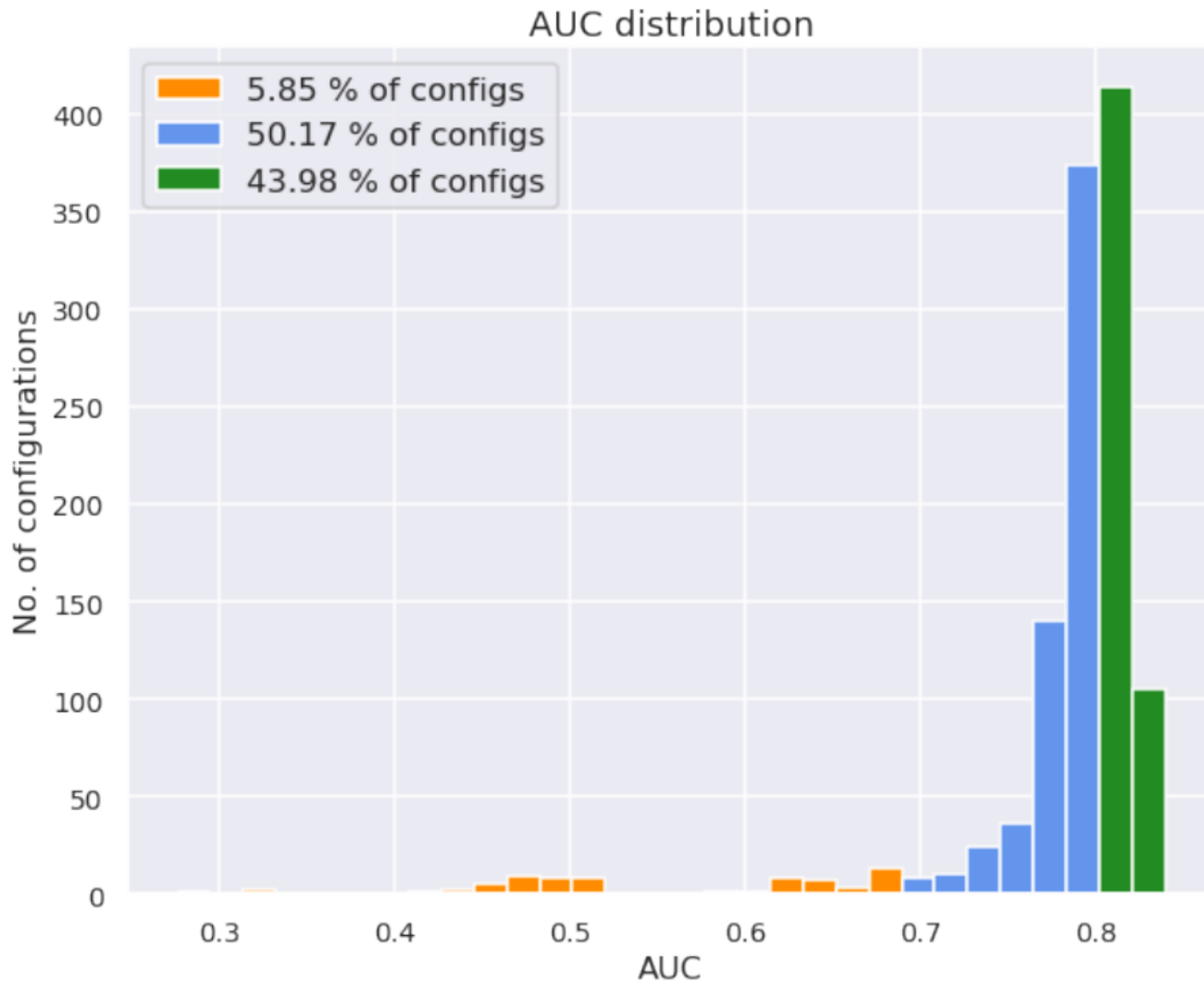
Hyper Parameter Optimization

I. Dinu



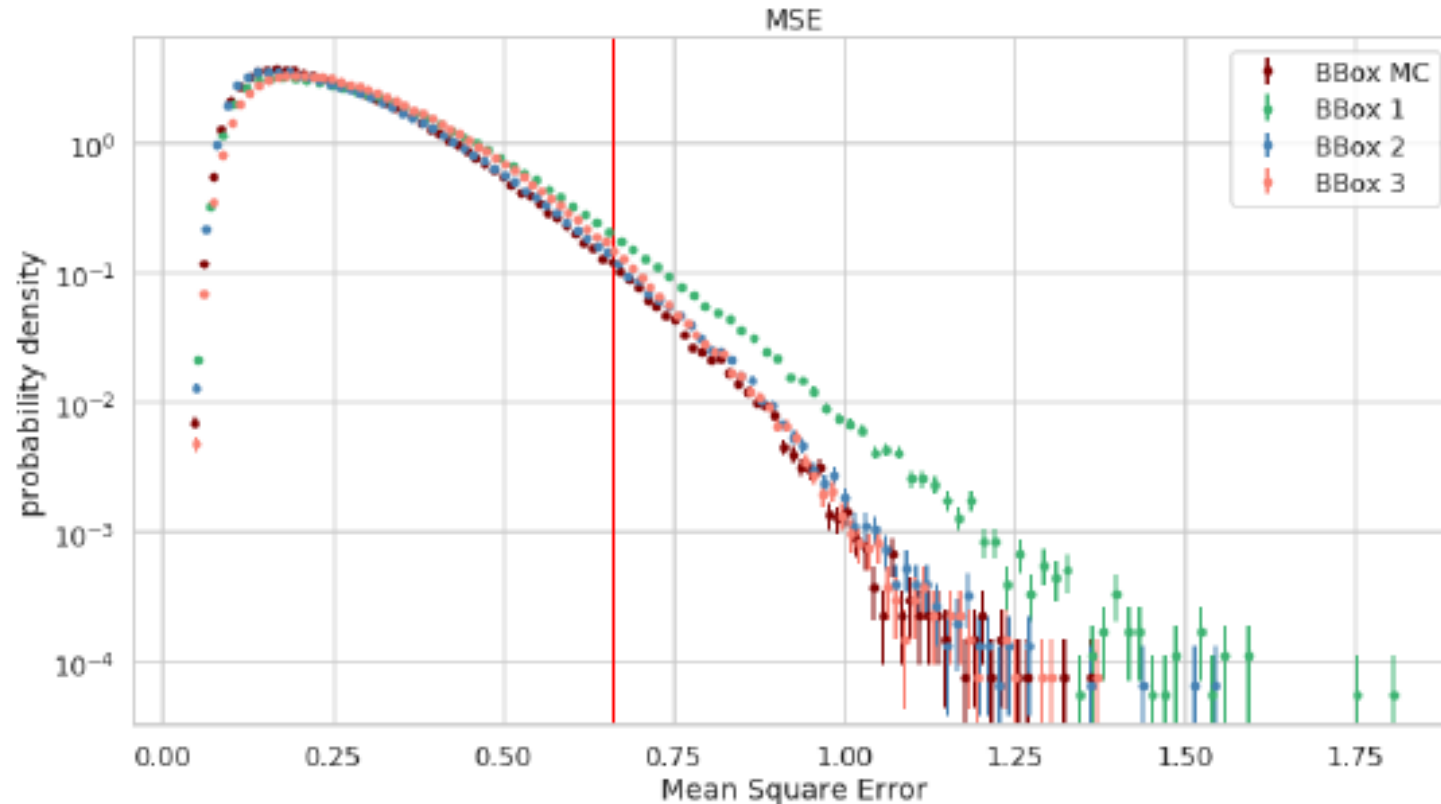
Hyper Parameter Optimization

I. Dinu



Mean square error returned by AE

→ **training** dataset (background) and **black box** samples 1-3:



