Machine Learning in ATLAS

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IHEP ATLAS ML kick-off meeting
2022.09.13

Introduction

- **Machine Learning is a very powerful tool in particle physics:**
  - ATLAS has performed several studies for the ML application:
    - Detection and simulation,
    - Combined Performance,
    - Reconstruction and analysis,
    - Anomaly detection,
    - …

  - And several corresponding tools are developed:
    - feature extraction,
    - hyper-parameter optimization,
    - …

  - All these topics are collected from the 5th ATLAS Machine Learning Workshop, Apr. 2021.

ML application in ATLAS

- **Event simulation with Generative adversarial networks (GANs):**
  - A very common method for fast event generation and simulation.
  - Unsupervised learning, with small statistic Madgraph/Phthia8+FastSim MC as training sample.
  - Example: DijetGAN.

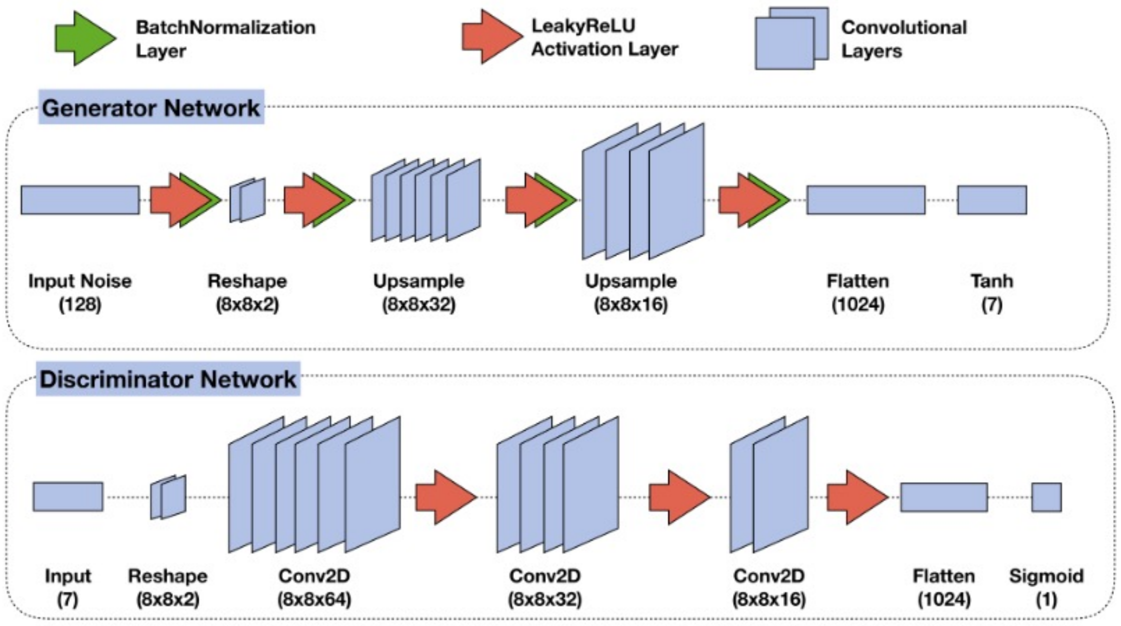


Figure 1. Network architecture: generator (top), discriminator (bottom). The GAN is composed by connecting the output of the generator to the input of the discriminator.

