Machine Learning as a Service for HEP

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Abstract. Machine Learning (ML) will play a significant role in success of the upcoming High-Luminosity LHC (HL-LHC) program at CERN. The unprecedented amount of data at the Exa-Byte scale to be collected by the CERN experiments in the next decade will require a novel approach to train and use ML models. In this paper we discuss Machine Learning as a Service (MLaaS) model which is capable of reading HEP data in their native ROOT data format, relying on the World-Wide LHC Grid (WLCG) infrastructure for remote data access, and serving a pre-trained model via HTTP protocol. Such modular design opens up a possibility to train data at large scale by reading ROOT files from remote storages, avoiding data-transformation to flatten data formats currently used by ML frameworks, and easily access pre-trained ML models in existing infrastructure and applications.

1 Introduction

With the CERN LHC program underway, we started seeing an exponential acceleration of data growths in High-Energy Physics (HEP) field. By the end of Run II, the CERN experiments were already operating in the petabyte (PB) regime, producing $O(100)$PB of data each year. And, the new HL-LHC program will bring us to the Exa-Byte scale. The usage of Machine Learning in the HEP is on the rise too. It has been successfully used in online, offline reconstruction programs, and there is huge interest to apply it for detector simulation, object reconstruction, identification, MC generation, and beyond \cite{1}. But the main obstacle of using ML frameworks and bringing CS expertise in ML to HEP lies in differences of data-structures used by ML practitioners and HEP users. In particular, the former mostly rely on flat-format data representation, e.g. CSV or NumPy data formats, while HEP data are stored in tree-based data-structures used by ROOT \cite{2} data-format. As was pointed out in HEP ML Community White Paper \cite{1}, the usage of ROOT data-format outside of HEP practically does not exists. This fact creates an artificial gap between ML and HEP communities. The recent kaggle challenges, e.g. ATLAS for identification of Higgs boson \cite{3} and the cross-experiment tracking ML challenge \cite{4}, were specifically adopted (in terms of input datasets) and presented to ML competitors in CSV data format. But, within the HEP community these datasets are easily accessible, without any pre-processing or transformation in the ROOT data-format. To close this gap, we present in this paper a novel approach to use HEP ROOT data natively for training purposes, reading ROOT files from remote storages via XrootD, and presenting pre-trained models as a service accessible via HTTP protocol. Such Machine Learning as a Service (MLaaS) modular design opens up a possibility to train ML models on

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PB datasets remotely accessible from the Worldwide LHC Computing GRID (WLCG) sites without requiring data transformation and data locality.

2 Related work and solutions

Machine Learning as a Service is a well known concept in industry, and major IT companies offer these solutions to their customers. For example, Amazon ML, Microsoft Azure ML Studio, Google Prediction API and ML engine, and IBM Watson are good examples of MLaaS, see [5]. Usually, MLaaS is used as an umbrella of various ML tasks such as data preprocessing, model training and evaluation, and prediction results can be accessed by clients through REST APIs. Even though they can provide very good results and interfaces, most of the time these services are designed to cover standard use-cases. For instance, data are expected to be fed in flat based data formats. All data preprocessing operations are performed automatically where a concrete service identifies which fields are categorical and which are numerical, and it does not ask a user to choose the methods of further data preprocessing. The model predictions are limited to well-established patterns, such as binary classifications, multi-class classifications, and regressions. Although quite often MLaaS service providers offer pre-defined models that can be used to cover standard use-cases, e.g. image classifications, etc. Obviously, all them are designed to make a profit by charging customers on the amount of predictions they want to make, or use tiered structure on the amount of calls placed by clients.

In HEP, usage of these services is quite limited though for several reasons. Among them, the HEP ROOT data-format can’t be used directly in any of these services, and pre-processing operations may be more complex than offered by service providers. For instance, the two HEP kaggle challenges [3, 4] used custom HEP metrics for evaluation procedure which is not available in out-of-the box industry solutions, and ML workflow in both competitions is far from trivial, e.g. the pre-processing step required writing custom code to include event selection and perform other steps. Therefore, after rounds of evaluations we found that provided solutions most often are ineffective for HEP use-cases (cost and functionality-wise), even though the CERN OpenLab initiative and others continue close cooperation with almost all aforementioned service providers.

At the same time, various R&D activities within HEP is underway. For example: hls4ml project [6] targets ML inference in FPGAs, while SonicCMS project [7] is designed as Services for Optimal Network Inference on Coprocessors. Both are designed for optimization of inference phase rather than targeting the whole ML pipeline from reading data, to training and serving predictions. At the moment we are unaware of any final product which can be used as MLaaS in HEP. The novelty of the proposed solution is three fold. First, we are proposing to use HEP ROOT files directly, either using them locally or remotely, without requiring data transformation operations to flat data format. Second, the training layer can use external 3rd party ML frameworks, from well established ML, e.g. scikit-learn, libraries to Deep-Learning (DL) frameworks such as TensorFlow, PyTorch and others. Third the inference phase is provided via RESTful APIs of TensorFlow as a Service (TFaaS) similar to industry solutions. The latter does not require significant changes of existing HEP infrastructures, frameworks and applications due to usage of HTTP protocol between clients and TFaaS server(s).