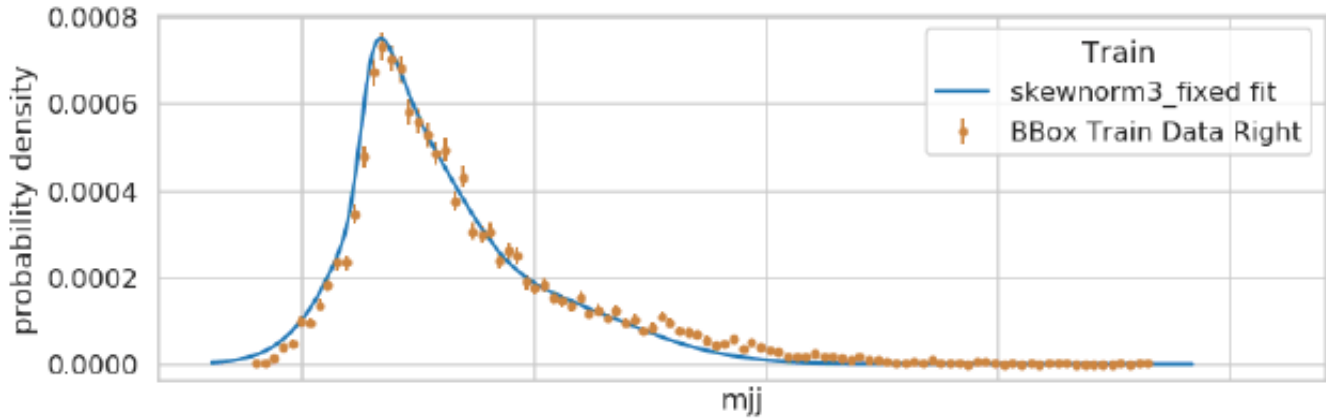
A **threshold** value is applied and feature distributions are compared.

Results on Bbox-1 dataset

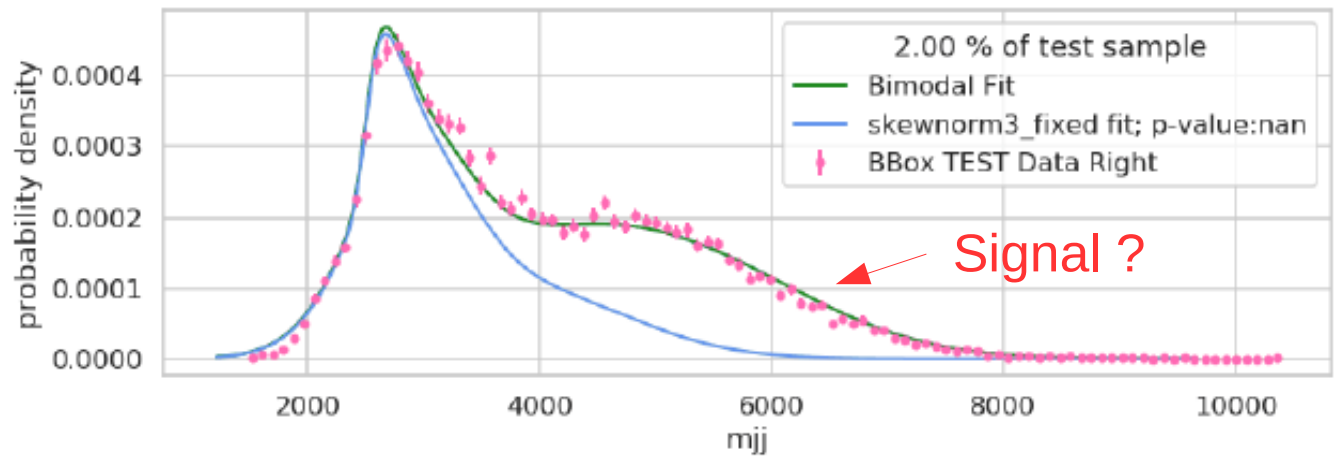
I. Dinu

Invariant mass distribution after **threshold** on MSE error:

Train BG dataset



Black box 1 data



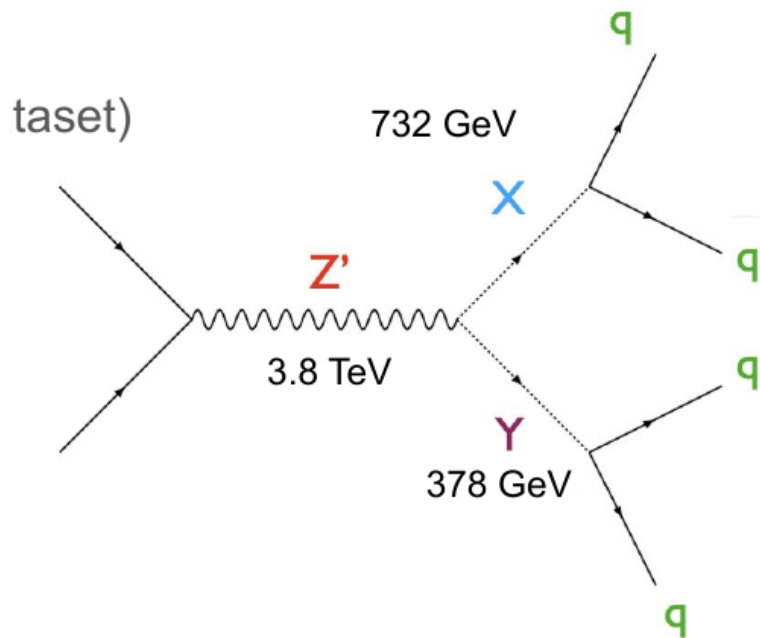
Possible signal around 5.2 TeV ?

Challenge (sad) truth

LHC Olympics outcome: [these slides](#)

Black box 1 signal

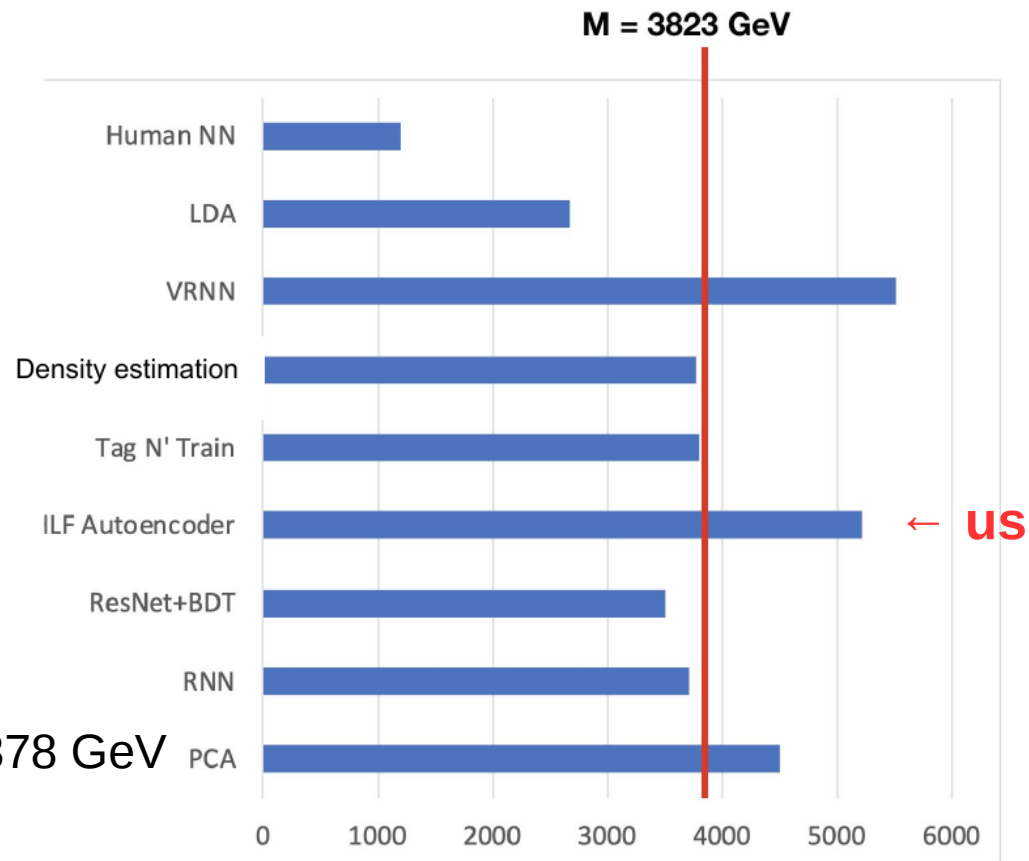
$Z' \rightarrow XY; X, Y \rightarrow qq$



