Searching for the Higgs Boson Particle using Data Analytics

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ABSTRACT

Physicists use accelerators such as the Large Hadron Collider (LHC) to produce new particles in order to understand the elementary structure of matter. These colliders produce different types of particles which are identical in many aspects but differ in their kinematic properties. In this project, we attempt to distinguish between those collisions that produce a particle of interest (signal) and those that produce other particles (background). This task is considered to be very difficult as conventional wisdom dictates the need for using complex parameters that are not directly observable for classification. To solve this problem, we explore a number of different techniques and evaluate these techniques in terms of accuracy and throughput. Our best classifiers outperform the state-of-the-art [3] by over 2% in terms of accuracy. We also provide a qualitative discussion on the possible trade-offs for different techniques.

1. INTRODUCTION

Physicists use high-energy particle colliders such as the Large Hadron Collider (LHC) to produce new particles in order to understand the elementary structure of matter. In these colliders, protons collide at high speed producing several interesting particles which quickly decays into other stable particles. The particles produced in these experiments are identical in many aspects but differ in their kinematic features. Of particular interest is the Higgs-Boson particle which aids in understanding the fundamental structure of matter. Studying this particle is expected to provide insight into the functioning of universe and its possible fates. While the"real world" impact of the particle is not known yet, the academic interest is significant that billions of dollars has been invested in constructing colliders that produce this particle. Identifying the Higgs boson particle *reliably* and *efficiently* enables solving the bigger problem of studying the particle.

One fundamental limitation in using magnetic detectors is their inability to distinguish signal (Higgs-Boson producing collision) from background noise (other collisions) when the signal-to-background ratio is too low. An alternative approach is to measure the properties of stable particles and infer the decaying particle originally produced by collision. For this purpose, scientists have created models of Higgs-Boson and other particles. They simulate their decay using these models and record the kinematic properties of the stable particles produced at the end. Based on these kinematic properties, they can create models to find the source particles. This model can then be used in real accelerators for real-time detection of Higgs-Boson particle. Based on the above, we formally state our data mining task as follows.

Data Mining Task. The problem of interest is classification. Given the kinematic features of stable particles produced in a collision, we classify it as signal (decays from Higgs-Boson) or background (otherwise).

Given the rarity in occurrence of signal events and their importance in understanding the nature of matter, the primary goal is to identify most signal events correctly. Secondarily, since millions of events occur every second, we are also interested in identifying techniques that maximize the number of classifications per second.

Our major contributions are as follows:

1. Implementation of several classifiers covering the following broad categories of classifiers for Higgs-Boson detection: Bayesian, tree-based, instance-based, deep learning, ensemble methods, meta-

*Ananya worked on shallow and deep learning techniques.
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classifiers.

2. Comparison of classification accuracy for the different classification schemes.

3. Evaluation of throughput (Number of classifications per second) for different classification schemes.

Our contributions help in identifying the appropriate classifiers for the given task and provides clarification on the complexity of features necessary for classification.

Our major findings are as follows:

1. There is no discernible difference in accuracy when we compare a neural network and an ensemble scheme.

2. Neural networks, however, is a better choice as the throughput (classifications made per second) is significantly higher.

3. It is possible to outperform the state-of-the-art implementations by carefully handling missing values, selecting the right parameters, and tuning the classification parameters. Our best classifiers outperform the state-of-the-art by 2%.

In addition, we also make several observations on other methods in the results and discussion section. The rest of the paper is organized as follows. Section II provides the necessary background in theoretical physics. Section III describes the related work. Section IV describes our approach. We present our results in Section V and conclude in section VI.

2. BACKGROUND

The LHC collides bunches of proton every 50 ns producing a random number of proton-proton collisions called events. These events produce new particles, most of which are very unstable and decays quickly. The ATLAS detector measures three properties of these surviving particles: type, energy and 3D direction of the particle. Based on these properties, the property of the heaviest primary particles is inferred. An online trigger system selects about 400 events per second producing 3 pb of raw data per year.

Each event contains about ten particles of interest in the final state. The particles of interest for this challenge are electrons, muons, hadronic tau, jets and missing transverse energy. Electrons and muons live longer enough to reach the detector, so their properties (direction and energy) can be measured directly. The other particles such as tau, hadron and jets decays into different particles and hence their properties are inferred using the law of momentum conservation. The measured momenta of all the particles of the event is the primary information provided in the dataset.