3 MLaaS architecture

A typical ML workflow consists of several steps: acquire the data necessary for training, use ML framework to train the model, and utilize the trained model for predictions. This
Figure 1. MLaaS architecture diagram representing three independent layers: data streaming layer to read local or remote ROOT files, a data training layer to feed Tree based HEP data into ML framework, and data inference layer via TensorFlow as a Service.

The workflow can be further abstracted as data streaming, data training, and inference phases. Each of these steps can be either tightly integrated into application design or composed and used individually. The choice is mostly driven by particular use cases. In HEP we can define these layers as following, see Fig. 1:

- **Data Streaming Layer** is responsible for reading local and/or remote ROOT files, and streaming data batches upstream to the Data Training Layer. The implementation of this layer requires ROOT I/O layer with support of remote I/O file access;

- **Data Training Layer** represents a thin wrapper around standard ML libraries such as TensorFlow, PyTorch, and others. It reads data from the Data Streaming Layer in chunks, transforms them from ROOT TTree based representation to the format suitable for underlying ML framework and uses it for training purposes;

- **Data Inference Layer** refers to the inference part of pre-trained models and can be either tightly integrated within underlying HEP framework or represented as a Service (aaS).

Even though the implementation of these layers can differ from one experiment to another (or other scientific domains/fields using ROOT files), it can be easily generalized and be part...
of the foundation for generic MLaaS framework. Further, we will discuss individual layers and outline particular sets of problems which should be addressed in their implementation.

3.1 Data Streaming Layer

The data streaming layer represents a simple task of streaming data from local or remote data storages. Originally reading ROOT files was mostly possible from C++ frameworks, but recent development of ROOT I/O now allows to easily access ROOT data from Python, and use XrootD protocol for remote file access. The main development was done in uproot \[8\] framework backed by the DIANA-HEP initiative \[9\]. The uproot library uses NumPy \[10\] calls to rapidly cast data blocks in the ROOT file as NumPy arrays, and provides integration with the XrootD protocol \[11\]. Among the implemented features it allows a partial reading of ROOT TBranches, non-flat TTrees, non TTrees histograms and more. It relies on data caching and parallel processing to achieve high throughput. In our benchmarks we were able to read HEP events at the level of $\sim O(100) - O(1000)\text{kHz}$ from local and from remote storages\[1\].

In our implementation of MLaaS, see Sect. 3.4, this layer was composed as a Data Generator which is capable of reading either local or remote file(s) with a pre-defined size. The batch data size can be easily fine tuned based on the complexity of the event and available bandwidth. The output of the Data Generator was a NumPy array with flat and Jagged Array attributes, see next Section for further discussion.

3.2 Data Training Layer

This layer is required to encapsulate HEP data and present it into ML to be used by the application. The main obstacle here is usage of non-flat representation of HEP data in ML frameworks. In particular, the ROOT data-format can be represented in so called Jagged Arrays\[2\] see Fig. 2. The HEP tree-based data representation is optimized for data storage but it is not directly suitable for ML frameworks. Therefore a certain data transformation is required to feed tree-based data structures into ML framework as flat data structure. We explored two possible transformation: a vector representation with padded values, see Fig. 3 and matrix representation into one of the multiple phase spaces, see Fig. 4.

\[1\] Speed varies based on many factors, including caching, type of storage and network bandwidth.

\[2\] Jagged Array is an array of arrays of which the member arrays can be of different sizes.
The idea of the vector representation approach is to identify a dimensionality of Jagged Array attributes in a vector via one time pass across the data, and the subsequent composition of the final vector with sufficient allocation for Jagged Array attribute values based on their dimensionality. If a certain event will have Jagged Array attribute shorter then its dimensionality a padded values can be used. For instance, a physics event is composed by a set of particles. A priori we may not know how many particles can be created in an event, and therefore we don’t know how much space we need to allocate for particle attributes even though their attributes have a fixed size, e.g. particle momentum values can be represented by three numerical values \((p_x, p_y, p_z)\). However, knowing the distributions of the particles in all events of certain physics dataset can allow us to choose the dimensionality of their Jagged Array attributes. For instance, we can run MC process and identify how many electrons per even we may have. A maximum number of electrons in this distribution will represent a dimensionality for corresponding Jagged Array attributes. Using these dimensionality numbers we can represent an event as a flat vector of certain size. The allocated values of Jagged Array attributes will vary event by event where extra slots of Jagged Array attributes will be filled with pre-defined pad values, e.g. NaN\(^3\). Additionally, the one time pass across a series of events can be used to determine the min, max, and mean values of jagged array attributes which can be later used for normalization purposes.