$m_{Z'} = 3823 \text{ GeV}$, $m_X = 732 \text{ GeV}$, $m_Y = 378 \text{ GeV}$

Signal: 834 events

Team results: fitted mass

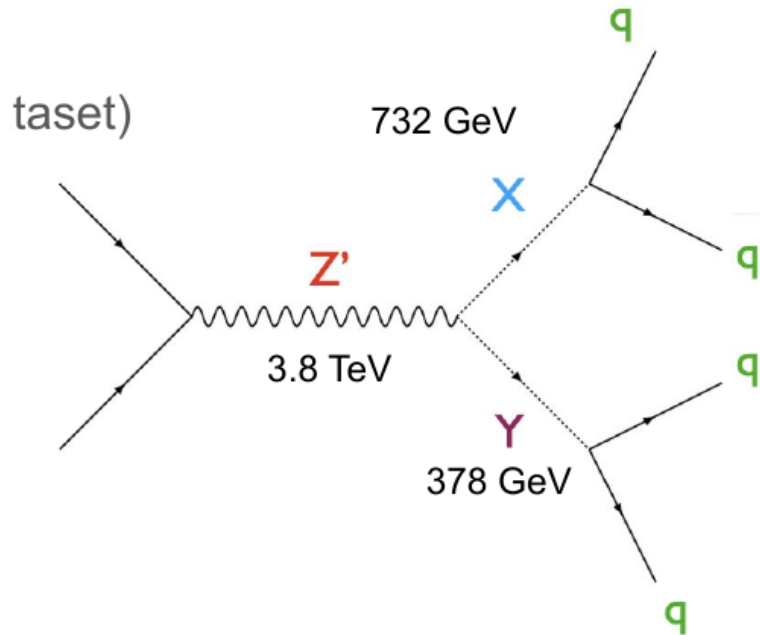


Challenge (sad) truth

LHC Olympics outcome: [these slides](#)

Black box 1 signal

$Z' \rightarrow XY; X, Y \rightarrow qq$

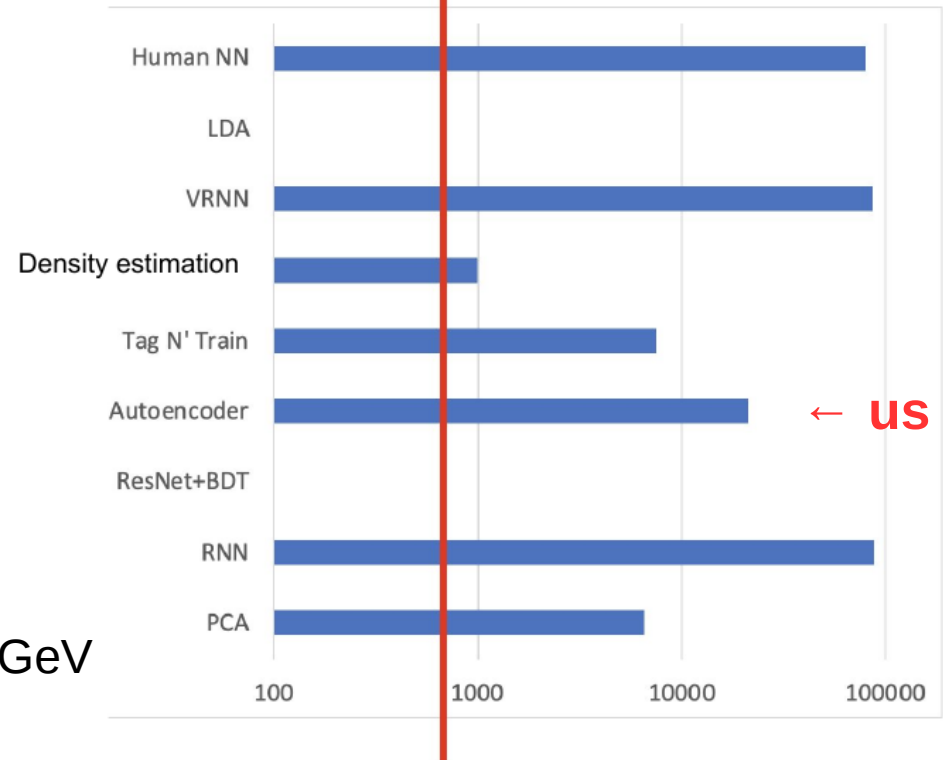


$m_{Z'} = 3823 \text{ GeV}$, $m_X = 732 \text{ GeV}$, $m_Y = 378 \text{ GeV}$

Signal: 834 events

Team results: number of events

834 Signal Events



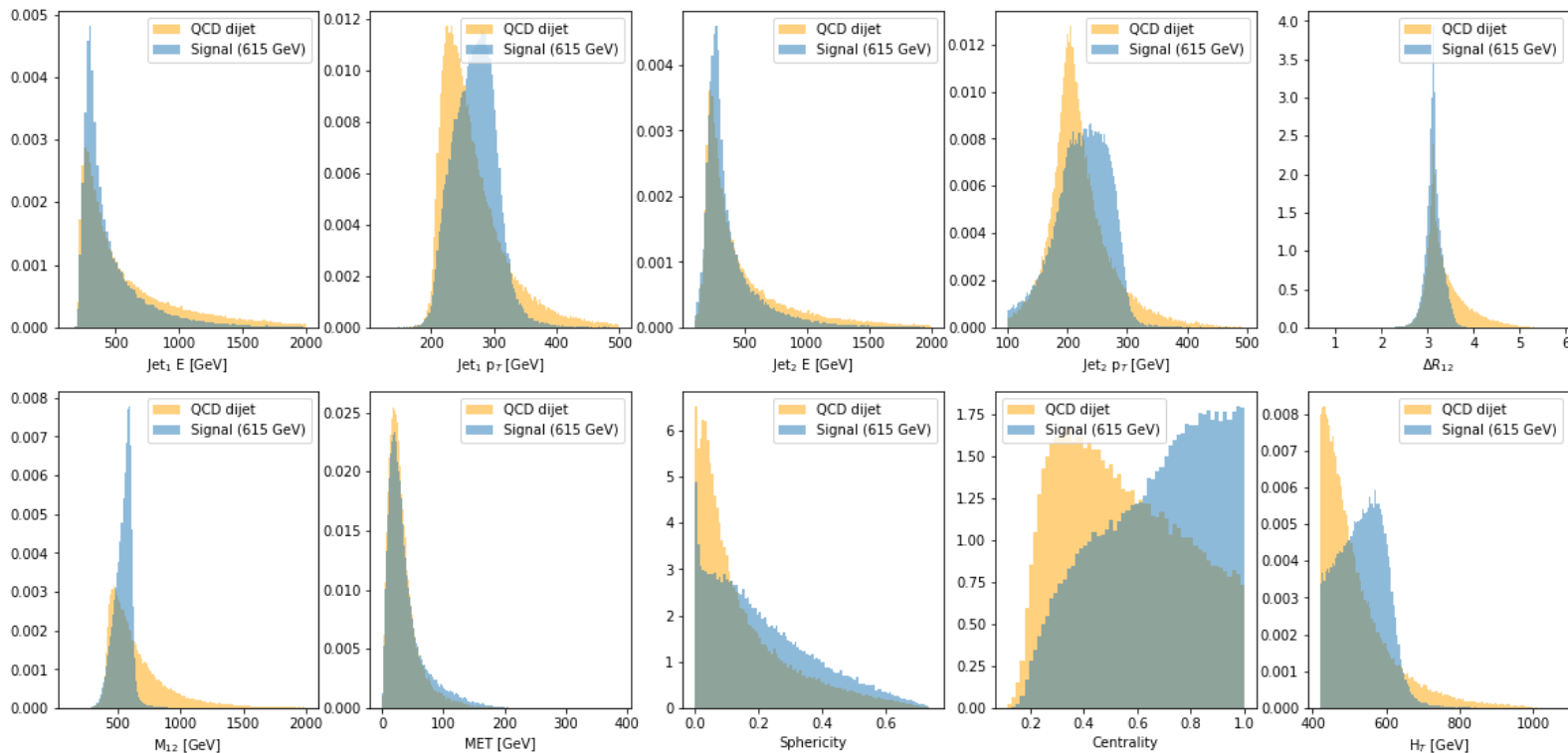
→ **Our approach finds something but clearly biased ...**

