HEPDrone: a toolkit for the mass application of machine learning in High Energy Physics

Sean Benson\textsuperscript{a}, Konstantin Gizdov\textsuperscript{b}

\textsuperscript{a}Nikhef National Institute for Subatomic Physics, Amsterdam, The Netherlands
\textsuperscript{b}School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom

Abstract

Machine learning has proven to be an indispensable tool in the selection of interesting events in high energy physics. Such technologies will become increasingly important as detector upgrades are introduced and data rates increase by orders of magnitude. We propose a toolkit to enable the creation of a drone classifier from any machine learning classifier, such that different classifiers may be standardised into a single form and executed in parallel. We demonstrate the capability of the drone neural network to learn the required properties of the input neural network without the use of any training data, only using appropriate questioning of the input neural network.

1. Introduction

Data collection rates in high energy physics (HEP), particularly those at the Large Hadron Collider (LHC) are a continuing challenge and require large amounts of computing power to handle. For example, the LHCb experiment \cite{1} at the LHC processes an event rate of 1 MHz in a software based trigger \cite{2}. The purpose of this trigger is to reduce the output data rate to manageable levels, \textit{i.e.} to fit in the available storage resources offline. This amounts to a reduction from 60 GB per second to an output data rate of 0.6 GB per second.

In order to accomplish such a remarkable real-time data reduction in the software based trigger, novel ideas have been introduced, such as the real-time alignment and calibration of the detector \cite{3}, in addition to the concept of real-time analysis \cite{4}, whereby a subset of the particles from the proton collisions need only be saved, and not the detector raw data.

Machine learning (ML) is becoming an evermore important tool in the data reduction, be it with the identification of interesting event topologies, or the distinction between individual particle species. For the case of LHCb data-taking, over 600 unique signatures are searched for in parallel in real time, each with its own set of requirements. However only a handful at present make use of machine learning.

A large ecosystem is available to analysts in the creation of machine learning classifiers, the TMVA \cite{5} and Neurobayes \cite{6} tools being among the most widely used. More recent examples gaining popularity include Scikit-Learn \cite{7} and Keras \cite{8}. It has been proven in many analyses of LHCb data that ML classifiers are better able to account for differences in the correlations between training variables that are seen in signal and background events, enabling more powerful data reduction. Despite this, the majority of the identification of interesting topologies is performed without the use of ML classifiers. Often the reason for this is the relative difficulty in the application of a preferred ML classifier to the C++/Python combination of event selection frameworks \cite{9}. Another reason is the required algorithm speed. Methods such as Bonsai Boosted Decision Trees (BBDTs) \cite{10} have been implemented in LHCb in order to enable the quick evaluation of models. The BBDT approach relies on the discretization of inputs such that all possible combinations along with the associated classifier response is known before the model is evaluated. One potential drawback of the BBDT approach is that the number of input variables is limited in order to limit the number of possible combinations.

We present in this article a package that allows an analyst to train a drone neural network that learns the important features of a given ML learning classifier from any chosen package such as SciKit-Learn. The resulting parameters are then fed into a C++ algorithm that performs execution in HEP production environments. The details of the drone training are provided in Sec. 2. This is followed by a real example using simulated data in Sec. 3. The advantages of the approach are discussed in Sec. 4.

2. Drone learning

The training of the drone network requires that the original network is extensively probed in the parameter space in which accuracy is desired. The principle utilised in the training of the drone is that sufficient approximation of the original network is achieved with sufficient expansion of the hyperparameter space of the drone, and that the same global minimum of the loss function can be found, as reported in Ref. \cite{11}.

2.1. Initial drone structure and corresponding training

The drone chosen for use in this article is initialised as a deep neural network with a single intermediate layer of 300 nodes using a standard sigmoid activation function. The network has the number of inputs determined from the number of desired characteristics of the decay signature. A single output is taken from the network and a linear model is used to relate layers.
The model is made to approximate the original classifier through a supervised learning technique, though not in the traditional sense. Instead of a label as signal or background taken from the training data, the output of the original classifier is used as a label. This means that the loss function is defined as

\[ \mathcal{L} = \sum_i (F(\vec{x}_i) - G(\vec{x}_i))^2, \]

where \( F(\vec{x}_i) \) and \( G(\vec{x}_i) \) are the outputs of the original and drone models on datapoint \( i \) of the mini-batch, respectively. The advantage of such a loss function is per-event equivalence of the original and drone model, in addition to equivalence of performance. For the drone training detailed in this article, standard mini-batch stochastic gradient descent is used. A feature of this method is that the drone classifier does not see any training data, but rather learns the same properties from the original classifier, and thus is a neural network that learns from another neural network in an empirical manner.