Higgs boson is a particle which is responsible for the mass of the other elementary particles. In the original discovery, the Higgs boson was seen decaying into $\gamma\gamma$, WW, and ZZ, which are all boson pairs [1, 8] . The signal class comprises of events in which Higgs boson decays into two taus. Our goal is to identify those signals from a significantly higher number of background events.

3. RELATED WORK

Detecting exotic particles in high-energy physics (HEP) using data analytics techniques instead of the traditionally used physical detectors [19] is not new. Cutts et al. were among the first to use neural networks to identify interesting events in HEP experiments [10]. This was quickly followed by several attempts improve the classification accuracy of neural networks [15, 18]. Apart from the widely popular techniques based on neural networks, only decision trees were explored for a long time. Bowser-Chao and Dzialo used binary decision trees to detect top quarks and compared their results with neural networks [5]. The conventional wisdom was that neural networks were, by far, the best when it comes to classification in HEP until Roe et al. came along and projected boosted decision trees as an alternative to artificial neural networks [21]. By combining several *weak* classifiers, Roe et al. showed that it is possible to obtain better accuracy than a neural network. However, more recently, Baldi et al. showed that a deep learning neural network with several hidden layers outperforms the boosted decision tree [3]. While a number of classification techniques have been developed and applied over the last several years, the HEP community has so far explored only neural networks and boosted decision trees in any depth. This lead to the development of statistical packages for the HEP community such as StatPatternRecognition so that several other techniques based on Rotation Forest, Discriminant Analysis etc. could be explored [16]. Despite this effort, no documented work exists in HEP where alternative techniques are explored even though other techniques are thought to be inferior.

Since the work of Baldi et al. [3] is the closest to ours, we describe it in detail here. The authors of this paper used deep learning methods of neural network to find exotic particles in high energy particle colliders. Deep learning models are neural networks with multiple hidden networks. Current techniques like shallow models which are single hidden layer feedforward network fail to capture all features. The deep learning model here is used on 2.6 million training examples and 100,000 validation examples. The mode is a five-layer neural network with 300 hidden units in each layer, learning rate of 0.05, and a weight decay coefficient of 0.00001 . Testing is done on 500,000 examples. For Higgs benchmark, Area Under the Curve(AUC) - complete for deep

neural network is 0.88 and for shallow neural network, it is 0.81.

4. METHODOLOGY

4.1 Data Preprocessing

In some situations, it becomes difficult to measure the physical properties of a particle such as momentum and energy accurately. In our original dataset, as many as 177000 out of 250000 instances had missing attributes. We considered three approaches to deal with missing values. First, we tried ignoring instances with missing attributes. But this resulted in very few useful instances. Second, we tried to replace the missing values with the mean/median. However, this biases the experiments. Finally, we decided to adopt a method known as multiple imputations [4] which replaces the missing values with a random number that follows the distribution for that attribute. We use the `Amelia` [12] package to perform this task.

4.2 Feature Engineering and Selection

The raw dataset includes 17 features. From these 17 basic features, 13 additional features were derived. These 13 derived features describe some property of the particle and requires knowledge of physics. The features are provided by physicists. From these 30 features, a subset is selected based on the following factors. First, we decide the ability of the feature/attribute to distinguish between signal an background. The distribution of different attributes is shown in Fig. 1 for signal and background separately. Second, while building the classifier we try to avoid using features that correlate with each other. Fig. 2 shows the correlation matrix of the features. The final set of features selected differs for each classifier. The details are given in their respective subsections.

4.3 Data Analytics Techniques

In this section, we describe the various classification schemes we explored. For each technique, we also describe the parameter settings explored in brief.

4.3.1 *Bayesian Classifiers*

Naive Bayes.

This classifier is based on the Naive Bayes technique developed by John et al. [13]. The modeling and prediction overhead is negligible as this method is known to be highly scalable. During data preprocessing step, we included only those features whose Pearson correlation coefficient was below a particular threshold as the naive Bayes classifier performs poorly when the features are dependent on each other.