Simulated samples: dijet events

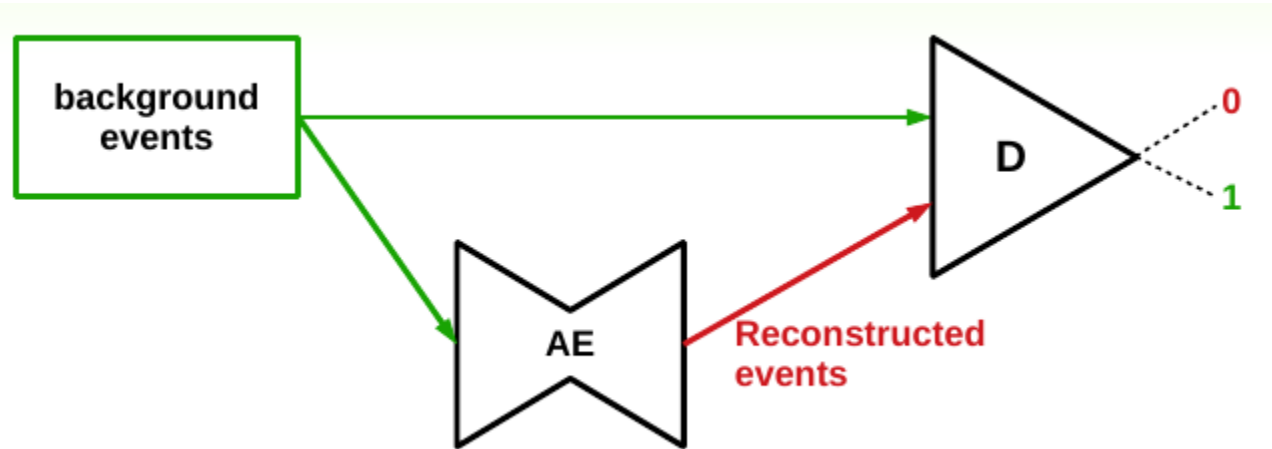
Dijet events (Madgraph+Pythia+Delphes):

- Background: 500k QCD dijets ($H_T > 400$ GeV)
- Signal: 500k RPV-MSSM stop (615 GeV, 1 TeV)

10 input variables (selected using supervised BDT ranking)

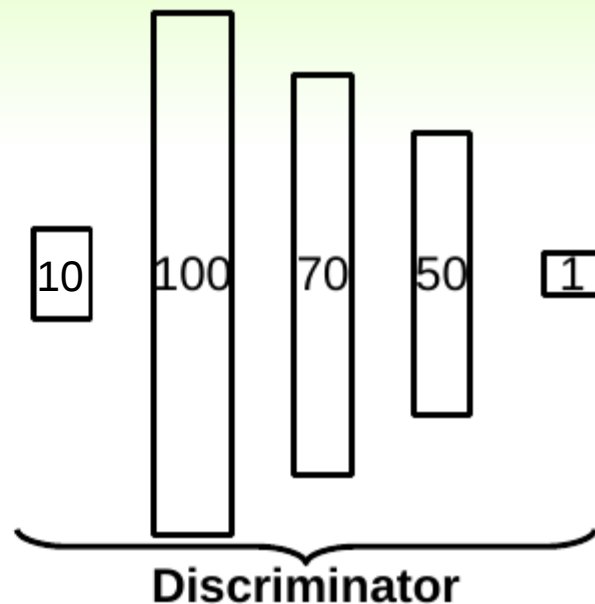
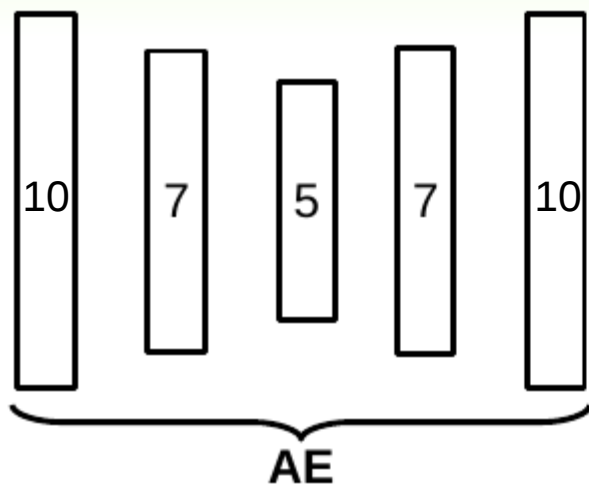


Network architecture



- Discriminant objective : learn AE's weaknesses
- AE objective : correct these weaknesses

- Architecture



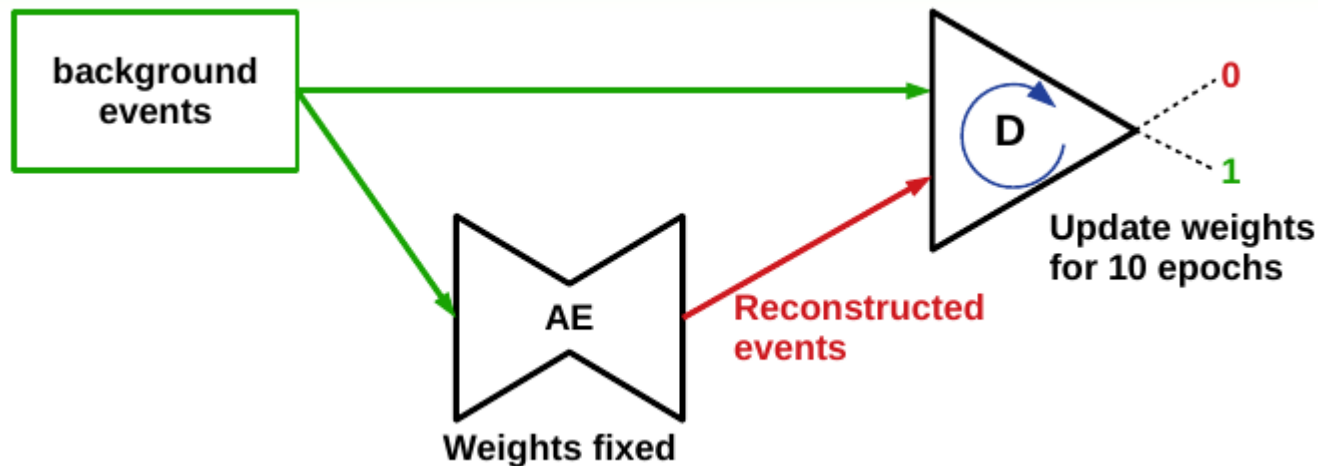
Activation : ReLU / sigmoid (out)
Optimizer : Adam (lr=0.0002, $\beta_1 = 0.5$)
Initialization : Glorot normal

$$\sigma_{\text{Glorot}} = \sqrt{\frac{2}{N+P}} \quad \mu_{\text{Glorot}} = 0$$

Activation : LeakyReLU / sigmoid (out)
Optimizer : Adam (lr=0.0002, $\beta_1 = 0.5$)
Initialization : Glorot normal