GAN vs. reco-level MC

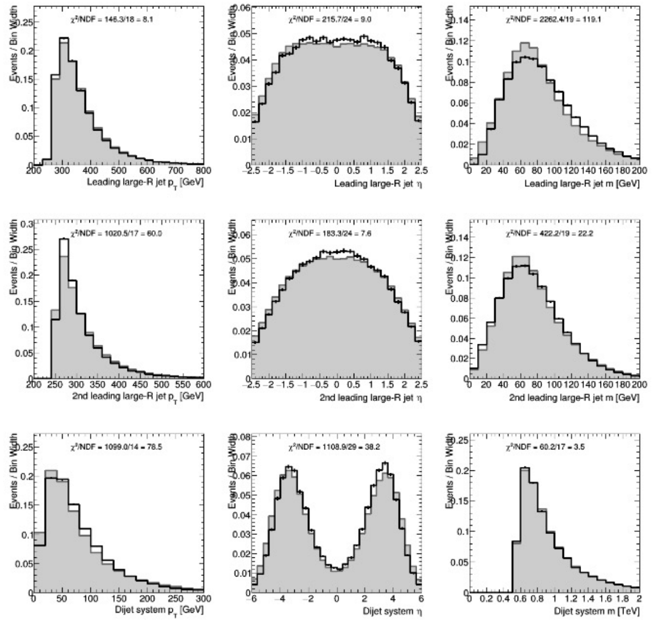
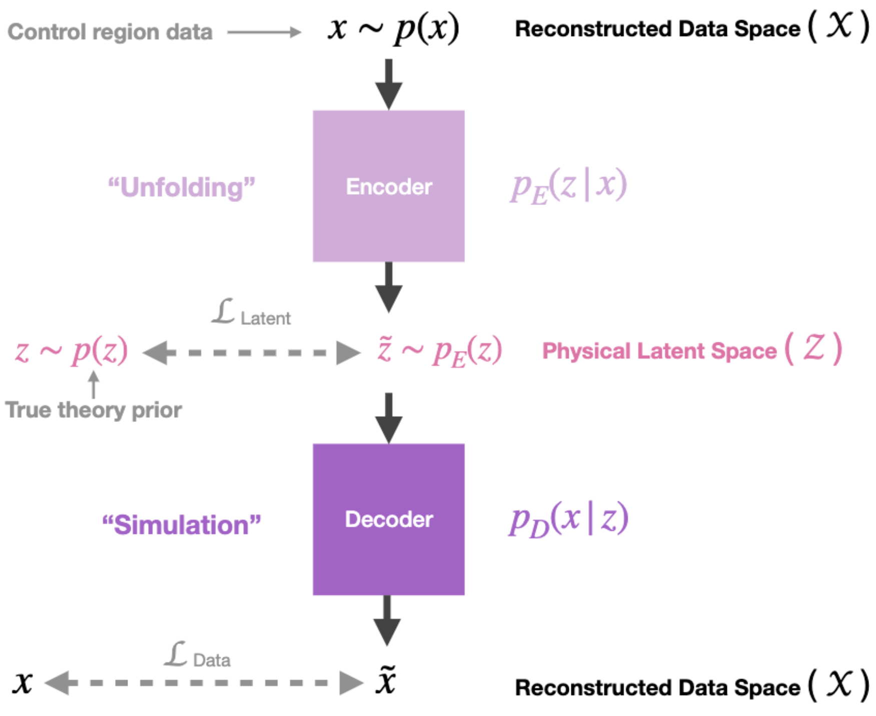


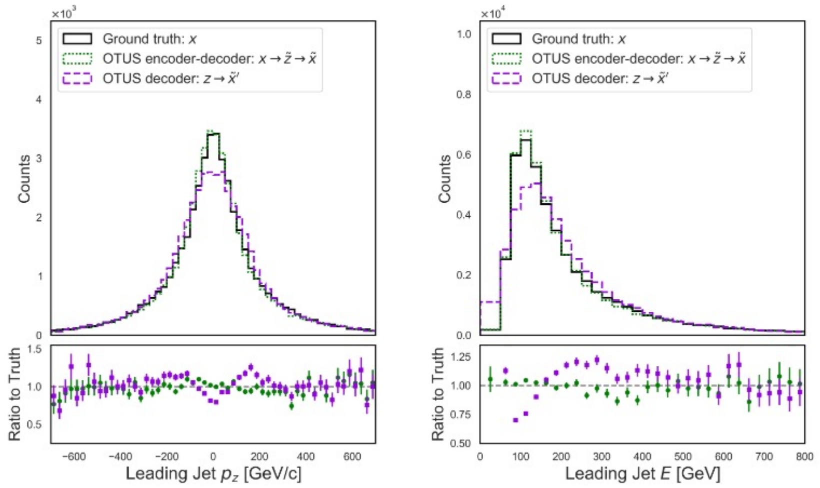
Figure 5. Comparison of kinematic observables with respect to reco-level (MadGraph5+Pythia8+ Delphes3) Monte Carlo simulation. The gray area represents the MC prediction, and the black line indicates the GAN output.

ML application in ATLAS

- **Optimal Transport based Unfolding and Simulation (OTUS)** arxiv: 2101.08944
  - A data-driven ML simulator with altering Variational Auto-encoders (VAEs): predict the **reco-level data (X)** from **parton interactions (Z)**. GANs only mimic the X but not learn the transformation $Z \rightarrow X$
  - Design the loss: Latent loss + Data loss + any additional physically motivated constraints.
  - Extra bonus: unfolding mapping from data to truth.