2.2. Model morphing during the learning phase

In order to keep the hyperparameter space to the minimum required level, additional degrees of freedom are added only when required. This removes the possibility of choosing an incorrect size of the drone network. During the learning phase, the following conditions are required to trigger the extension of the hidden layer in the \( j \)th epoch:

\[ \delta \equiv (L_j - L_{j-1})/L_j < \kappa, \]  \hspace{1cm} (2)

\[ L_j < \hat{L} - \delta L_j, \] \hspace{1cm} (3)

where \( \kappa \) is the required threshold and \( \hat{L} \) is the value of the loss function when the hidden layer was last extended.

When the conditions in eqs. 2 and 3 are met, the linear model is updated to extend the weights matrices and bias vectors to accommodate the layer addition. The associated neurons are initialised with a zero weight to ensure continuity of the loss function value.

3. High energy physics application

3.1. Data sample

In order to demonstrate the functionality of the toolkit, data samples generated from the RapidSim package [12] are used. The interesting signal is chosen to be the \( B^0 \rightarrow J/\psi(\rightarrow \mu\mu)\phi(\rightarrow KK) \) decay, and the background is the \( D^{\ast \pm} \rightarrow \pi\pi\pi\pi \) decay. A total of 10000 candidates is generated for each decay.

3.2. Training of the original classifier

The machine learning classifier chosen is the Multi-layer perceptron of SciKit-Learn, which is constructed as

\begin{verbatim}
classifier = MLPClassifier(activation='relu',
batch_size='auto', beta_1=0.9, beta_2=0.999,
early_stopping=False, epsilon=1e-08,
hidden_layer_sizes=(3, 3),
learning_rate='constant',
learning_rate_init=0.001, max_iter=200,
nesterovs_momentum=True, power_t=0.5,
random_state=1, shuffle=True,
solver='lbfgs', tol=0.0001, momentum=0.9,
validation_fraction=0.1, verbose=False,
warm_start=False, alpha=1e-05)
\end{verbatim}

The neural network is trained using kinematical properties of the respective decays. These include the pseudorapidity, \( \eta \), and momentum transverse to the direction of the input proton beams, \( p_T \), of the decaying particle. In addition, the minimum and maximum \( p_T \) and \( \eta \) of the final state particles is used. The signal and background distributions of the input variables are shown in Fig. 1.

In the training of the original classifier, half of the data is reserved in order to test for overtraining. The output probability distributions of the signal and background samples after the training are shown in Fig. 2. It can be seen that the test and training samples are in good agreement, showing that the original SciKit-Learn classifier is not significantly overtrained.

3.3. Drone conversion

The drone neural network is trained following the procedure outlined in Sec. 2. In total, 300 epochs are used with the learning rate of the stochastic gradient descent set to 0.05. The value of \( \kappa \) is chosen to be 0.02.

The loss history of the training is shown in Fig. 3 as a function of epoch number. The convergence is also shown in Fig. 4, which shows the difference in the value of the loss function with respect to the previous epoch. The epochs that triggered an increase in the number of hyperparameters are also overlaid. In total in this example, an increase was triggered 104 times. The total number of parameters in the final drone neural network is therefore 3233. It is interesting to note that with the algorithm design of Sec. 2, the introduction of the new parameter space causes the drone network to learn faster, as evidenced by increases in Fig. 4 with continuing descent of the loss function.

3.4. Drone storage and transferability

The hyperparameters and structure of the drone are required to be portable and easily stored for later usage. For this the JSON format was chosen as mediator. It is human-readable and easily accessible in the Python and C++ environments commonly used in HEP. Thus, it is readily deployable in both personal and production environments.

Provided is a tool to export and save a drone neural network to a JSON formatted file which preserves the input & output structure, the layers and nodes, all hyperparameters and activation functions. The drone configuration is later read in by an equivalent tool into the production software framework, which then constructs a class object based on the Keras model. The C++ class implements a flexible member structure that is capable of completely reproducing the original drone. The production implementation may be used for all data reduction levels, be it in the form of the LHcb high level trigger for example up to the latest stages of data handling and output. This allows for the drones to be applied using a wide range of observables and event reconstruction properties.
4. Summary

It has been demonstrated that for the case of a high energy physics event selection application, a drone neural network is able to accurately approximate and learn the features of a neural network with a different structure. The proposed algorithm design allows the drone to learn the aforementioned features without ever having access to the training data, or indeed any data, but only with appropriate questioning of the original model.

The equivalency of the outputs of the drone and original model enables an analyst to treat both the original and the drone in the same way. The creation of a drone in a standardised form permits an analyst to use any desired machine-learning package to isolate a decay signature, and from this create a classifier guaranteed to be suitable for execution in the C++ real-time data selection frameworks.

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Figure 2: Output distributions of the signal and background training and test samples from the classifier after training.

Figure 3: Convergence of the loss function during the drone training.

Figure 4: Difference in the loss function with respect to the previous iteration. The green triangles depict the epoch number in which the number of hyperparameters was increased.
Figure 5: Difference between the output response of the drone model with respect to the original classifier for data points in the test sample.