Deployment of unsupervised learning in a search for new physics with ATLAS Open Data

Analysis of two lepton final state from OpenData at ATLAS

Sakarias Frette

Spring 2022

Abstract

University of Oslo

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I. INTRODUCTION

The standard model is arguably the best model ever created by man, showing remarkable accuracy comparing with experiments. Its crown jewel was discovered in 2012 by both ATLAS¹ and CMS² at CERN. There has however not been any new particle discoveries since the early 70's, and this is somewhat alarming. The standard model has several issues, some of them includes explanation of dark energy, cosmic inflation, the hierarchy problem and no including of gravity.

This leads scientists to look beyond the standard model, and there are several models proposed, such as dark matter candidates, extra vector bosons and super symmetry. Attempts are made by multiple collaborations to discover evidence for these models, and there are several obstacles to overcome, such as method of analysis and sufficient amount of data. With the impressive progress of machine learning software such as Tensorflow[5], machine learning methods have become more and more popular as possible methods to use for new physics.

In the last decade machine learning has excelled from being tedious and hard to program to become available to almost everyone. It's scale-ability and ability to discover hidden structure in large datasets makes it an intriguing candidate to use on data from the Large Hadron Collider. One possible candidate is semi unsupervised learning, which is done by an auto encoder. The idea is to train a model-independent algorithm on only background, with the hope that what ever new physics that is in the data is detected, without knowing what it is. This machine learning model is the method of choice for this report.

This report is structured in a theory, implementation, results and discussion, and conclusion section. In the theory section we introduce the necessary theory, with respect to both data, method of analysis and choice of evaluation. In the implementation section we discuss data handling, with respect to cuts, event selection, scaling and feature choices, choice of hyper parameters for grid search and the software and api's used for training and tuning. In the results and discussion section we display the results and discuss them as as well as distinct observations. In the conclusion we summarize our findings.

II. THEORY

Some of theory sections about anomaly detection and machine learning algorithms are based on previous work done in other courses, such as [3] and [2].

A. Anomaly detection

Anomaly detection is a tool with a wide range of uses, from time series data, fraud detection or anomalous sensor data. Its main purpose is to detect data which does not conform to some predetermined standard for normal behavior. The predetermined standard varies from situation to situation, and can be set by the context it self, and what is expected as an anomaly. We typically classify anomalies in three categories[1]:

- 1. Point anomalies
- 2. Contextual anomalies
- 3. Collective anomalies

For the purpose of this report we will mostly consider collective anomalies, as anomalies in the standard model has to be collective to claim anything due to noise etc.

In high energy physics we can using machine learning separate anomaly detection into two categories, supervised and unsupervised searches.

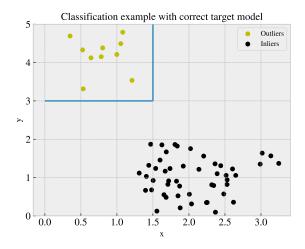


Figure 1: Example of supervised classification of anomaly where the target model is correct. Here the machine learning model manages to correctly identify the anomalies.

B. Stacked auto encoder

One method to attack the anomaly detection problem is the so called (stacked) auto encoder. The idea is based on reconstruction, and has been implemented for denoising of images, image compression, and anomaly detection. An auto encoder is a subgroup of feed forward neural networks, and the goal is to compress the information into fewer variables, called the latent space,

¹ Paper from ATLAS colaboration can be found here.

² Paper from CMS colaboration can be found here.

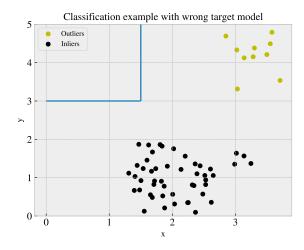


Figure 2: Example of supervised classification of anomaly where the target model is wrong. Here the machine learning model manages to wrongly identify the anomalies.

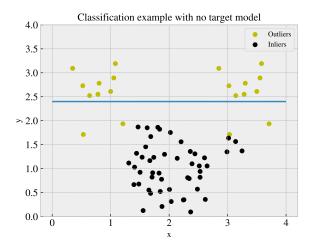


Figure 3: Example of unsupervised classification of anomaly with no target model. Here the machine learning model manages to with good precision identify the anomalies.

which then can explain much of the data through decoding that information. This allows the algorithm to learn the most important components of the data. An illustrative image of an auto encoder is shown below.

We see here in figure 4 that the input data is deconstructed through an encoder to a lower dimensional space called the latent space, depicted here as **z**, and then reconstructs the data with the decoder. It is important to note that the number of layers, nodes per layer and activation function per layer for the encoder does not need to match the structure of the decoder. The only requirement is that the input and output layer has the same shape. The end result is the reconstructed data **x**'.

