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Searches for Anomalies in hadronic final states with GNNs in ATLAS(*)

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Summary. — Graph neural networks are a promising technique for Anomaly Detection whenever it is possible to express detector information in the form of a graph. In our approach, graphs can be used to represent heavy resonance boson jets as interconnected topocluster nodes. By leveraging graph information and message passing, the network can identify unexpected signals deviating from the Standard Model.

1. – Anomalies in High Energy Physics

The Standard Model (SM) has demonstrated its ability to accurately depict observed phenomena in High Energy Physics (HEP) experiments, to forecast the existence of novel particles, and to provide essential guidance for successful discovery analyses. Numerous investigations conducted within the ATLAS collaboration aim to identify new resonances that could potentially address the remaining open questions of the Standard Model. However, up to this point, none of these efforts has succeeded in undermining its robust theoretical foundation and this can be attributed to many reasons, e.g. because New Physics (NP) signatures closely resemble SM signatures, making it challenging to distinguish between background signals and new phenomena. In this regard, it can be useful to exploit innovative Machine Learning (ML) algorithms, such as the Anomaly Detection (AD) whose primary goal is to identify candidates considered anomalous compared to others. In High Energy Physics, these algorithms can be used in the search for NP in the form of anomalous events (i.e., signals) that are inconsistent with the Standard Model (i.e., background). The idea behind the AD is to define a quantity, the Anomaly Score (AS), that quantifies the "distance" of the event from a standard reference. If the AS is a good discriminator, it is possible to distinguish two well separated distribution for the signal and the background, and then to determine a cut on the AS that maximises the significance of discovery over the signal itself.

AD and ML techniques, in general, have proven to be effective in addressing the challenges associated with NP searches and, therefore, several ATLAS analyses have

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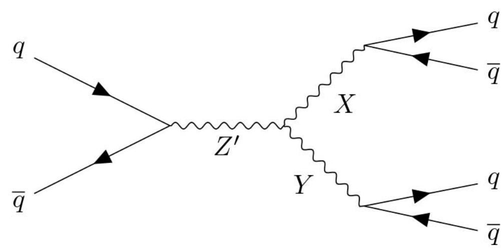

Fig. 1. – Diagram of the signal process used for the LHC Olympics R&D dataset.

incorporated these approaches. Notably, [2] was the first attempt among ATLAS analyses to employ AD for the exploration of a heavy resonance Y decaying into a SM Higgs boson and a distinct new particle X. This achievement was made possible through the utilisation of a Variational Recurrent Neural Network (VRNN) [1], which was trained in a fully unsupervised manner to discern anomalous jets as sequences of constituent four-vectors.

Given the results obtained with the VRNN, we have decided to use an unsupervised training to search for anomalies in hadronic final states, but this time exploiting graph representation and Graph Neural Networks (GNNs). First, we are going to use a simplified use case, the LHC Olympics dataset, in order to assess the performance of the ML architecture and then, once the best model is identified, use it on Run-3 ATLAS data.

2. – LHC Olympics use case

Some of the algorithms developed for HEP in the recent years have competed in the LHC Olympics project [3] and then published in [4]: the aim of LHC Olympics challenge is to promote the development of ML models to identify jet events coming from a new resonance decaying fully hadronically among QCD background. Hadron jets, in fact, are very favourable candidates for AD, since they have a very complex internal structure that the current clustering algorithms can only partially reveal.

The LHC Olympics R&D dataset includes events with large-radius jets (antik_T with $R = 1.0$) from either QCD multi-jet production or a hypothetical new resonance Z' decaying into two vector boson X and Y with masses at 3.5 TeV, 500 GeV and 100 GeV respectively. The dataset consists of 1M QCD dijet events and 100k signal events.

2·1. *Representation of the events as graphs.* – A graph is a method of representing data as nodes, that are a collection of objects, and the connections between them. In the context of our analysis, the strategy is to depict jets resulting from the decay of heavy resonance bosons, which, in turn, decay into fully hadronic final states, using undirected graphs. Here, each node within the graph corresponds to a calorimeter topological cluster, or topocluster, and the node's characteristics are described in terms of kinematic variables such as the fraction of p_T, η and ϕ. The criteria for establishing connections between nodes are primarily based on spatial distance: two topoclusters will be connected if their relative distance is less than a reference distance.