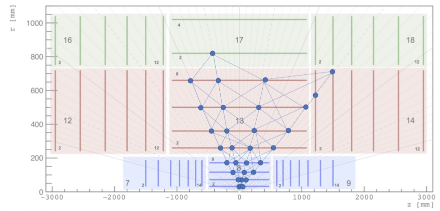
Leading jet

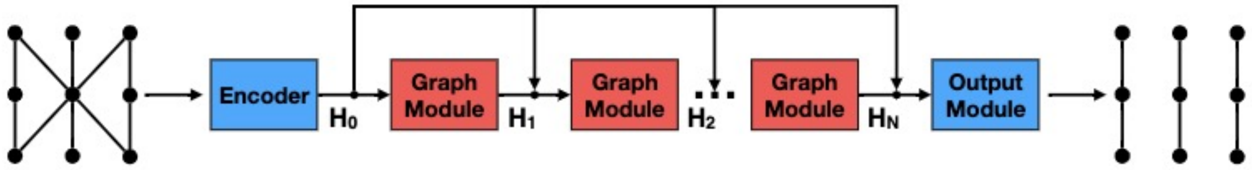


$pp \rightarrow t\bar{t}$

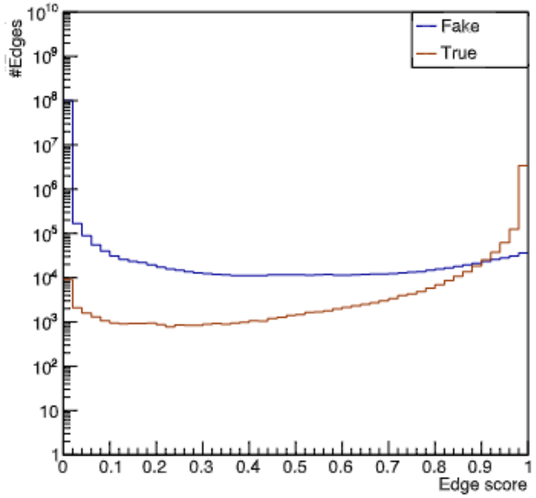
ML application in ATLAS

- **Track reconstruction algorithm with GNN in HL-LHC:** arXiv:2103.0091
  - Connect the hits and select the truth track from all connections (edge in graph).
  - Reduce the connections with detector module maps and geometric cuts for less memory.

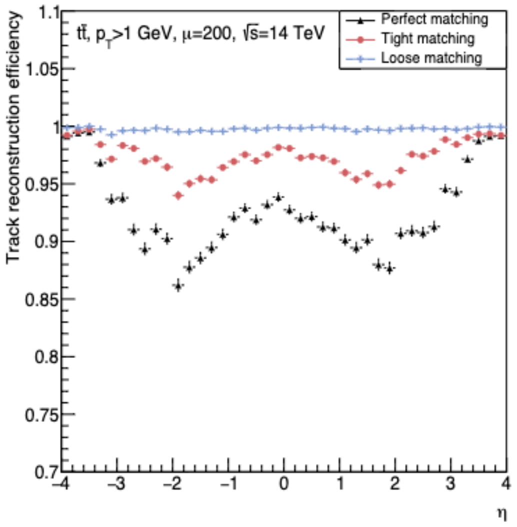




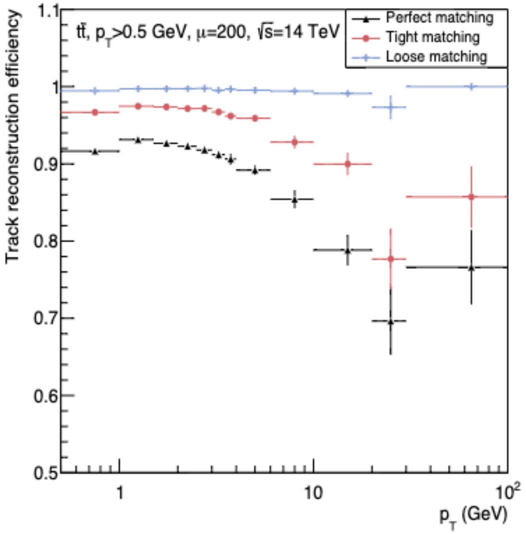
(arXiv:2003.11603)



Edges classification score (on a test dataset)