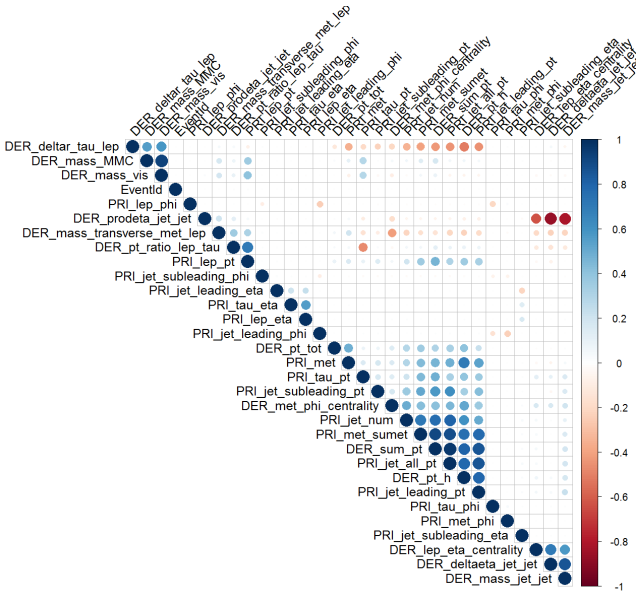

Figure 2: Correlation matrix. Dark blue indicates features that shows strong positive correlation. Dark red indicates features that show strong negative correlation.

4.3.2 *Functions-based Classifiers*

Logistic Regression.

This classifier is based on the Ridge estimation technique developed by Cessie et al. [7]. Being a linear method, the modeling and prediction overhead is small. In this technique, we used L1 regularized logistic regression. We explored the performance of this method by varying the number of features in the dataset.

Linear Discriminant Analysis.

This linear classifier fits a gaussian distribution of equal variance to each of the classes. We took the class priors to be equal when evaluating this method.

Quadratic Discriminant Analysis.

This linear method is similar to Linear Discriminant Analysis, expect that this technique uses quadratic decision boundaries. In evaluating this method, we used equal class priors. The optimal performance shown in the table is obtained when the dataset included features whose pairwise correlational coefficient is less than 0.95.

4.3.3 *Tree-based Classifiers*

Decision Tree Classifier.

In evaluating the performance of decision tree classifier, we used "gini" and "entropy" criterion. We also varied the minimum number of samples required to split an internal node to study their impact.