Dropout rate: up to 20% or 40% depending on the layer

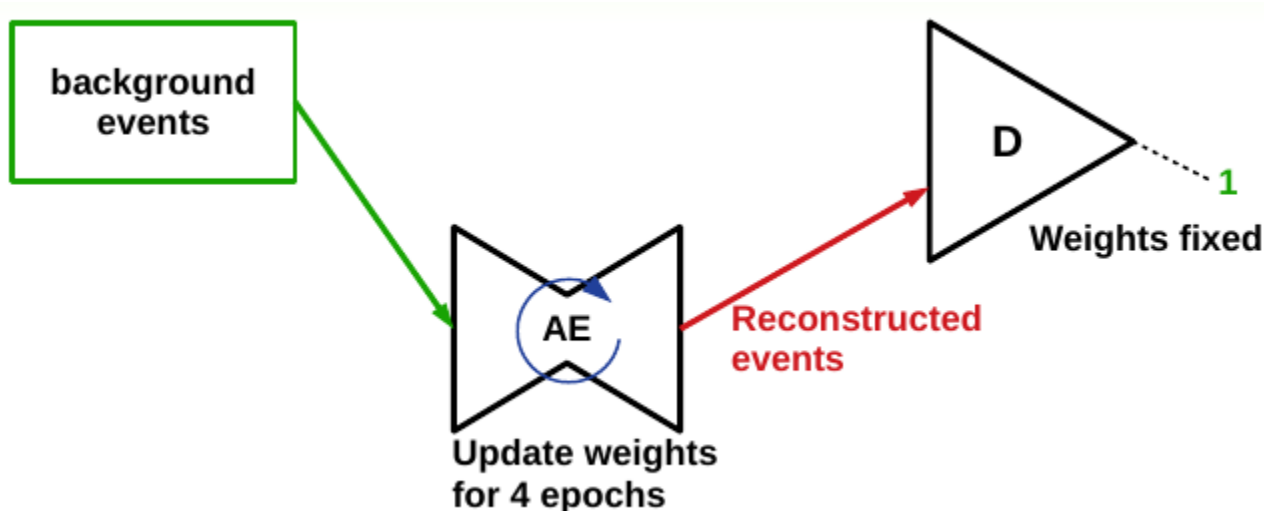
Training of discriminant



Loss function: binary cross-entropy

$$\ell = - \sum_j y_j \log(p_j) + (1 - y_j) \log(1 - p_j)$$

Training of AE

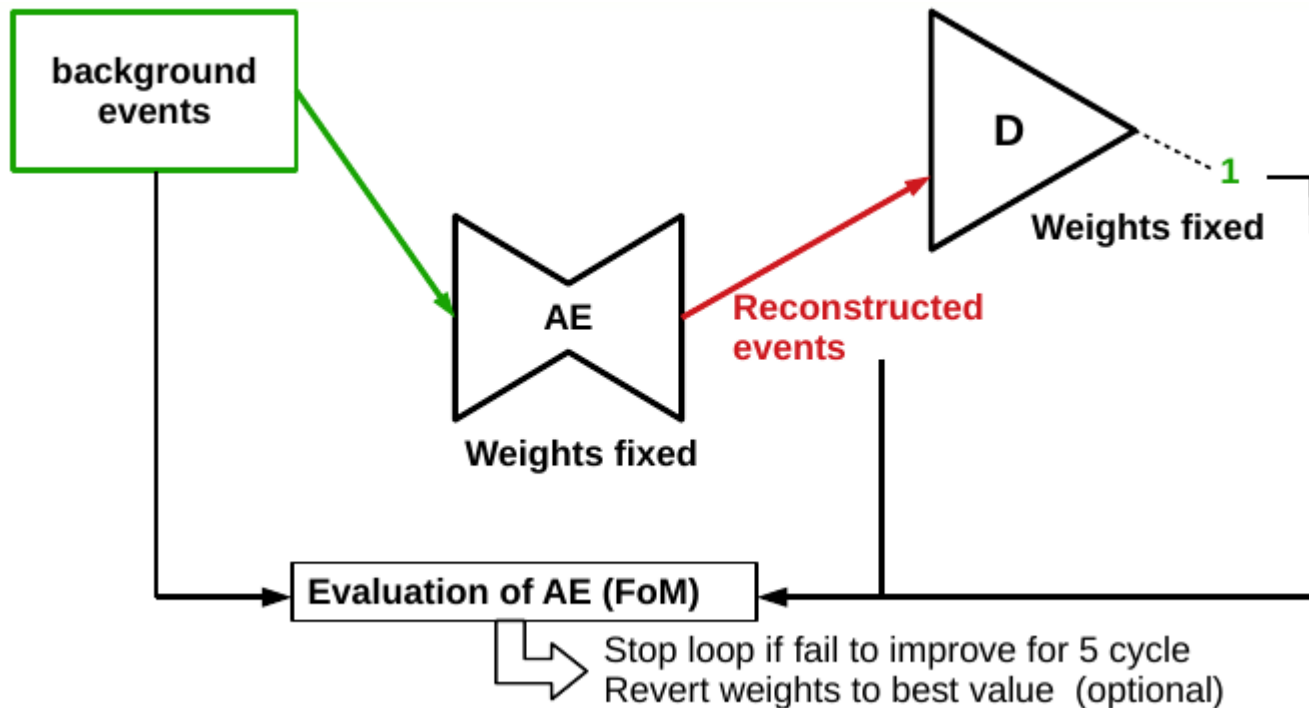


Loss function: binary cross-entropy + ϵ x mean distance [$\epsilon=2\%$]

$$\ell = - \sum_{j=1}^N y_j \log(p_j) + (1 - y_j) \log(1 - p_j) + \frac{\epsilon}{N} \|\mathbf{x}_j^{\text{in}} - \mathbf{x}_j^{\text{out}}\|$$

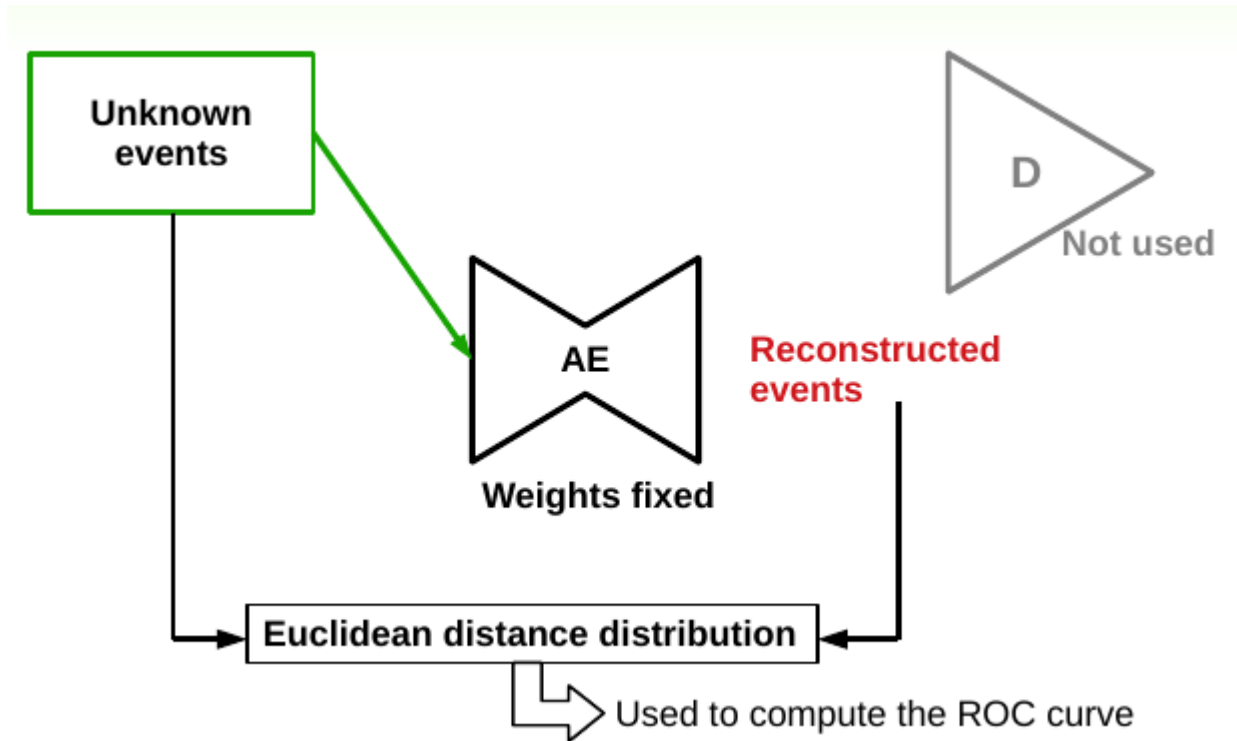
Training cycle: 10 epochs on D, 4 epochs on AE (asymmetric training)

