Application of Domain Adaptation Techniques for Classifying Particles Basing On the Data From ALICE Experiments

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Abstract. One of the main elements of each high-energy physics experiment in ALICE collaboration is the identification of particles that arise during the collisions in the Large Hadron Collider. The particles must be marked with high purity, as it decides about usability of a classification in further analysis. The current methods used by physicists are based on linear classifiers and require manual calibration for new data. Therein work introduces a new method of particle classification which is based on novel domain adaptation techniques. Those methods were mostly used in natural language processing and computer vision so far but the work proves that they can also be successfully applied to the realm of high-energy physics. Proposed techniques employ unsupervised methods of domain adaptation which are based on two sources of data - the labeled source domain and unlabeled target domain. In the case of the ALICE experiment, the first dataset consists of the data from virtual simulations, and the second one is made out of data from real hadron colliders. Within the work, the six different domain adaptation models were successfully implemented and compared. Each of them improves the quality of classification compared to the machine learning models which does not imply domain adaptation. In the further part of the paper, the method for the identification of unadapted particles based on machine learning algorithms is proposed. Verification of such elements makes a way for understanding the nature of particles that couldn't be adapted correctly and is the necessary step before future inventions of a new method of classifying particles in the Large Hadron Collider.

Keywords: domain adaptation · machine learning · classification · low-mass dielectrons · heavy-ion collisions · particles identification.

1 Introduction

High energy physics is also called elementary physics and is a field of study which focuses on examining the properties of matter in extreme circumstances. The experiments are performed to better understand the creation of the Universe and its structure.

Because of the scale of the research, it can only be done indirectly with the use of complex detectors thanks to which the physicists can confirm or reject theoretical models. Among many experiments made in that area, some of them focus on the identification and analysis of elementary particles and are based on the data from detectors during beam collisions.

The machine which enables to recreate light speed collisions of the particles is called the Large Hadron Collider (LHC) [1]. It is located between Switzerland and France and belongs to the European Organization for Nuclear Research (CERN). The experiments made in LHC aim to better understand elementary particles. In particular, physicists try to confirm the existence of Higgs Boson [2] and a black matter [3].

One of the main experiments which use data from LHC detectors is A Large Ion Collider Experiment (ALICE). Its main task is to examine collisions of heavy ions and arising during the experiment Quark-Gluon Plasma (QGP) [4], which is the state of the matter directly after the Big Bang [5].

The examination of QGP consists of two main phases - identifying the particles created during the collisions and tracking their flight. The most descriptive detectors which enable classification are Time of Flight (TOF) [6] and Time Projection Chamber (TPC) [7]. After a successful distinction of the particles, further analysis can be made.

The data in the ALICE experiment derives from two sources. The production data comes from the readings of the detectors during the real experiment in LHC and does not include information about particle types. However, the simulation data comes from physical simulations which are made for all of the experiments and includes information about particle type.

Due to some simplifications, noise, and inaccuracies of simulating tools the distribution of the simulation data diverges from the original one.

2 Related works

Currently, the main method used for particle classification is simple linear classifiers, in which cutoff points are adjusted manually. Such classifiers are made by splitting the production data into smaller subsets basing on the values of particle momentum. For small momentum, the values of TOF and TPC signals can be represented as values derived from the normal distribution, which is unique for each particle type. The distributions are disjoint so an experienced physicist can easily build the linear models by manually adjusting a certain standard deviation, above which a particular data point will be classified as noise.

The downside of this method is that it requires a manual adjustment of parameters fit, which slows down the work of the physicists. What's more, in the case of classifiers based on linear models, identification of the particles with a higher value of momentum is almost impossible because of superimposing distributions of the signals.

Another approach is to build a non-linear classifier that would be automatically trained on simulation data and applied to the production one. The problem which occurs in those techniques is a difference between the distribution of the attributes in two datasets. The classical deep learning methods such as Support-Vector Machine or Deep Neural Networks are sensitive for the probes whose attributes values lie outside of the training dataset distributions.

The most recent studies were focused on techniques utilizing unsupervised domain adaptation [8]. Those methods use production and simulation data during the training taking into account the shift between their distributions. So far, this approach seems to be the most promising as it is robust to the downsides of the two preceding techniques and improves the classification of production data [9]. The field of domain adaptation in high-energy physics is still not precisely explored and will be the main focus of current work.

3 Domain Adaptation

Domain adaptation is a group of Machine Learning techniques, which allows for addressing problems connected with decreasing accuracy of the model, when the testing data has different distribution than the training one. It finds wide applications in natural language processing [10, 11] and computer vision [12, 13]. However, in the domain of High Energy Physics (HEP) [14], its application was restricted only to analyses [15]. In ALICE collaboration we believe that HEP could also become a field in which the results of domain adaptation techniques will result in clearly visible benefits.