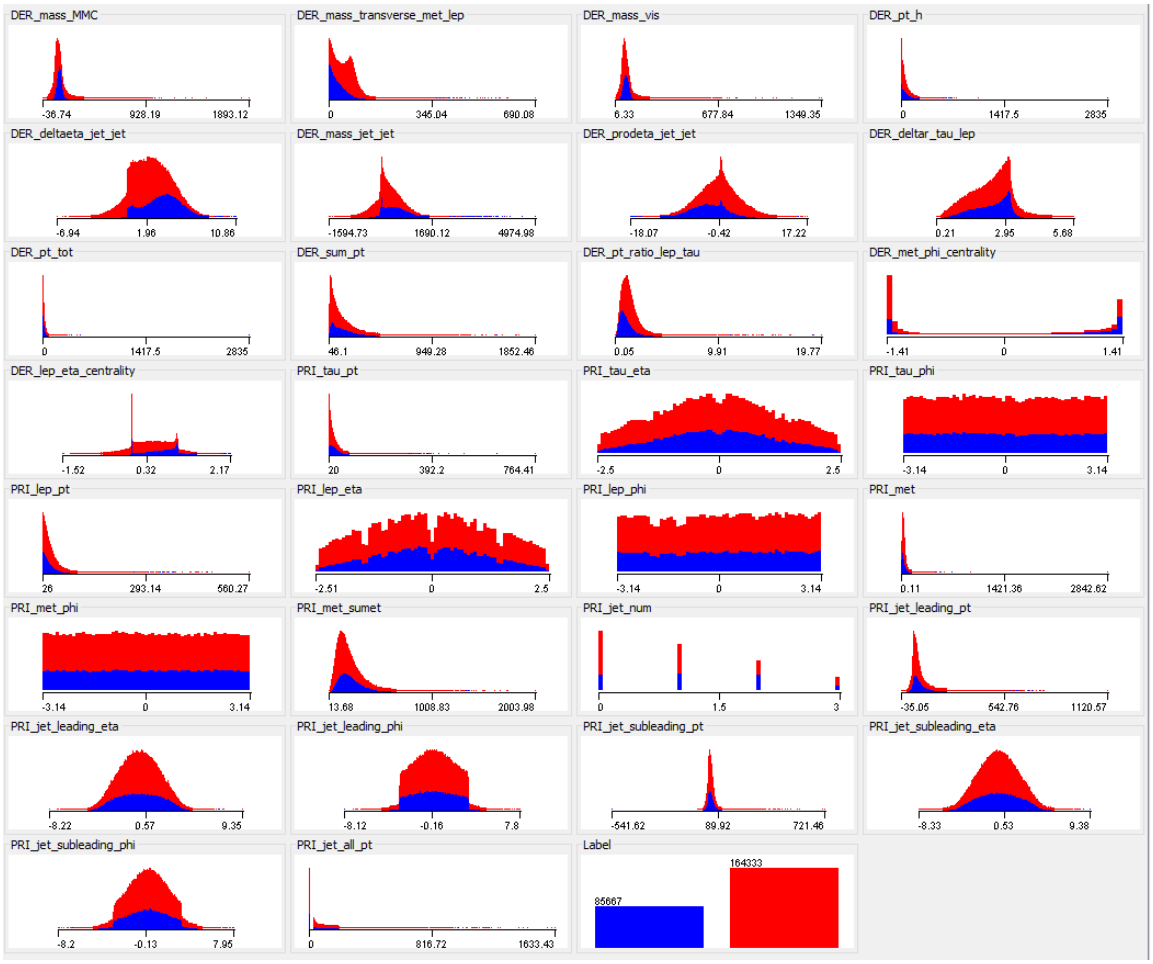

Figure 1: Distribution of different attributes for signal. Blue represents signal and red represents background.

4.3.4 *Instance-based Classifiers*

k-Nearest Neighbor.

For the instance-based classifier we explore the k-nearest neighbor (kNN) technique [2]. This is a lazy classification technique in which the k nearest neighbors are looked at to decide the class of a new instance. This technique has practically no training overhead. The classification overhead is very high though, particularly if the distance for all previously seen instances are computed exhaustively. Since this technique is known to perform bad with noisy attributes and irrelevant attributes, we explore removing such attributes from our dataset. We also tried to construct the classifier using top few principal components in order to keep only relevant features. In addition, we also experiment with the number of neighbors considered.

4.3.5 *Neural Networks*

For Higgs Boson project, we used both deep and shallow neural networks. We analyzed our data using multiple networks each of which are discussed below.

feedforwardnet.

Feed Forward networks consist of a series of layers. The first layer has a connection from the network input. Each subsequent layer has a connection from the previous layer. The final layer is the output layer which produces the network output. The hidden layer is of size 60. The transfer function used in this layer is 'tansig' (tan-Sigmoid Transfer Function). Tansig is a neural network transfer function which calculates a layer's output from its net input. The output layer produces only 1 output (0 or 1). The transfer function used in this layer is 'purelin'. It is a linear transfer function which calculates the final output.

patternet.

It is a Pattern Recognition Network which is trained to classify inputs from target classes. The target data should consist of a vector of 0 or 1. It contains one hidden layer of size 40. The output layer is of size 1.

cascadeforwardnet.

Cascade Forward Network is very similar to feed for-

ward networks but includes a connection from the network input and from every previous layer to following layers. The output layer has two inputs : one from the previous hidden layer and the other from the input. The hidden layer is of size 80. The rest of the network is same as that of FeedForwardNetwork.

Custom Neural Network.

We designed a deep neural network with 4 layers: three hidden layers, one output layer. All the hidden layers are connected to the network input. There is no direct connection between any of the three hidden layers. The output layer takes 4 inputs, three of the inputs are outputs of each hidden layer. The output layer is also recursive layer. So it's own output is fed back as its fourth input. The network model is trained using 'trainrp' network training function which updates weight and bias according to resilient back propagation algorithm (Rprop). The 1st hidden layer contains 20 neurons. The transfer function used in this layer is 'tansig' (tan-Sigmoid Transfer Function). The second hidden layer has 10 neurons. The transfer function used here is 'logsig'. It is log-sigmoid transfer function. The third hidden layer has 20 neurons. The transfer function used here is again 'tansig'. The output layer produces only 1 output (0 or 1). The transfer function used in this layer is 'purelin'.

The number of layers in a network, number of neurons in each layer, transfer function to be used to calculate output of each layer, etc are based on heuristics. We have used biases in the network as networks with biases are more powerful. Each layer's weights and biases are initialized with the Nguyen-Widrow layer initialization method [17].

4.3.6 Meta Classifiers and Ensemble Methods

Classification via Clustering and Regression.

We simply cluster the raw dataset and mark certain clusters as signal and others as noise. Prediction based on the distance of the new data point to the centroid of the two cluster groups. For the regression technique, we form an equation from the basic parameters and based on the value from the equation, we predict if the event is a signal or a background.