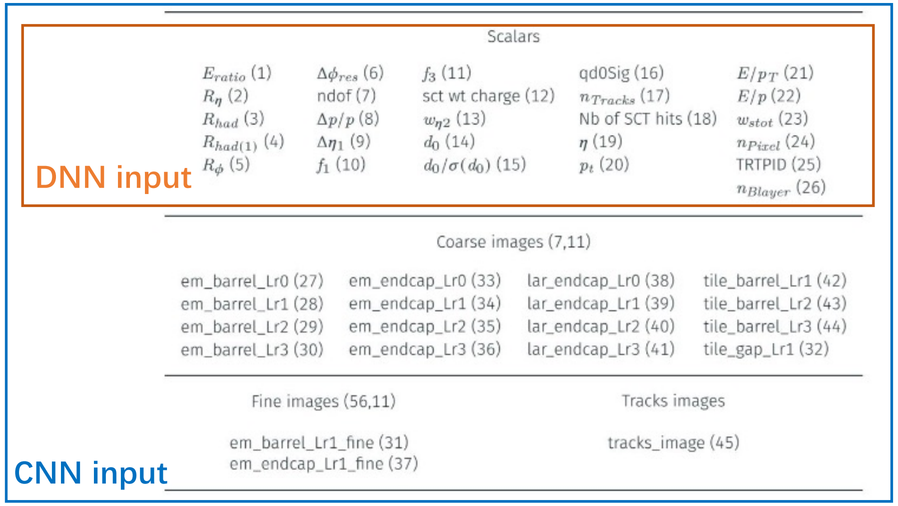
Track reconstruction efficiency vs. η

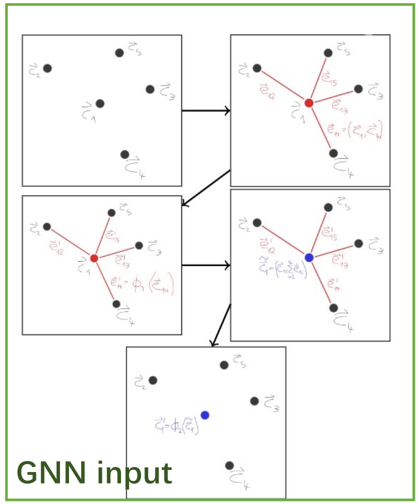


Track reconstruction efficiency vs. p_T

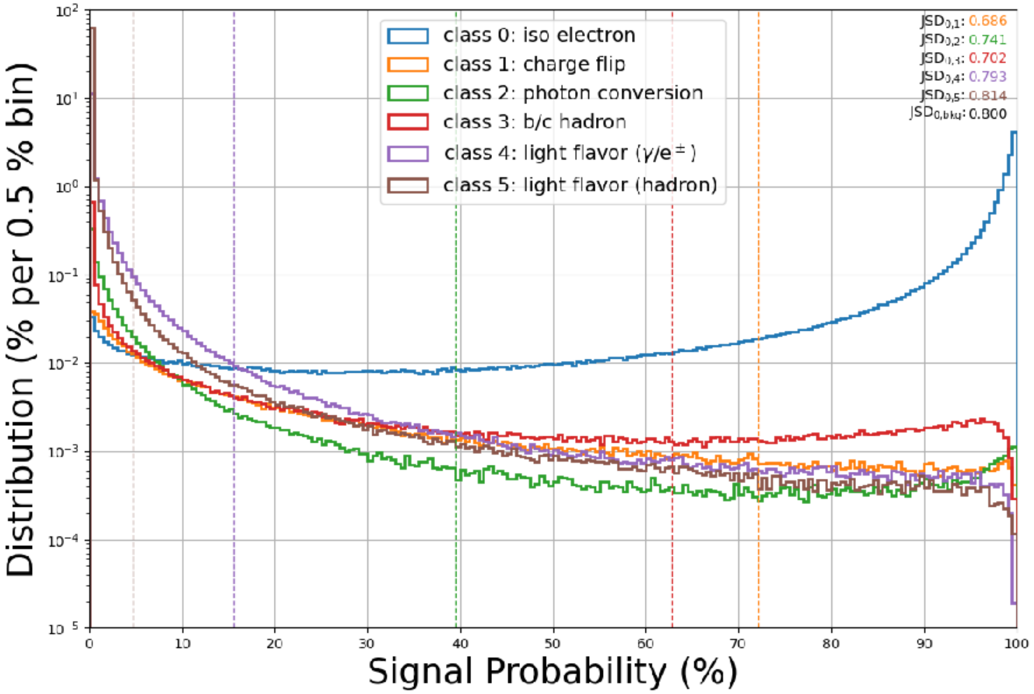
ML application in ATLAS

- **Object identification with ML:**
  - Electron ID with high level features + DNN, low level features + CNN/GNN.
  - Jet tagging for b-jet, c-jet, di-tau, gluon and bosons.
  - Similar procedure: select the input information and proper method, tune it and get the result.
  - Take e-ID as example:
    - High level info + multi-class: DNN.
    - Low level cell info (hit maps): CNN.
    - Low level cell info (hit structure): GNN.