The matrix representation of Jagged Array, see Fig. 4, can use certain phase space if it is present in a dataset. For example, the spatial coordinates or attribute components are often part of HEP datasets, and therefore can be used for Jagged Array mappings. This approach can resolve the ambiguity of vector representation (in terms of dimensionality choice) but it has its own problem with the choice of granularity of a phase space matrix. For example, if the X-Y phase space (where X and Y refers to an arbitrary pair of attributes) will be used in matrix presentation we don’t know a cell size in this space. A choice of matrix granularity may introduce a collision problem with Jagged Array attribute values, e.g. if two particles have the same phase space values of the cell, i.e. two particles point into the same cell in X-Y space. Such ambiguity may be easily resolved either by reducing matrix granularity or adding other phase space, e.g. using matrices in X-Y, Y-Z and X-Z phase spaces and concatenate

\(^3\)Since all numerical values can be used, e.g. in case of an angle distribution we may have negative, positive and zero values, the only choice for padded values we have will be NaN.
them together into a final vector. But such enhancement will increase the sparsity of the final matrix and therefore will require more resources at the training time.

In our prototype, discussed in Sect. 3.4, we used vector representation with padded values and applied two pass procedure over the data. The first pass read data streams and determined dimensionality of Jagged Arrays along with min, max, and mean values used for normalization. The second pass was used for reading and transforming data from the streaming layer to the underlying ML framework.

In Neural Network models it is natural to assign padded NaN values to zeros since they are used in the multiplication operations between input values and weight matrix elements. But knowledge of locations of padded values in vector representation approach may be valuable in certain circumstances. For instance, when training AutoEncoder networks the knowledge of locations of padded values in input vector can be used at a decoding phase. Therefore our initial implementation of vector representation, discussed in Sect. 3.4, used additional mask vector to preserve the knowledge of padded values locations.

3.3 Data Inference Layer

A choice of a data inference layer should be driven by the usage of underlying technology, e.g. ML framework. It can be either tightly integrated with application frameworks (both CMS and ATLAS experiments followed this approach in their CMSSW-DNN [12] and LTNN [13] solutions) or it can be developed as a Service (aaS) solution. The former has the advantage of reducing latency of the inference step per processing event, but later can be easily generalized and become independent from the internal infrastructure. As such, it can be easily integrated into cloud platforms, be used as repository of pre-trained models, and serve models across experiment boundaries. We decided to implement the latter solution via TensorFlow as a Service (TFaaS) architecture, see [15].

We evaluated several ML frameworks and decided to use TensorFlow [16] graphs for the inference phase. The TF model represents a computational graph in a static form, i.e. the mathematical computations, graph edges and data flow are well-defined at run time. Reading TF model can be done in different programming languages due to support of APIs provided

Figure 4. A matrix representation of Jagged Array into certain phase space, e.g. eta-phi.
by TF library. Moreover, the TF graphs are very well optimized for GPUs and TPUs. We chose the Go programming language to implement the Tensor Flow as a Service (TFaaS) [15] part of MLaaS framework based on the following factors: the Go language natively supports concurrency via goroutines and channels, it is the language developed and used by Google and very well integrated with TF library, it provides a final static executable which significantly simplifies its deployment on premises and to various (cloud) service providers. We also opted out in favor of REST interface where clients may upload their TF models to the TFaaS server and use it for their inference needs via the same interface. Both Python and C++ clients were developed on top of the REST APIs (end-points) and other clients can be easily developed thanks to HTTP protocol used by the TFaaS Go RESTful implementation.

We performed several benchmarks using TFaaS server running on CentOS 7 Linux, 16 cores, 30GB of RAM. The benchmarks were done in two modes: using 1000 calls with 100 concurrent clients and 5000 calls with 200 concurrent clients. We tested both JSON and ProtoBuf data format while sending and fetching the data to/from TFaaS server. In both scenarios we achieved a throughput of $\sim 500 \text{ req/sec}$. These numbers were obtained with serving mid-size pre-trained model which consists of 1024x1024 hidden layers.

Even though a single TFaaS server may not be as efficient as an integrated solution it can be easily horizontally scaled, e.g. using kubernetes or other cluster solutions, and may provide desire throughput for concurrent clients. It also decouples application layer/framework from the inference phase which can be easily integrated into any existing infrastructure by using HTTP protocol to TFaaS server for inference results. Also, the TFaaS can be used as a repository of pre-trained model which can be easily shared across experiment boundaries or domains. For instance, the current implementation of TFaaS allows visual inspection of uploaded models, versioning, tagging, etc. A simple search engine can be put on top of TFaaS with little effort. For full list of planned improvements see Sect. 4.