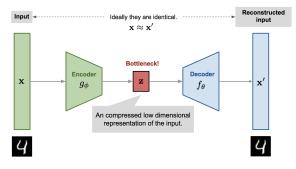


Figure 4: The architecture of an autoencoder with image reconstruction as the example use. Source, accessed 28.04.22

The training of the model is parameterized in the following way. We define the decoder as

$$\mathbf{z} = g_{\mathcal{E}}(\mathbf{x}),$$

and the reconstructed information as

$$\mathbf{x'} = f_{\theta}(g_{\xi}(\mathbf{x})),$$

where the parameters (ξ, θ) are tuned to reconstruct the data as close to the original data as possible. The model then adjusts following the simple mean squared error of the reconstruction and the actual data, given below

$$L_{AE}(\xi, \phi) = \frac{1}{N} \sum_{i=0}^{N-1} \left(\mathbf{x}^i - f_{\theta}(g_{\xi}(\mathbf{x}^i)) \right)^2$$

C. Beyond standard model physics

D. Evaluation

ROC curves

2. Error distributions

III. IMPLEMENTATION

A. Handling of data

In appendix ?? the features used in the data set are listed, with their respective type and description. The data can be seperated into two categories, Monte Carlo simulated (MC) data and actual data. The MC data contain background samples which are standard model processes, and signal samples which are proposed new physics. The actual data is data from the ATLAS detector. The totality of the data used in this report is given as

ATLAS OpenData³. This is a dataset that has been analyzed for new physics, and can thus be released to the public.

1. Cuts, pre-selection and scaling

To preserve as much information and add as little bias as possible we did as few cuts as possible. The entire data gathering process is biased from the moment the data is collected at the collider, but even then it is good to try to minimize the bias.

The first cut we impose is to require "good leptons". This is done by requiring lep_etcone20/lep_pt < 0.15 and lep_ptcone30/lep_pt < 0.15. We then require only two leptons per event. The event selection was done using RDataframe, to speed up the selection⁴

We tested two methods of scaling in this report, Min Max Scaling⁵ and Standard scaling⁶[7].

2. Choice of features

The choice of features is a mixture of specification and broadness. In this context specification is defined as information that specify for a given part of the physical system, in this case leptons. Thus, most of the features are directly related to the leptons, as they are the main focus of the BSM final states. Broadness is in this context defined as information about the rest part of the final state, such as jets, photons or tau leptons. Ideally one would pick as much information as possible for each event, but there is a trade-off between amount of information and size of data, and as consequence, execution time.

The features were picked such that there are no missing values, only 0 or larger than 0. For regular machine learning problems, missing values usually gets replaced by the mean value of the feature. This is however a problem when analysing physics, as such a choice could violate the laws of physics. To avoid this, all features are designed to either have 0 if missing, or sum up the contributions of both missing and present values, given that they represent the same type of information.

An example of this is if we have two jets in one event and three in another, using the transverse momentum of the jets as features. We cannot in the first event input the mean values of all third jet-transverse momentum in the entire dataset, but we could put 0, or sum all the transverse momentum for the jets in the given event into one feature. Another possibility is to only give the count of jets in the event, and there are even more ways to solve this issue.

B. Tuning and training

For the auto encoder to accurately distinguish background from signal, the model needs to train on the background data. However, neural networks are highly susceptible to hyperparameters, which needs tuning. In this project we used Keras-tuner[6] to tune the hyperparameters. The hyperparameters we have for our network are the learning rate, the alpha parameter for the LeakyReLU⁷ activation function, the activation function for each layer and the amount of nodes per layer. The activation functions used in the hyperparameter grid search where

- ReLU
- LeakyReLU
- tanh
- linear

whilst the different learning rates that was tested was $[9 \cdot 10^{-2}, 9.5 \cdot 10^{-2}, 10^{-3}, 1.5 \cdot 10^{-3}]$.

The auto encoder was written using Tensorflow api[5], using a functional structure⁸. In practise, this model could just as well have been written as a Sequential model⁹, but at a cost of flexibility and lack of potential non-linear structure in the architecture.

IV. RESULTS AND DISCUSSION

A. Semi unsupervised

- Difference between broad and narrow search
- Bias
- bias with features to choose
- difference of how well the model detects different signal models in mc data signals
- any interesting in actual data?
- difference in scaling
- tuning effect
- optimizing tensorflow code with use of autoclustering and possibly mixing floating point precision.

³ Link to ATLAS OpenData here.

⁴ This code was written by Eirik Gramstad, and can be found here.

⁵ More on Min max scaling here.

⁶ More on Standard scaling here.

