Machine Learning

Topics in Particle Physics and Astroparticles II



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Kinematic Properties

The required background levels at SHiP are of < 0.1 events over the course of the experiment.

Resources:

- PID
- Kinematic Features

Total Momentum

Transverse Momentum

Fraction of Transverse Momentum

Opening Angle

Impact Parameter

Distance of Closest Approach (DOCA)

Coordinates of the Decay Vertex

Data Analysis with Pandas

The 3rd tutorial can be found on the usual places, with the name Template Data Analysis.ipynb

This template will show you the basics on handling dataframes with pandas.

The topics covered will be the following:

- Printing the DataFrame
 - Reading Entries one at a time
 - Concatenating DataFrames
- Adding and Removing Columns
- Bulk Dataset Cuts
- Plotting Variables

Tutorial 3 - Plotting Pandas Dataframes

Drawing Plots with Matplotlib:

In order to plot datasets I use 2 different methods:

- Matplotlib Reliable and default in python. Use it to plot 2D histograms
- Seaborn My preference to compare distributions

Seaborn can take the points argument in a flexible way, as either a traditional array or as a column from a pandas: :dataframe, saving a couple of lines of code.

Matplotlib can be customized to give a TH* look from ROOT. Hence I present a 2-dimensional plot in the template.

In order to do this, we first create a figure (similar to the ROOT TCanvas). While it is not needed here, it is helpful in order to save it using matplotlib.savefig("path_to_save_to"). Afterwards we need to translate our data from the pandas dataframe to classic python lists through a loop.

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Drawing Plots with Matplotlib:

Then we just create a matplotlib::pyplot::hist2d object as follows : matplotlib.hist2d(datax, datay, bins=[binsx,binsy], cmap=plotstyle, range=[[xmin,xmax],[ymin,ymax]])

Only non-intuitive argument is **cmap**, which defines the plot style.

The last point to make is that adding a line with matplotlib.colorbar() creates the side bar with the z axis scale.

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Drawing Plots with Seaborn:

Overlapping distributions can be done through the seaborn::distplot() function : $ax = sns.distplot(x, hist_kws={"range" : [0,250]}, norm_hist = True, kde=False, label="Signal")$

x is the list of points and can be defined as x = Signal['variable'], **norm_hist** is an option to normalize the distribution to a total area of 1, **kde** gives an automatic fit to a gaussian distribution, **label** assigns a specific label to that distribution and **hist_kws** allows you to insert any options available for the matplotlib counterparts.

Drawing a second overlapping distribution is easy, as it simply requires you to utilize the previous function with a different dataset \mathbf{y} . Although this would usually overwrite most objects in python, here the new distribution \mathbf{y} is added to the previously created distplot object.

Tutorial 3 - Drawing Correlation Plots

The last part of this tutorial is related to our next project involving Machine Learning.

While doing a separation analysis you need to be aware that some variables are more correlated with each other than others, and going over features that are highly correlated in order to separate samples is not very efficient.

Pandas provides an automatic way of looking at the correlation matrix of dataframes, through the pandas::dataframe.corr() function. This method gives the pearson correlation matrix by default, but the method might be changed through a **method** option.

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Tutorial 3 - Normalizing Data

Normalizing data can be helpful in a plethora of cases. We will be performing a data normalization in order to apply machine learning methods.

We will be utilizing Pipelines, which are objects from SKLearn that take as inputs transformation functions and perform them in a pipeline.

Our pipeline contains 2 different functions.

The first is the StandardScaler, which renormalizes all of data in order to obtain a gaussian distribution with an average value of 0 and a standard deviation of 1. The second function is a Principal Component Analysis (PCA). This one transforms the data so that you get components that are as independent of each other as possible, while maximizing the variance, with the idea of reducing the amount of dimensions needed in order to represent a space, while losing the least amount of information possible.

In order to do the normalization, we just need to define a subset of our data with the features that we want to transform and utilize the pipeline.fit_transform(subset) function.

Notice that the output of this function is an array (of floats in our case since we deemed it so in the options).