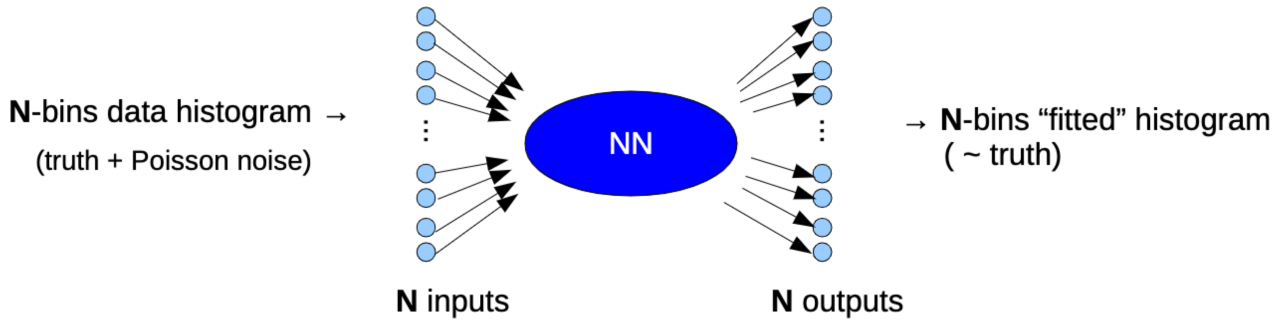


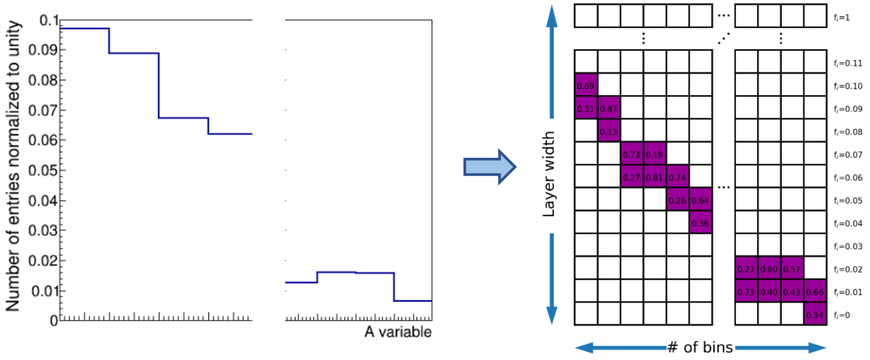
CNN classification performance

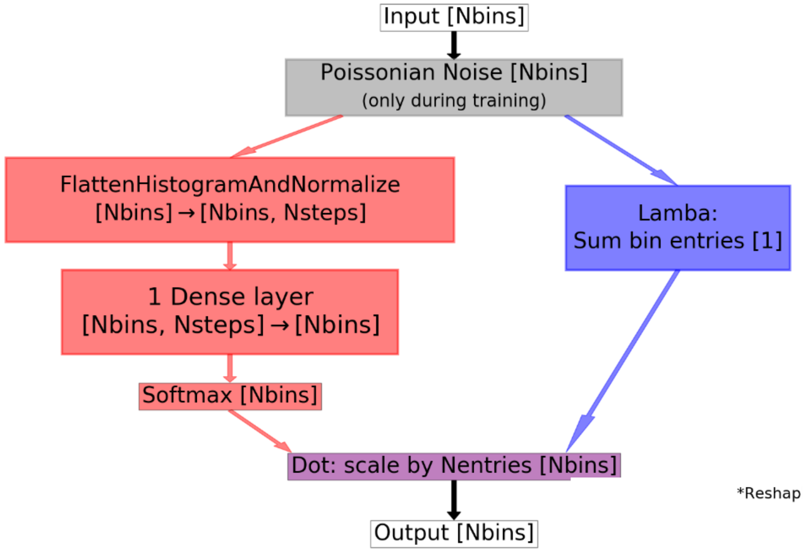


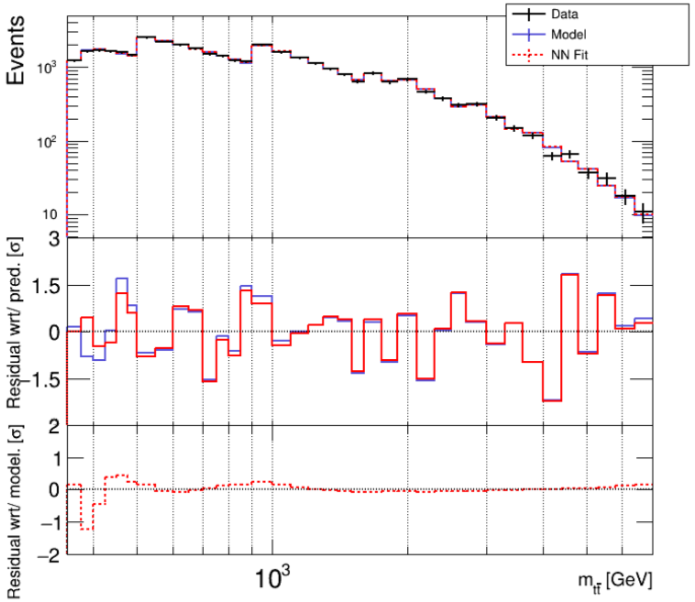
ML application in ATLAS

- **DNN-based fitting method:** extract a model from the existing histogram