⁷ More on the LeakyReLU api can be found here.

⁸ More on the functional api can be found here.

⁹ More on sequential models can be found here.

V. CONCLUSION

REFERENCES 7

REFERENCES

[1] Varun Chandola, Arindam Banerjee, and Vipin Kumar. "Anomaly Detection: A Survey". In: ACM Comput. Surv. 41 (July 2009). DOI: 10.1145/1541880.1541882.

- [2] Sakarias Frette and William Hirst. "Seaching for Higgs through supervised and unsupervised machine learning algorithms". In: (2022). URL: https://github.com/WilliamHirst/Advanced-Machine-Learning/blob/main/article/Project_1.pdf.
- [3] Sakarias Frette, William Hirst, and Mikkel Metzch Jensen. "A computational analysis of a dense feed forward neural network for regression and classification type problems in comparison to regression methods". In: (2022), p. 5. URL: https://github.com/Gadangadang/Fys-Stk4155/blob/main/Project%202/article/Project_2_current.pdf.
- [4] Christopher G. Lester. "The stransverse mass, M T2, in special cases". In: *Journal of High Energy Physics* 2011.5 (May 2011). DOI: 10.1007/jhep05(2011)076. URL: https://doi.org/10.1007%2Fjhep05%282011%29076.
- [5] Martín Abadi et al. *TensorFlow: Large-Scale Machine Learning on Heterogeneous Systems*. Software available from tensorflow.org. 2015. URL: https://www.tensorflow.org/.
- [6] Tom O'Malley et al. KerasTuner. https://github.com/keras-team/keras-tuner. 2019.
- [7] F. Pedregosa et al. "Scikit-learn: Machine Learning in Python". In: Journal of Machine Learning Research 12 (2011), pp. 2825–2830.
- [8] Review of the 13 TeV ATLAS Open Data release. Tech. rep. All figures including auxiliary figures are available at https://atlas.web.cern.ch/Atlas/GROUPS/PHYSICS/PUBNOTES/ATL-OREACH-PUB-2020-001. Geneva: CERN, Jan. 2020. URL: https://cds.cern.ch/record/2707171.

REFERENCES 8

Appendix A: Features

Table I: Features and their description [8]

Feature	Туре	Description
njet20	int	Number of jets with $p_T > 20 \text{ GeV}$
njet60	int	Number of jets with $p_T > 60 \text{GeV}$
nbjet60	int	Number of b-jets with $p_T > 60 \text{ GeV}$
nbjet70	int	Number of b-jets with
nbjet77	int	Number of b-jets with
nbjet85	int	Number of b-jets with
isOS	int	1 if leptons have opposite charge, 0 if leptons have same charge
isSF	int	1 if leptons are of same flavor, 0 is leptons are of different flavor, flavor code 11 is electron, flavor code 13 is muon
mll	float	Invariant mass of the two leptons
mt2	float	The maximal lower bound on the mass of each member of a pair of identical parent particles which, if pairproduced at a hadron collider, could have each undergone a two-body decay into (i) a visible particle (or collection of particles) and (ii) an invisible object of hypothesised mass $\chi[4]$.
met_et	float	Transverse energy of the missing momentum vector
met_phi	float	Azimuthal angle of the missing momentum vector
lep_flav	vector <int></int>	Flavor of the lepton, 11 for electron and 13 for muon
lep_pt	vector <float></float>	Vector containing transverse momentum for the leptons
lep_eta	vector <float></float>	Vector containing pseudo-rapidity , η , for the leptons
lep_phi	vector <float></float>	Vector containing azimuthal angle, ϕ , for the leptons
lep_E	vector <float></float>	Vector containing the energy for the leptons
lep_ptcone30	vector <float></float>	Vector containing scalar sum of track p_T in a cone of $R = 0.3$ around lepton, used for tracking isolation
lep_etcone20	vector <float></float>	Vector containing scalar sum of track E_T in a cone of $R = 0.2$ around lepton, used for calorimeter isolation
lep_trackd0pvunbiased	vector <float></float>	d_0 of track associated to lepton at point of closest approach (p.c.a.)
lep_tracksigd0pvunbiased	vector <float></float>	d_0 significance of the track associated to lepton at the p.c.a.
lep_isTightID	vector <bool></bool>	Vector containing boolean indicating whether leptons satisfies tight ID reconstruction criteria
lep_z0	vector <float></float>	Vector containing z-coordinate of the track associated for the leptons wrt. primary vertex
channelNumber	int	
costhstar	float	
weight	float	MC sample weight
category	string	SM or BSM category
physdescr	string	MC process name
isSignal	int	1 if category is a BSM signal, 0 if the category is SM background