Among Domain Adaptation (DA) techniques we can differentiate unsupervised methods, which base on two streams of data - data from the source domain, which is labeled and data from the target domain, which is unlabeled. The model aims to create a function that maps source domain distribution into the distribution of the target domain. The classical example of a domain adaptation is a classification made on SVHN [16] and MNIST [17] datasets. MNIST consists of monochromatic scans of handwritten digits, while SVHN is made from colorful photos of house numbers. Those datasets have identical class labels, but different distributions of features. One possible way of translation to the new artificial space is by retrieving similar features from both domains. It is usually done by minimizing a divergence metric which was implemented in models like WDGRL, DAN or JAN [18–20]. Models like CDAN or DANN [21, 22] focus on confusing a domain discriminator to learn domain invariant features. Combination of both methods was implemented in MDD model [23].

The architecture of the first group of models brings to mind Generative Adversarial Networks (GANs) [24], which pioneered adversarial learning and successfully implemented it for generative modeling. GANs constitute two networks in a two-player game: a generator that captures data distribution and a discriminator that distinguishes between generated samples and real data. The networks are trained in a minimax paradigm such that the generator is learned to fool the discriminator while the discriminator struggles not to be fooled. The architecture of adversarial domain adaptation models is analogous. They consist of a source domain classifier, which task is to classify elements from a labeled dataset and is a substitute for a generator. Alternative for discriminator in DA model is domain classifier which predicts an element's domain. Another group of domain adaptation techniques aims to minimize a divergence metric for example a Maximum Mean Discrepancy (MMD) [23]. The minimization is usually done on the fully connected layers of deep networks and aligns distributions of two domains.

Unfortunately, both methods have their drawbacks. In the case of adversarial learning, several works [25, 21] claimed that there is no guarantee that the two domains will be aligned even if the domain discriminator is fully confused, which is caused by the equilibrium challenge [25, 21]. On the other hand, almost all of the existing approaches based on minimizing a metric, work on leveraging the very few off-the-shelf metrics, e.g., MMD, KL-divergence, and H-divergence [29], more effectively. Because of that a method raised which not only implements the conventional metrics but also alleviates the equilibrium challenge in adversarial learning. Those types of methods are a combination of both previously mentioned approaches.

4 Evaluating Models

Validation Method. To validate the domain adaptation models, the quality of classification should be measured on the target domain. Unfortunately, the production data from the ALICE detector does not contain labels, which disables direct evaluation of the models.

After a closer look at the distribution of attributes in the source and target domains, we can notice that the production data contains additional noise, which smoothens their distribution.

To simulate this phenomenon, we created a new dataset which is normalized data from simulations with an extra noise from a normal distribution N(0, 0.005). Simultaneously, a new dataset includes particle labels, which enables model evaluation.

As it can be seen, the distribution shift between the new dataset and simulation data is similar to the difference between production and simulation data. In regard to that fact, we can assume that improvement of the classification on perturbed data will positively influence the classification of the production data. The attributes distribution of the three datasets are shown in the figure Fig. 1.

Validation Results. To be able to adjust the cutoff point after which a particle is assigned to a certain class it was decided to create a separate binary classifier for each type of a particles. It facilitates to obtain classifiers with expected purity. Due to that, the four different models (one for each particle type) were created for each type of domain adaptation technique.

In the Table 1 we can see the Area Under Precision Recall (AUC) [30] for each model which shows the tradeoff between precision and recall for different threshold. A high area under the curve represents both high recall and high precision, where high precision relates to a low false positive rate, and high recall relates to a low false negative rate. The last column represents mean from four

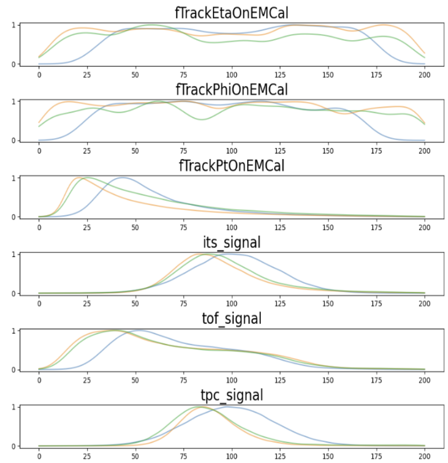

Fig. 1. Distribution of model's input attributes. The green line marks distribution of production dataset, the yellow - simulation dataset and blue - perturbed dataset.

preceding columns. The model named 'Source' is a classifier without a domain adaptation, trained only on source domain.