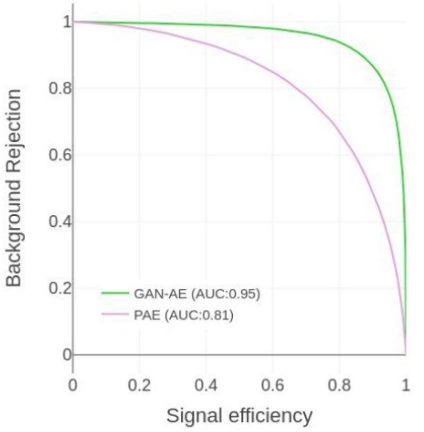


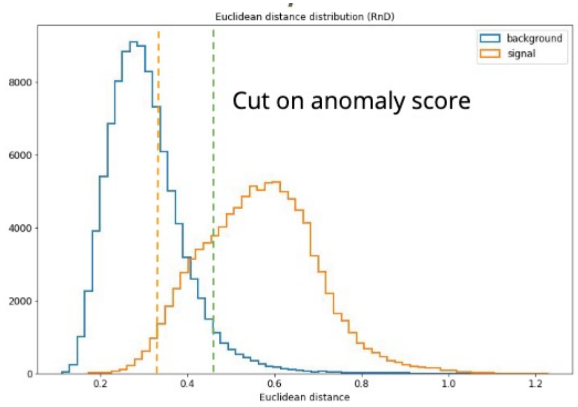


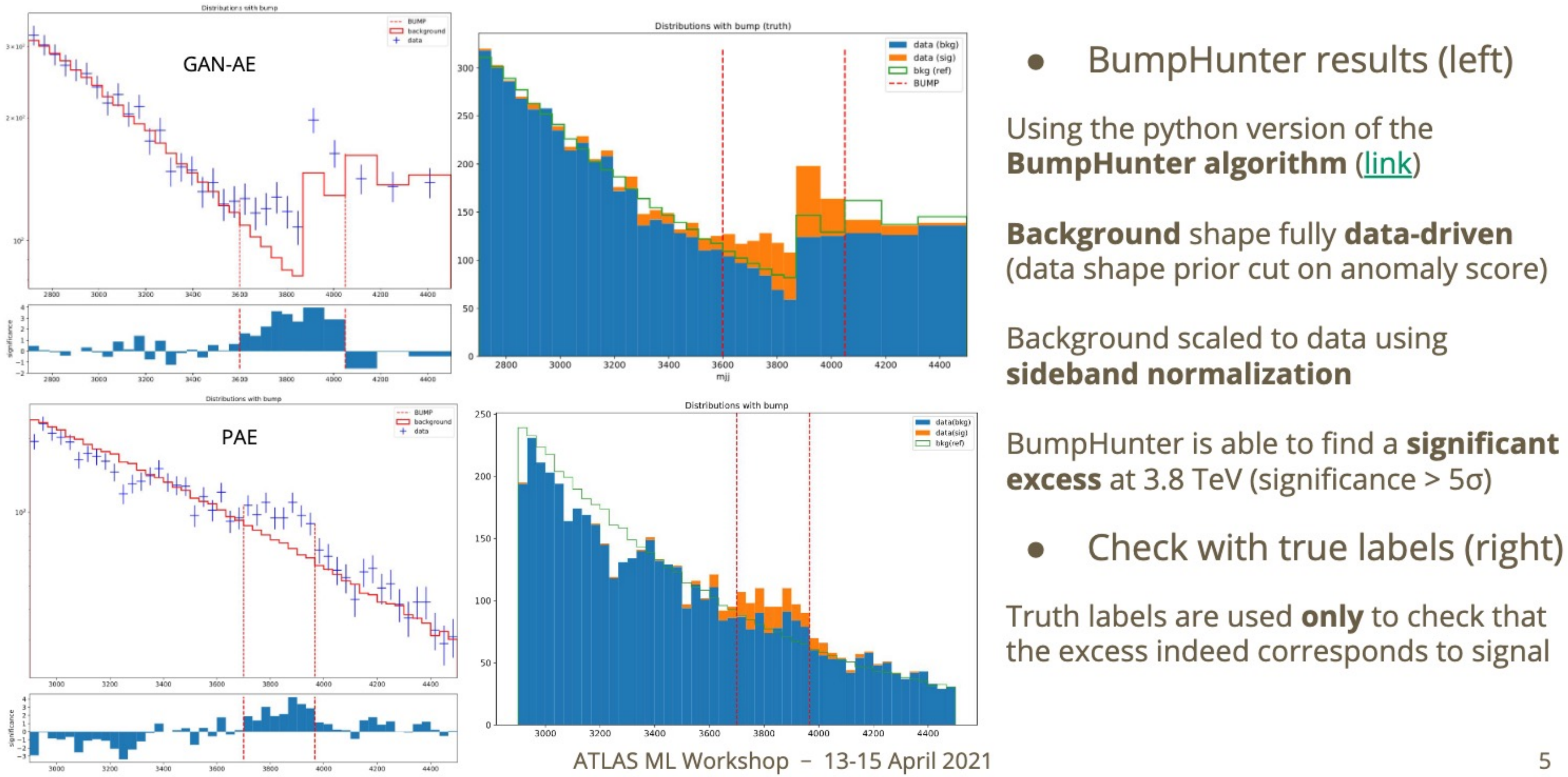
ML application in ATLAS

- **Physics analysis: unsupervised anomaly detection for BSM.**
  - Auto-encoder based ML for anomaly score: GAN-AE and PAE.
  - Checked with RnD dataset for AUC and blackbox dataset:

Another example for $H \to \gamma\gamma$

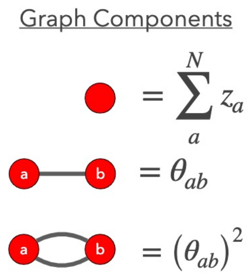


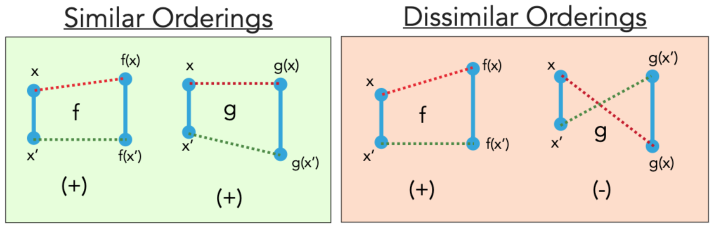


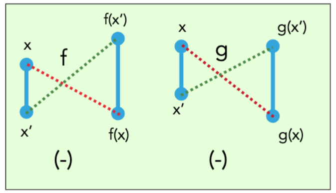


Tools for ML

- **Visualize the hidden physics in low-level NN**:
  - Jet substructure can be fully represented with Energy Flow Polynomials.
  - Define a Decision Ordering (DO) of 2 NN f(x) and g(x): 0 or 1.
  - Use Average DO (ADO) to represent the similarity between 2 NNs for one variable.







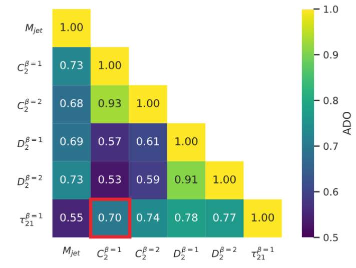
After Averaging

ADO = 1 : *Identical decisions*

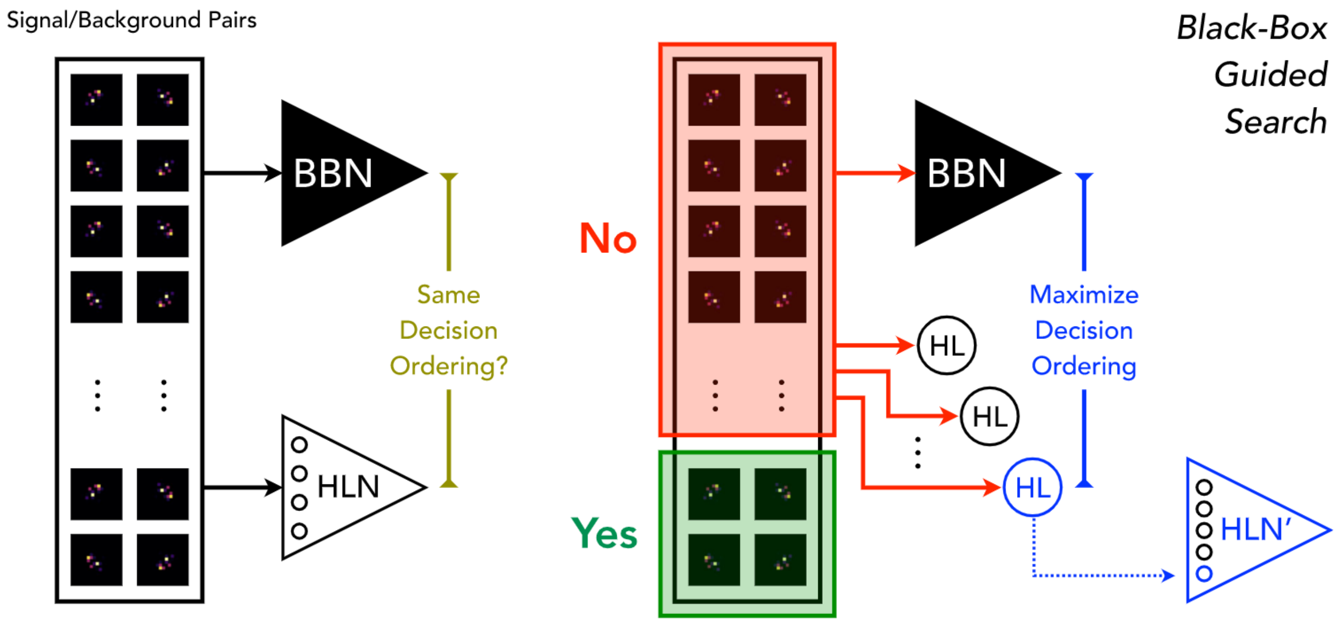
ADO = 0.5 : *Random similarity*

AUC of 6HL

Observable	AUC
$M_{\rm jet}$	0.898 ± 0.004
$C_2^{\beta=1}$	0.660 ± 0.006
$C_2^{\beta=2}$	0.604 ± 0.007
$D_2^{\beta=1}$	0.790 ± 0.005
$D_2^{\beta=2}$	0.807 ± 0.005
$\tau_2^{\beta=1}$	0.662 ± 0.006