Stopping criterion: evaluation of AE performance (validation sample)



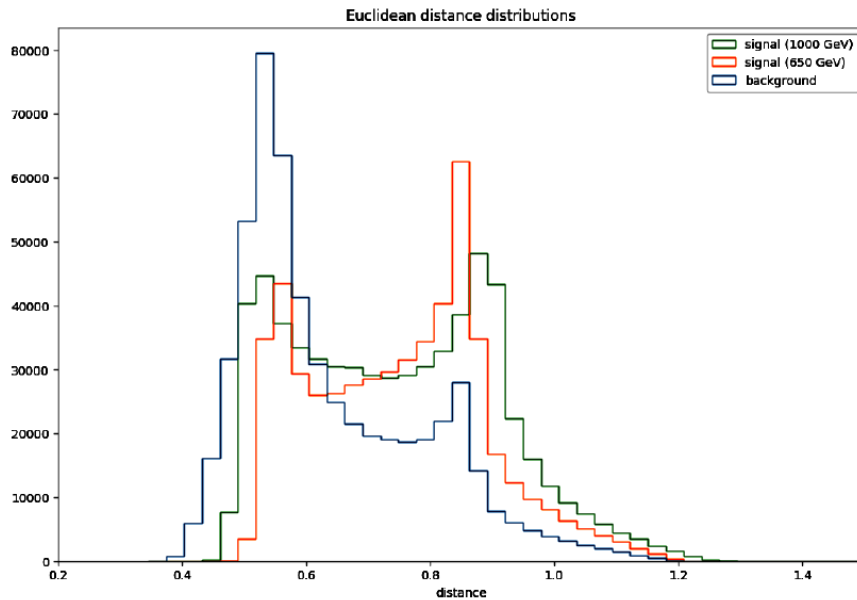
$$\text{FOM} = \text{Mean distance} + (1 - \text{mean D output})$$

Application: only the AE is used on test events

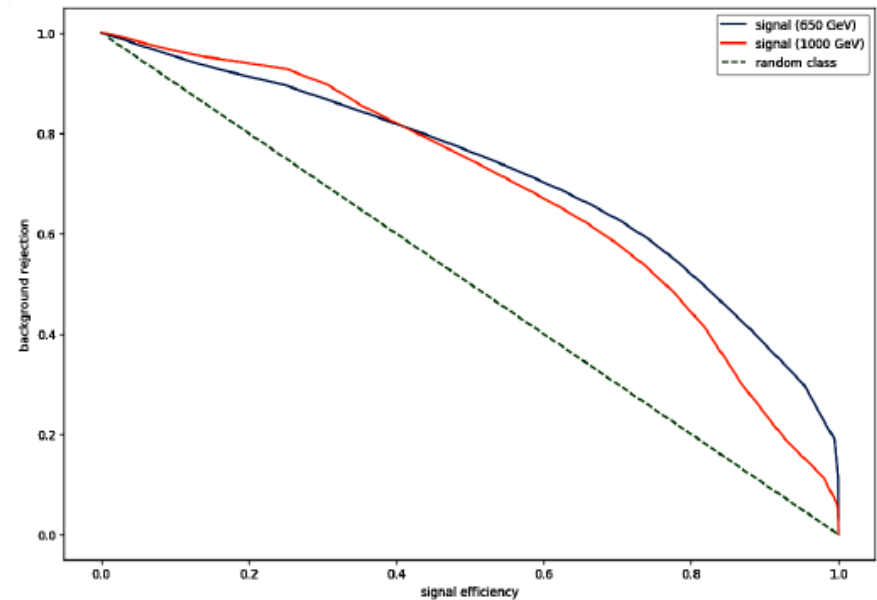


Trained AE is applied on both background and signal test samples

Mean Euclidean distance

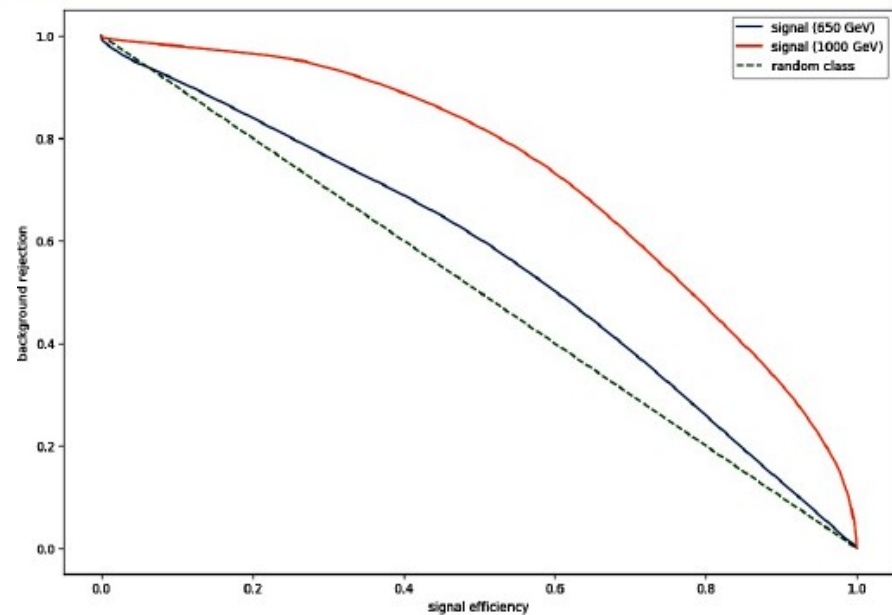
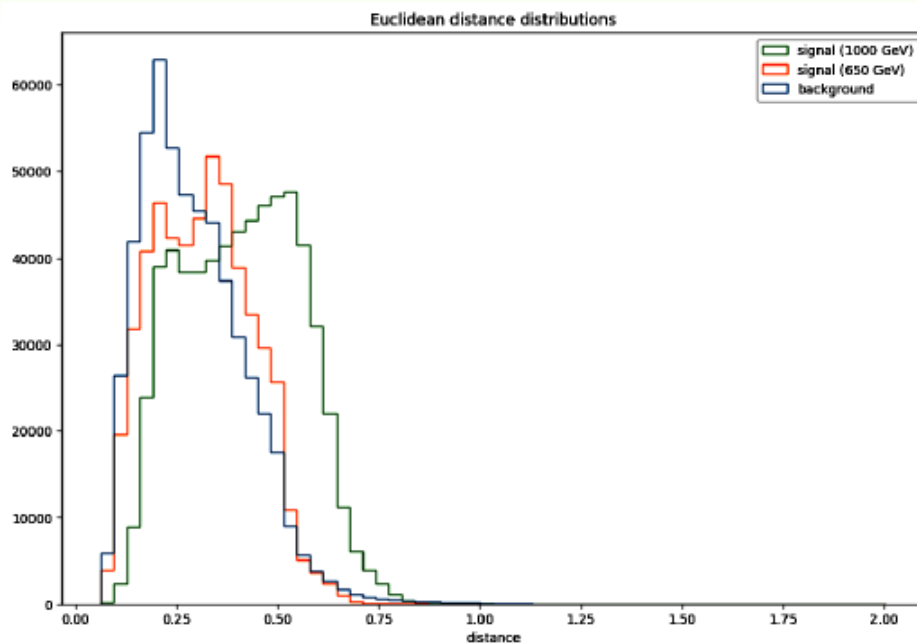