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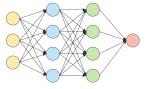
Machine Learning

Machine Learning algorithms have an advantage over traditional selection methods: They take into account multi-variable correlations in a non-trivial way.

We will be utilizing Multi-layer Perceptrons, which are feedforward Neural Networks.

Neural Networks are interconnected groups of nodes (neurons) arranged in layers, where each node processes information and passes the result on to the next layer Input layer is the first layer, that receives the data,

and has to have 1 node for each feature of the data



put layer hidden layer 1 hidden layer 2 output layer

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Output layer is the last layer, and usually has as many neurons as the classes that we are trying to classify our data into. The one exception is for binary problems, where just 1 neuron is enough (the chance of not being from a set is the maximum score possible minus the score attained, hence low scores are a measure of being of the other set)

The connections between nodes are defined by Weights that are adapted through the training phase, and each of the nodes might have a threshold or a bias. Alongside the structure of the network, the weights are what define the network

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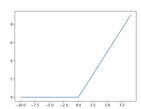
Machine Learning - Activation Functions

Each node processes the received information before transmitting it to the next layer. The biggest difference between MLPs and simple NNs is that the **Activation Functions** for MLPs are non-linear for all layers besides the first, which allows for backpropagation.

This implies that MLPs always have at least 3 layers, since all linear functions can be simplified through linear algebra in a way such that we would only need 2 layers: input and output. The layers in between these are called Hidden Layers

The more complex and bigger these hidden layers are, the longer it takes to process information. As such the activation functions need to be simple, fast to calculate and limited output ranges are preferred.

■ Rectified Linear Unit (ReLU)

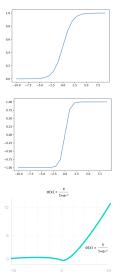


Machine Learning - Activation Functions

■ Sigmoid

■ Hiperbolic Tangent (Tanh)

Swish (x×Sigmoid)



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Machine Learning - More Basic Concepts

MLPs are NNs with Supervised Learning, which means that they train by processing examples with clearly defined inputs and results (features of the data, and we know it what is signal/noise à priori), forming a probability weighted association between the two.

This probability (weights) is updated according to a Loss-Function, which is commonly the Cross-Entropy. This is just a logarithmic function that is skewed towards correct predictions by heavily punishing incorrect predictions

$$\sum_{i} t_i \log (p(x_i)) + (1-t_i) \log (1-p(x_i))$$

Here t_i is the true value of the event i (usually 1 for signal 0 for background) and $p(x_i)$ is the probability that the MLP attributed to said event.

Since it is impossible to find the optimal value for the weights of NNs, we try to find close to optimal solutions with **Optimization Algorithms**. These are usually stochastic gradient descent algorithms.

Each time the algorithm sees the whole dataset once is called an **Epoch**, but this does not necessarily define the rate at which the **weights** are updated. That rate is known as a **Batch**.

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Machine Learning - Last Basic Concepts

The last thing to mention is that **there is** such a thing as **Overfitting**. This happens when the NN becomes so optimized for our data that it is turned obsolete when faced with new data.

In order to circumvent this there are several tools. The first one is setting aside a sample of our data that we do not use in training, but rather use to validate our training after each **epoch**, called **Validation Sample**. This way, we can let our NN run freely for as long as we want, and we can save the weights that give the best performance for the validation sample, that the NN is blind to, and as such should have no biases towards.

The second tool is varying the structure of our MLP. If the MLP is too complex for a problem, there is no avoiding overfitting our data, as it is akin to trying to use a pneumatic hammer to drive a nail.

The third tool is to try and mask information as we progress deeper into the MLP. This can be done through a function that we have already seen in Pandas: drop()). This ensures that random fractions of our data are removed, in order to try and avoid biases stemming from a high degree of omniscience.

The last thing to note is that due to all the randomness involved in ML algorithms, which can be as simple as being lucky in the early guesses of the optimization algorithms regarding the optimal solution, even while maintaining everything equal in one NN, training it several times will always yield different results, although they will never be too dissimilar provided we are constructing the Network correctly.