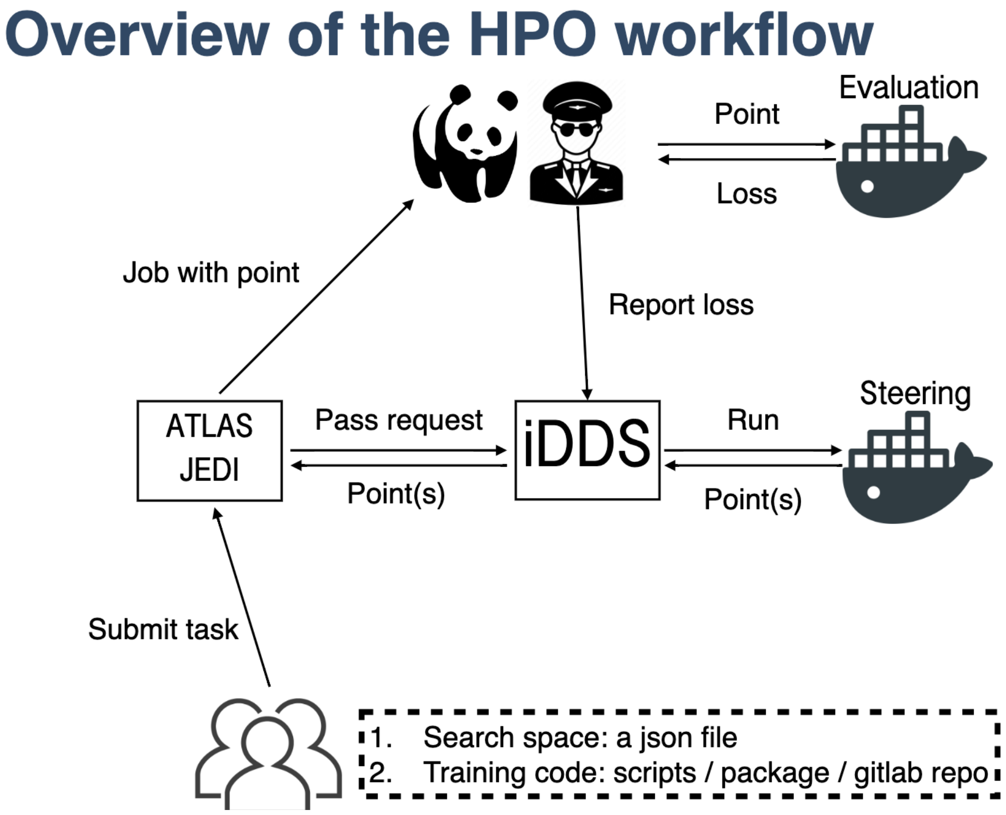
ADO similarity of pairs of HL Observables

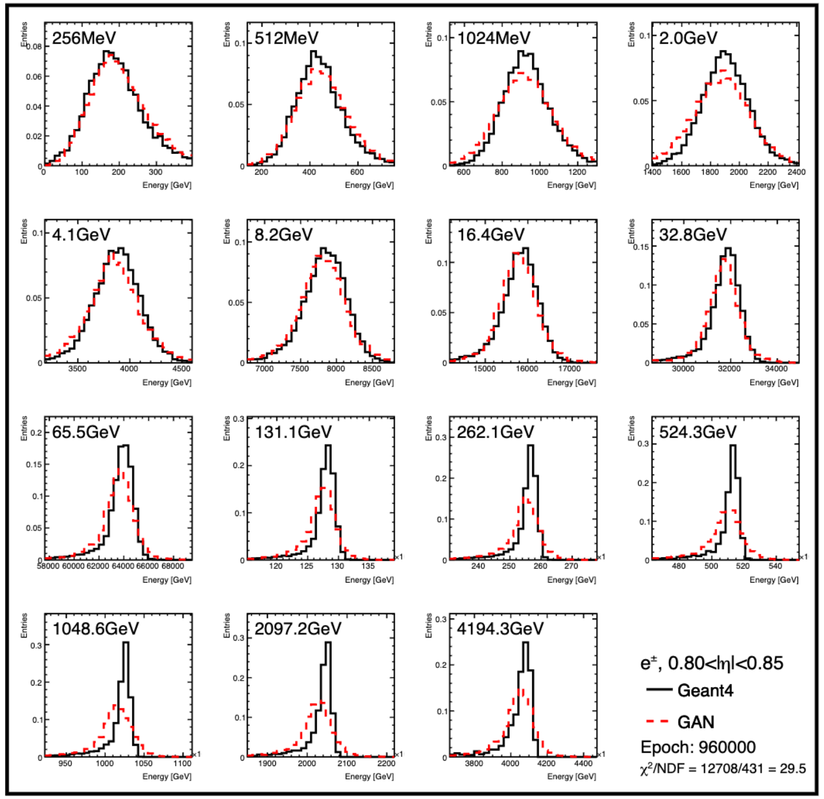


Phys. Rev. D **103**, 036020

Tools for ML

- **Hyperparameter optimization with intelligent Data Delivery Service (iDDS)**
  - Supported in ATLAS environment PanDA.
  - Specific the HPO job when submitting: phpo





Summary and Conclusion

- **There are many interesting topics in ATLAS**
  - This report only includes a few topics, please find more in AML workshops.
  - Large amount of ML methods are available nowadays. Analyze your questions and find a proper one:
    - Classification or regression? 2-class or multi-class?
    - What information you can have for input?
    - Supervised or un-supervised?
    - Training / Inference time?
    - …
  - Enjoy your trip in ML!