ROC Curve



Double peaks in distance calculation: to be understood
AUC ~ 0.7 for both signal masses

Comparison with standalone AE

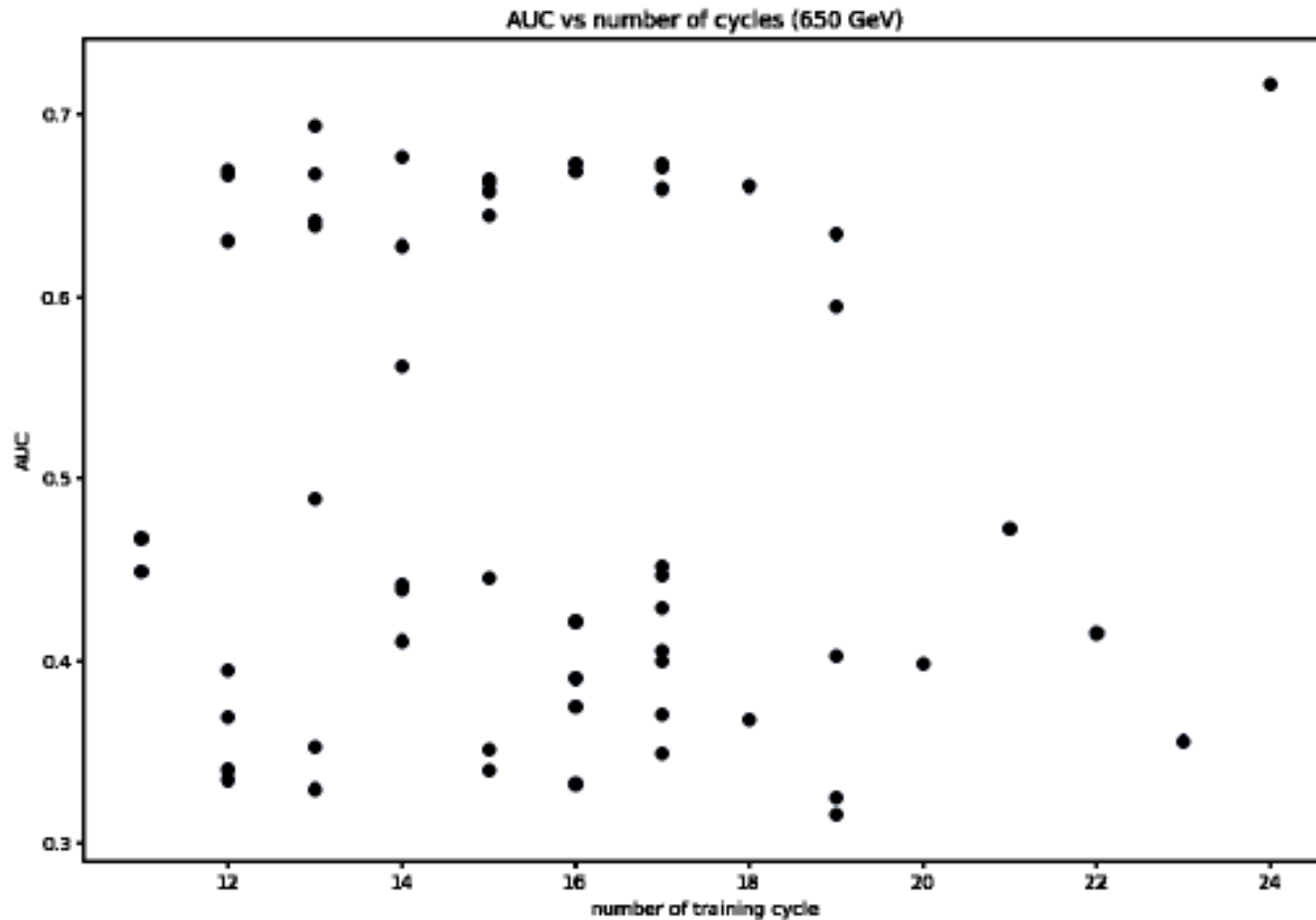


GAN-AE performs better for low mass signal (most difficult)

Issues with instability

L. Vaslin

Results (AUC) show high variance: here for 60 GAN-AE (signal $m=615$ GeV)



AE seem a good idea for unsupervised searches

However simple use case are not conclusive

- Appearance of spurious signal ? (LHC Olympics dataset)
- Instabilities (dijet sample)

More work needed on NN architectures (GAN-AE could be promizing)

Try to generalize to more complex signatures

General searches in CMS & ATLAS

- [1] CMS Collaboration, MUSiC, a Model Unspecific Search for New Physics, in pp Collisions at $\sqrt{s} = 8$ TeV, CMS-PAS-EXO-14-016 (2017).
- [2] CMS Collaboration, Model Unspecific Search for New Physics in pp Collisions at $\sqrt{s} = 7$ TeV, CMS-PAS-EXO-10-021 (2011).
- [3] ATLAS Collaboration, M. Aaboud et al., A strategy for a general search for new phenomena using data-derived signal regions and its application within the ATLAS experiment, Eur. Phys. J. C79 (2019) 120, [arXiv:1807.07447].
- [4] ATLAS Collaboration, A general search for new phenomena with the ATLAS detector in pp collisions at $\sqrt{s} = 8$ TeV, ATLAS-CONF-2014-006 (2014).
- [5] ATLAS Collaboration, A general search for new phenomena with the ATLAS detector in pp collisions at $\sqrt{s} = 7$ TeV, ATLAS-CONF-2012-107 (2012).

Latent Dirichlet Allocation (LDA)

- [6] B. M. Dillon, D. A. Faroughy, and J. F. Kamenik, Uncovering latent jet substructure, Phys. Rev. D100 (2019), no. 5 056002, [arXiv:1904.04200].
- [7] D. M. Blei, A. Y. Ng, and M. I. Jordan, Latent dirichlet allocation, J. Mach. Learn. Res. 3 (Mar., 2003) 993-1022.