As we can see in the table, electrons and pions are easily distinguishable from the rest of the particles. The validation metric for each of the models equals around 0.98, which is a satisfying score. What should also be noticed in the case of the first two particle types is that domain adaptation hardly improves classification quality. For the Electrons Source model the area under precision-recall equals 0.98, while any other model with domain adaptation does not score much above that value. Some of them, especially DANN are even significantly worse. For the Pions, each domain adaptation model brings a value. In that case, the score for Source classifier equals 0.97, while for DAN, which is the best model, it is 0.99. Classification of Protons and Kaons is much more challenging, as the validation metrics have much lower values. However, in case of those particles domain adaptation significantly improves a quality of the models. The scores for Protons and Kaons Source models are 0.59 and 0.10. While the best values obtained for those particles by classifiers which take into account the distribution shifts are respectively 0.77 and 0.32. What's more, each model with adaptation seems to improve the classification.

Classification vs Adaptation Quality. To find out if higher adaptation quality always improves the classification, the AUC for particle classifier was compared with the metric describing adaptation. To measure adaptation quality the metric which equals to (1 - A) was used. In that case A is the AUC of a classifier (e.g. kernel SVM) trained on the binary problem of discriminating the source and target. Greater A means easier distinction between two domains, which is

Table 1. Area Under Precision-Recall Scores for Each Model.

Model Name	Electrons	Pions	Protons	Kaons	Mean
Source	0.98	0.97	0.59	0.10	0.66
MDD	0.98	0.97	0.63	0.10	0.67
JAN	0.97	0.96	0.70	0.17	0.70
DANN	0.93	0.98	0.67	0.25	0.71
WDGRL	0.98	0.98	0.73	0.21	0.72
CDAN	0.96	0.99	0.69	0.28	0.73
DAN	0.98	0.99	0.77	0.32	0.77

indication of low adaptation quality. It was decided to use 1 - A, as a greater value of that metric means better adaptation and it is more intuitive.

The results of such comparison were visualized at the Fig. 2. Each plot describes models for particular particle type (protons, kaons, pions or electrons) while points at each plot marks the results for particular model (cdan, dan etc.). As it can be deduced from the picture, in case of protons and kaons, the quality of the classification seems to increase with the quality of adaptation up to certain point and then it decreases. For the pions it is hard to notice any particular relationship, as the classification AUCs for most of the models are in tight range and the quality of the classification is rather not dependent on the quality of adaptation. However, for the electrons, adaptation has negative or no influence for the classification, as the models with the lowest adaptation quality (source, wdgrl) result with similar or even better classification quality than the rest of the models which adaptation quality is significantly higher.

From above comparison it can be concluded that the domain adaptation improves quality of the models if the classification of certain particle is relatively hard, which is in case of protons and kaons. The classification AUC for models (without adaptation) of those particles is consecutively 0.59 and 0.10. Whats more, the higher adaptation quality doesn't always yield higher classification quality, as the mdd model which adapts the domain the most precisely returns comparatively weak results. For the electrons and pions which classification AUC for the models without adaptation is 0.98 and 0.97, domain adaptation doesn't influence or even compounds the quality of the classification.

5 Identifying Unadapted Particles

As the purpose of the work is to not only implement certain domain adaptation models but also to understand their limitations in case of particles identification, the data points which were not properly adapted are identified.

Visualization of Domain Adaptation. First, to better understand the nature of domain adaptation, the 2-dimensional UMAP embedding [26] of the output from the Feature Extractor for the model with and without domain

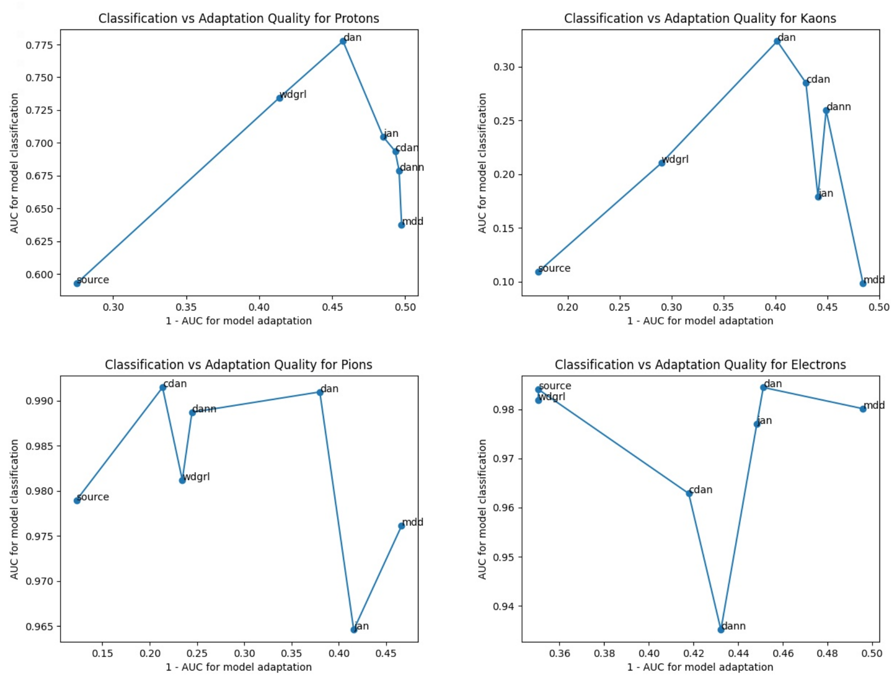

Fig. 2. Comparison of classification and adaptation quality for each particle type.