Bagging.

Bagging technique developed by Brieman involves creating several models using different subsets of the training dataset [6]. Each model does its own classification and they all vote with equal weight to decide on the class. We explored the number of iterations it takes to form the solution. We also experimented with two types of tree based classifiers - REP Tree and Decision Stump Classifier.

Boosting.

Boosting is similar to bagging in that we create several models and they all vote to make the final decision. However, there is a difference in how the dataset is constructed for each model. All those instances that failed in model 1 are propagated to subsequent models. The models that come later all try to improve the regions where the older models failed. Here we explore ADA Boosting developed by Freund and Schapire [11] and MultiBoosting technique developed by Webb [22]. We use these techniques in conjuction with REP Tree and Decision Stump Tree classifiers.

Rotation Forest.

Rotation Forest is an ensemble method developed by Rodriguez et al. [20] where several classifiers are combined to produce a highly accurate classifier. Here, again several decision trees combine to decide the final class. However, the difference here is that each tree does this classification based on a *different* subset of the *principal components*. We use this technique in conjunction with J48 decision tree and REP Tree.

5. RESULTS

In this section, we describe the dataset used, hardware details, accuracy, and throughput results for the different classifiers.

5.1 Dataset

We make use of the dataset provided by Kaggle [9]. This is the cleaned up data from the original dataset provided by physicists at the UC Irvine Machine Learning Repository. This data set contains *250000* instances. Each instance (row) in the dataset describes a collision event detected by the collider. Events are described by the kinematic properties (such as direction and momentum) of the particles produced in a collision. A set of 17 features describe these kinematic properties. In addition, 13 derived features that the physicists deemed important are also included in the dataset. *200000* instances from the original dataset is used for *training* and the remaining *50000* instances is used for *testing*.

5.2 Hardware details

All experiments were run on a MacBook Pro using a *4-core* Intel Core i7 processor running at 2.5 GHz. This machine has *256 KB* of L2 cache per core, *6 MB* of L3 cache, and *16 GB* of DDR3-1600 MHz memory. Modeling and prediction overheads of all techniques were measured and this machine and the corresponding throughput results presented in subsequent sections.

5.3 Accuracy Results

5.3.1 Bayesian Classifiers

Table 1: Accuracy results for different models

Classifiers	Precision(s)	Recall(s)	f1-score(s)	Precision(b)	Recall(b)	f1-score(b)	Precision	Recall	f1-score	ROC Area
Naive Bayes	0.66	0.75	0.7	0.86	0.8	0.83	0.79	0.78	0.79	0.85
Decision Tree Classifier	0.76	0.73	0.75	0.87	0.88	0.88	0.83	0.83	0.83	0.9
Logistric Regression	0.69	0.62	0.65	0.81	0.86	0.83	0.77	0.78	0.77	0.84
LDA	0.66	0.51	0.58	0.78	0.74	0.82	0.74	0.75	0.74	0.85
QDA	0.65	0.78	0.71	0.88	0.79	0.83	0.8	0.79	0.79	0.86
k-nearest Neighbor	0.72	0.69	0.72	0.84	0.86	0.85	0.8	0.8	0.8	0.87
Custom network	0.79	0.71	0.74	0.85	0.9	0.87	0.83	0.83	0.82	0.89
Feed Forward Network	0.79	0.74	0.77	0.87	0.9	0.88	0.84	0.84	0.84	0.91
Cascade Forward Network	0.79	0.74	0.76	0.87	0.9	0.88	0.84	0.85	0.84	0.91
Pattern Neural Network	0.75	0.71	0.73	0.85	0.88	0.87	0.82	0.82	0.82	0.9
Rotation Forest	0.8	0.73	0.76	0.86	0.91	0.88	0.84	0.84	0.84	0.91
Boosting	0.78	0.74	0.76	0.87	0.89	0.88	0.84	0.84	0.84	0.9
Bagging	0.79	0.74	0.77	0.87	0.9	0.88	0.84	0.85	0.84	0.91

As expected, the removal of correlating features had a positive impact on the accuracy of the classifier. When we decrease the threshold value of correlation for parameter removal, the accuracy decreased as the number of correlated features increase. The best performance is achieved when the dataset includes 12 features whose pairwise correlation coefficient is less than 0.6. We also observe that this method can classify background noise better than signal.

5.3.2 *Function-based Classifiers*

For this class of techniques, we explored varying the features used for classification. Our results suggest that the number of features used for classification did not affect the accuracy of the classifier. The best results obtained for this technique is shown in Table. 1.