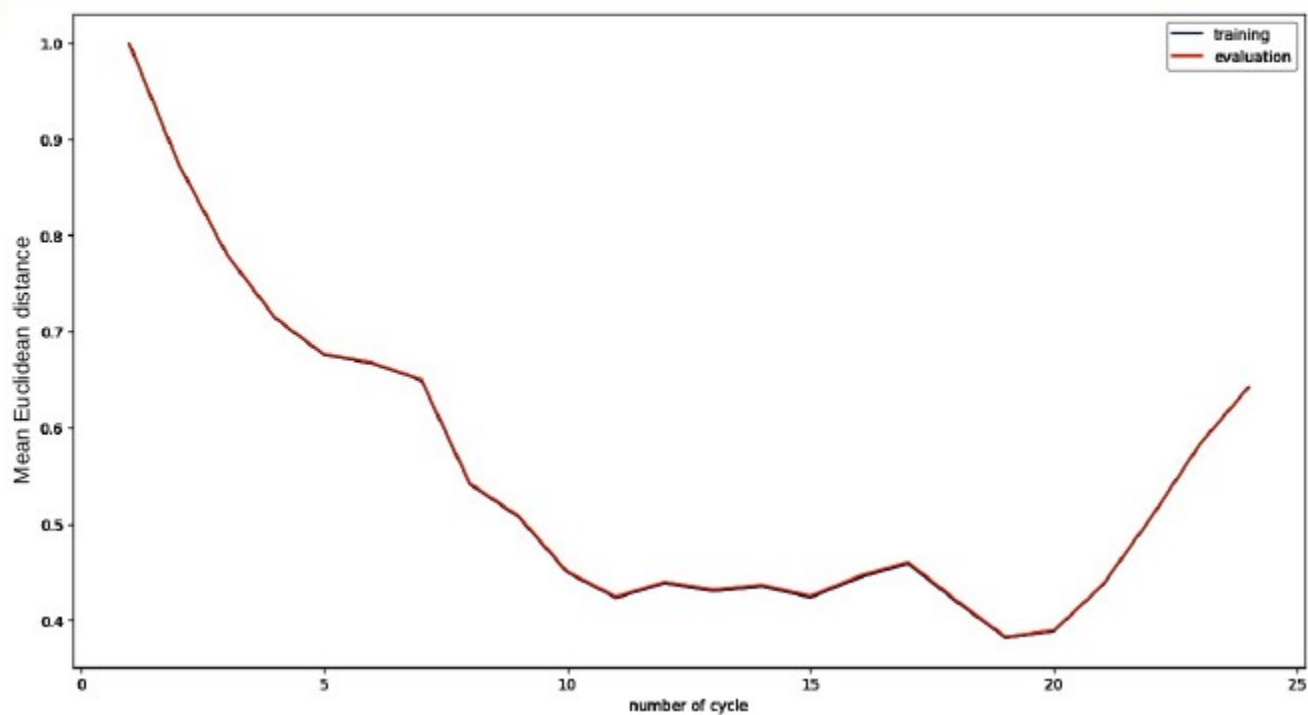
Autoencoders approaches

- [8] M. Farina, Y. Nakai, and D. Shih, Searching for New Physics with Deep Autoencoders, arXiv:1808.08992.
- [9] T. Heimel, G. Kasieczka, T. Plehn, and J. M. Thompson, QCD or What?, SciPost Phys. 6 (2019), no. 3 030, arXiv:1808.08979.
- [10] T. S. Roy and A. H. Vijay, A robust anomaly finder based on autoencoder, arXiv:1903.02032.
- [11] O. Cerri, T. Q. Nguyen, M. Pierini, M. Spiropulu, and J.-R. Vlimant, Variational Autoencoders for New Physics Mining at the Large Hadron Collider, JHEP 05 (2019) 036, arXiv:1811.10276.
- [12] A. Blance, M. Spannowsky, and P. Waite, Adversarially-trained autoencoders for robust unsupervised new physics searches, JHEP 10 (2019) 047, arXiv:1905.10384.
- [13] J. Hajer, Y.-Y. Li, T. Liu, and H. Wang, Novelty Detection Meets Collider Physics, arXiv:1807.10261

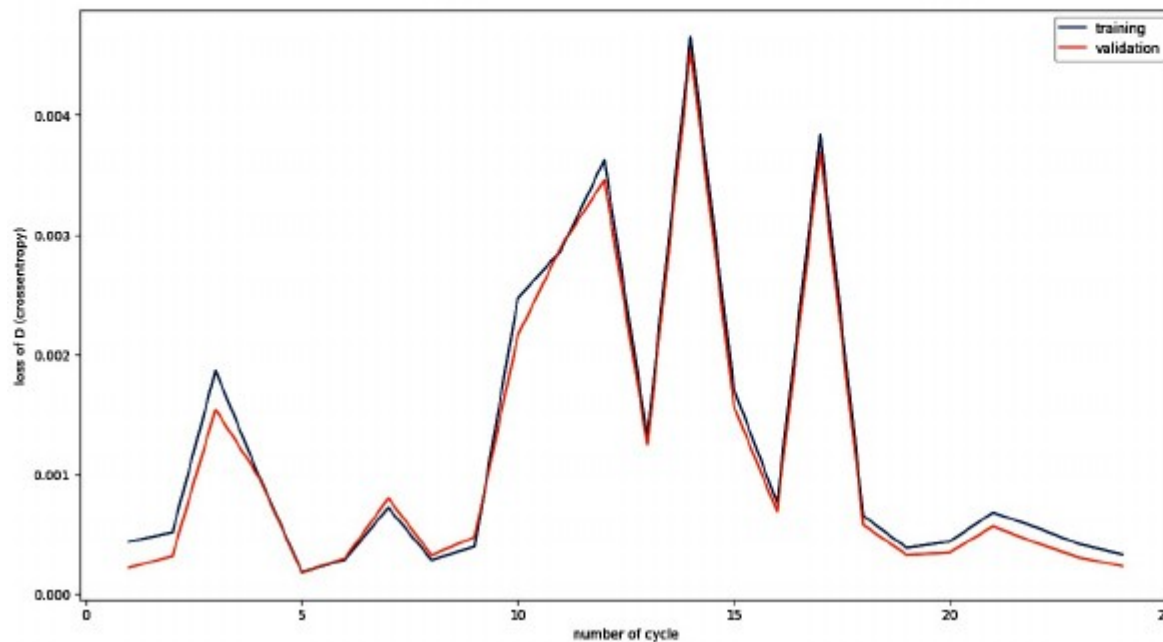
Bump hunt approaches

- [14] J. H. Collins, K. Howe, and B. Nachman, Extending the search for new resonances with machine learning, Phys. Rev. D99 (2019), no. 1 014038, arXiv:1902.02634.
- [15] B. Nachman, D. Shih, Anomaly Detection with Density Estimation, arxiv:2001.04990

- Reconstruction error evolution



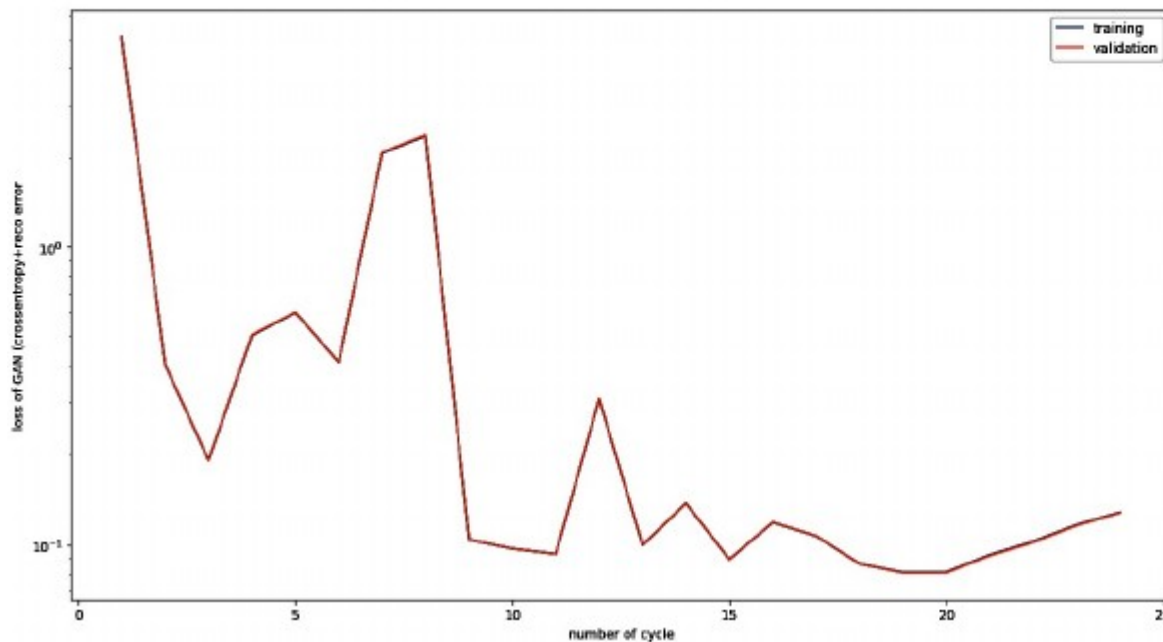
- Loss curve of the discriminator



Loss evaluated at each cycle after D training phase

Spiky behavior :
AE as changed between each evaluations
=> Performance of D varies at each cycle

- Loss curve of the AE+D model



Loss evaluated at each cycle after AE training phase

More stable behavior : Comes from the 2nd term