### 3.4 Proof-of-concept prototype

When all layers of the MLaaS framework were developed, we composed a working prototype of the system by using ROOT files accessible through XrootD servers. The data were read by 1000 event batches, where single batch was approximately 4MB in size. Each batch was fed into both Tensor Flow (implemented via Keras framework) and PyTorch models. The Data Generator representing data streaming layer yields a vector representation of Jagged Array ROOT data structures along with mask vector representing positions of padded values, see Fig. 5 into corresponding model. This was done to avoid misinterpretation of real values of attributes from padded values. This mask vector was used in both models to cast NaN values...
to zeros. We tested this prototype on a local machine as well as successfully deploying it on the GPU node.

The implementation of data streaming and data training layers was done in python. The workflow consisted of running python scripts for reading the data, training ML models, and uploading them into TFaaS server via HTTP protocol. The prediction was served to python, C++, and curl clients. The further details of this proof-of-concept prototype can be found in the MLaaS4HEP github repository [20].

4 Future directions

We foresee that MLaaS approach can be widely applicable in HEP. As such, further improvements will be necessary to achieve and implement.

4.1 Data Streaming Layer

In a Data Streaming Layer we plan to introduce proper data shuffling. It should be done carefully when reading data from multiple remote ROOT files. Current implementation of MLaaS reads data sequentially from file to file and feeds the data batches directly to ML framework. In order to implement proper data shuffling a reading parallelism should be introduced into MLaaS framework. We also need to look at further optimization of the streaming layer to achieve better throughput from remote data-providers.

4.2 Data Training Layer

The current landscape of ML framework is changing rapidly, and we should be adapting MLaaS to existing and future ML framework and innovations. For instance, Open Network Exchange Format [17] open up a door to migration of models from one framework into another. So far we are working on automatic transformation of PyTorch [18] and fast.ai [19] models into TensorFlow which is used by the TFaaS service.

As discussed in Sect. [3.2] there are different approaches to feed Jagged Array into ML framework and R&D in this direction is in progress. For instance, for AutoEncoder (AE) models the vector representation with padded values should always keep around a cast vector since AE model transform input vector into an internal dense representation and then should decode it back into original representation. The latter transformation can use cast vector to assign back the padded values, and if necessary convert vector representation of the data back to Jagged Array or ROOT TTtree data-structures.

4.3 Data Inference Layer

On the inference side (TFaaS) we plan to extend the "aaS" part to become a repository of uploaded models. As such, several functionalities should be added, such as search capabilities, extended model tagging, and versioning. It can be easily achieved by adding proper meta-data description of uploaded models and storing it into a back-end database for later look-up, indexing and versioning.

4.4 MLaaS services

The proposed architecture allows to develop and deploy training and inference layers as independent MLaaS services where separate resource providers can be used and dynamically scaled if necessary, e.g. GPUs/TPUs can be provisioned on demand using commercial
cloud(s) for training purposes of specific models, while inference TFaaS service can reside at CERN premises. For instance, the continuous training of complex DL models would be possible when data produced by the experiment will be placed on the GRID sites, and the training MLaaS service will receive a set of notifications about newly available data, and re-train specific model(s). When new model is ready it can be easily pushed to TFaaS and be available for end-users immediately without any intervention on the existing infrastructure. The TFaaS can be further optimized to use FPGAs to speed up the inference phase. We foresee that such approach may be more flexible and cost effective for HEP experiments in HL-LHC era. As such, we plan to perform additional R&D studies in this direction and evaluate further MLaaS services using available resources.

5 Summary

In this paper we presented a novel Machine Learning as a Service approach to training ML models using native ROOT format of HEP data. It consists of three layers: data streaming, training, and inference layers, which were implemented as independent components. The data streaming layer relies on the uproot library for reading data from ROOT files (local or remote) and yielding NumPy (Jagged) arrays upstream. The data training layer transforms the input Jagged Array portion of the data into vector representation and passes it into ML framework of user choice. Finally, the inference layer was implemented as an independent service (TFaaS) to serve a TensorFlow models via HTTP interface. Such flexible architecture allows to perform ML training over HEP ROOT data without physically downloading data into a local storage. It reads and transforms ROOT Tree data representation (Jagged Array) into intermediate flat data format suitable as an input for underlying ML framework. A prototype proof-of-concept system was developed to demonstrate MLaaS capabilities to read arbitrary size datasets, and potentially allow to train HEP ML models over large datasets at any scale.

This work was done as a part of CMS experiment R&D program. I would like to thank Jim Pivarski for his numerous and helpful discussions and hard work on uproot (and many other) packages which open up a possibility to implement MLaaS.

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