adaptation is visualized in the Fig. 3. The particles from the source domain were marked as red and particles from the target domain as blue.

We can perceive those embeddings as a visual representation of the features on top of which the classification is made. The embedding from a model without domain adaptation consists of many unicolor segments, which indicates that it could distinguish between domains so that Domain Discriminator would be capable of classifying a particle's domain. In that, it may be assumed that the part of the deep neural network which is responsible for particle classification would use predicates that characterizes only the source domain. Because of that, the model would not be able to correctly classify particles from the target domain.

The colors at the picture with embedding from a model with domain adaptation are rather precisely tossed, which means that the domain of a particle will be hard to classify. Thanks to that, the features used for classification should be common for both domains and the classification of the target domain should be correct.

Identification of Unadapted Particles. To understand what types of particles are not adapted correctly they need to be identified before. To that end, a new dataset which is a multidimensional representation of attributes used for classification has been created. In practice, it is an output vector from the part

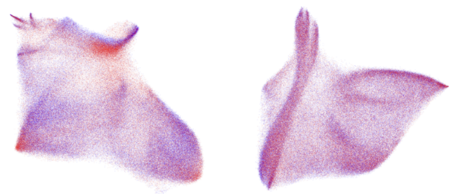

Fig. 3. UMAP embeddings of the output from Feature Extractor. The left picture presents the result for the model without adaptation, while right picture is an embedding for the model with adaptation. Red color marks particles from source domain while the blue marks particles form target domain.

of the model which is responsible for creating features. Having such representation the data points were clustered into segments with similar characteristics. It was decided to use Kohonen's Self-Organizing Maps algorithm [27] for that task, as it is robust for data with numerous dimensions. Then, the Fréchet Inception Distance (FID) [28] between particles from different domains was calculated. The FID was originally created to assess the quality of images created by the generator of a generative adversarial network (GAN) and it compares the distribution of generated images with the distribution of real images that were used to train the generator. Notwithstanding that the FID was originally destined for GANs it can be successfully applied to DA problems, as they are similar. The clusters with the highest value of that metric are the ones in which the distribution of source and target attributes differs the most and can be considered as unadapted.

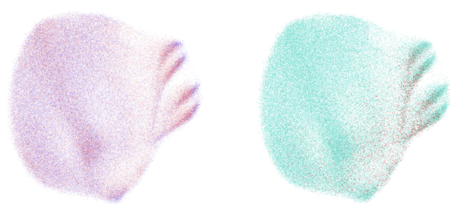

Fig. 4. UMAP embeddings of the output from Feature Extractor of a model with domain adaptation. At the left picture colors indicate a domain. At the right picture the red color marks particles marked as unadapted and a green color marks a rest.

To assure that the given method works correctly the unadapted particles are marked at the Fig. 4. which represents UMAP embeddings of the output from Feature Extractor of a model with domain adaptation. At the left picture colors indicate a domain while at the right picture the red color marks particles marked as unadapted and a green color marks a rest. By comparing those pictures it can be deduced that the parts which are marked as unadapted on the right picture, are the parts that mostly consist of unicolor particles at the left picture.

6 Conclusion

In this paper, it was proved that the usage of novel domain adaptation techniques can be applied in the field of high-energy physics. Six different domain adaptation models were successfully implemented, from which two were based on the concept of adversarial training, three on minimization of divergence metric and one was the combination of both methods. In case of some particles the quality of the classification have been improved significantly which proves that the approach for classification is appropriate and that domain adaptation techniques can be also applied for other domains than Image Recognition or Neural Language Processing, which may be breakthrough for some fields of study.

The experiments conducted during this work have also proved that using domain adaptation techniques does not always improves the classification. It was advantageous only in case of particles which classification was relatively hard for the model without domain adaptation. Whats more it was proved that better quality of domain adaptation doesn't always yields better classification, because the models which were capable of high adaptation quality returned comparatively weak results.

Also, a new method based on machine learning algorithms that enable to mark unadapted particles was proposed. Identification of such elements makes a way for understanding the nature of particles that couldn't be classified correctly and is the compulsory step before creating a new method of classifying particles in the Large Hadron Collider.

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