2·2. *Graph Neural Networks.* – GNNs, a powerful class of deep learning models, have gained prominence in the realm of graph-based data analysis. The GNN takes as input graphs with a variable number of nodes and can predict whether the graph is anomalous

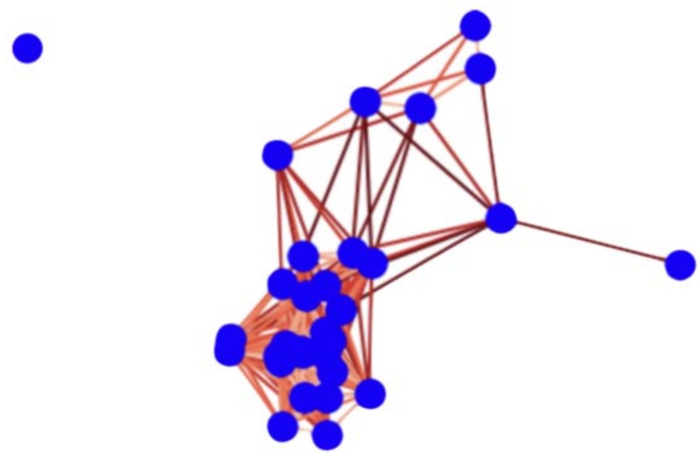

Fig. 2. – Example of one jet that has been reconstructed as an undirect graph.

or not. Information is propagated to each node from its neighbouring nodes through a mechanism known as message passing. This mechanism allows nodes to aggregate and update their information based on the information received from adjacent nodes. The iterative nature of message passing enables GNNs to capture and propagate information across the entire graph, making them adept at tasks like node classification, link prediction, and graph classification.

3. – Anomaly Detection analysis strategy

There are different ways of operating a ML algorithm with a supervised, weakly supervised or unsupervised approaches, depending if the labels are used, partially used or not at all exploited respectively during the training. The strategy behind this analysis is to employ unsupervised training, which typically exhibits lower performance compared to its supervised counterpart when evaluated on the training dataset. Nevertheless, it offers the advantage of increased generalisation power. Given that the nature of NP remains unknown, there is a desire for enhanced model independence. As a result, the ability to generalise, a characteristic inherent to unsupervised architectures, is crucial for accommodating the uncertainty associated with NP and promoting model independence.

In our unsupervised approach, the network exclusively employs background data during its training phase and optimises its parameters to reside within a hypersphere, as expressed in the DeepSVDD loss [5]. Subsequently, when the network is presented with signal events, these events fall outside the hypersphere and are thus identified as anomalous through the AS. The AS is computed at each epoch of the training process and its distribution serves as an indicator of the degree of anomaly associated with the considered event.

3˙1. *Results and perspectives.* – The GNN used for this analysis is a Graph Isomorphism Network (GIN) [6], with five layers of message passing. The training is done in a completely unsupervised manner and the DeepSVDD loss function is minimized. The AS

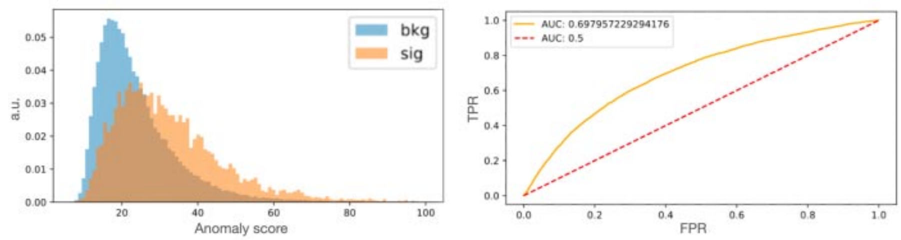

Fig. 3. – The Anomaly Score distribution, on the left, and the Receiver Operating Curve of the GNN used.

considered is the result of the loss itself and its distribution for the signal and background evaluated in the test dataset is given in fig. 3. The overall performance is considered in terms of Area Under the Curve (AUC) of the Receiver Operating Curve; the GIN model is able to obtain a promising AUC of around 70%. Once the model has been evaluated, it can be tested on real Run-3 ATLAS data.

REFERENCES

[1] Kahn A. *et al.*, *JINST*, **16** (2021) P08012.
[2] ATLAS Collaboration, *Phys. Rev. D*, **108** (2023) 052009.
[3] LHC Olympics 2020, `https://lhco2020.github.io/homepage/`.
[4] Kasieczka G. *et al.*, *Rep. Prog. Phys.*, **84** (2021) 124201.
[5] Ruff L. *et al.*, *Deep One-Class Classification*, in *Proceedings of the 35th International Conference on Machine Learning*, **,** (V) ol. **80** (PMLR) 2018, pp. 4393–4402.
[6] Xu K. *et al.*, *How Powerful are Graph Neural Networks?*, arXiv:1810.00826v3.