5.3.3 *Tree-based Classifiers*

For the tree-based classifiers, we did not see any different for the two criterion (gini and entropy) explored. The number of samples used to form the split, however, had a significant impact and the best performance was achieved when this value was 300. The corresponding accuracy metrics are shown in Table. 1.

5.3.4 *Instance-based Classifiers*

While using the raw and derived features, we did not see any notable impact of the number of neighbors on the accuracy. Also, removing irrelevant and noisy features did not help (F1-score was always around 0.70). However, simply by using principal components improved the accuracy to over 74%. Reducing the number of principal components to four increased the accuracy to over 77.5%. Also, increasing the number of neighbors improved the accuracy further to 80%. The best results were obtained for number of principal components = 4 and number of neighbors = 20. The corresponding results are tabulated in Table. 1.

5.3.5 *Neural Network*

As mentioned before we used multiple NN technics to classify the data between a signal and a background but the classification results are very similar. Among the 4 neural networks used here, cascade forward network has the best results – ROC curve (AUC) is 0.91, precision and recall s 0.84 and 0.85 respectively.

We noticed that for each network model, the testing performance stops increasing with the increase in the number of neurons in the hidden layers after a certain point . Liu et al. [14] call this as the stop criterion. Beyond this point the neural network overestimates the complexity of the target problem which causes overfitting.

Recently there has been substantial interest in feed forward network with many layers. However, we restricted ourselves to only two layers (one hidden and one output layer) as we noticed an increase in overfitting when the number of layers in a feed forward network is greater than 2. Similarly in the custom network that we designed, the neural network's performance improves when we increase the number of hidden layers from 2 to 3, the AUC is 0.89 but it is still less than other ANN models with 2 layers.

5.3.6 *Ensemble Methods and Meta-classifiers*

Bagging.

Our evaluation indicates that the choice of the decision tree algorithm matters the most when applying the bagging technique. REP tree showed a 20% better accuracy than a Decision Stump Tree. The effect of increasing the number of iterations was low, changing the bag size negligible for reasonable sizes. The best AUC value obtained was 0.91 (Corresponding f1-score was 0.84) when using REP tree with 50% bag size, and 20 iterations. The details of the result is presented in Table. 1.

Boosting.

Among the two boosting techniques evaluated, Multi-Boosting is found to be better. Our results showed REP Tree is better than Decision Stump Tree. For example,

the accuracy increased from 76.8% to 82.3% for ADA boost, and from 77% to 83.9% for MultiBoost when REP Tree Classifier is used as the base classifier.

Rotation Forest.

Unlike bagging and boosting, the choice of the underlying decision tree classifier did not matter much. The J48 algorithm was marginally better than the REP Tree. The results for the best configuration is presented in Table. 1.

Classification via Clustering and Regression.

The regression method is comparable to other linear methods explored earlier. The classification via clustering did not work well as expected with an ROC Area of just 0.628 which is the least value obtained among all classifiers explored.

5.4 Throughput Results

A particle physics accelerator produces millions to billions of events in a second. The classifier has to be really fast to process that many events in real time. While several dedicated ASICs can be used to perform real time classification for more sophisticated techniques if the accuracy improvement warrants them. In our case several techniques produce similar accuracy thereby making decisions from throughput results necessary. The ensemble methods and neural networks all have similar accuracy. While it is expensive to construct a neural network, it is just an one-time cost. Ensemble methods on the other hand are relatively faster to construct, however since several models have to be evaluated before a decision is made, its prediction overhead is very high as shown in table 2. This translates to low throughput. On the other hand, neural networks show much higher throughput even though it takes a long time to construct the model.

Table 2: Throughput results for different classifiers

Classifiers	Modeling(ms)	Prediction(ms)	Classifications/s
Naive Bayes	86	11	4587156
Decision Tree Classifier	8750	13	3937008
Logistric Regression	12300	9	5561735
LDA	316	20	2551020
QDA	266	52	967118
k-nearest Neighbor	200	68000	735
Custom network	603000	187	267380
Feed Forward Network	786000	102	490196
Cascade Forward Network	1034000	108	462963
Pattern Neural Network	828800	75	666667
Rotation Forest	362000	227000	220
Boosting	87000	44000	1136
Bagging	59500	44000	1136

5.5 Discussion

There has been much discussion about the efficacy of neural networks and ensemble methods in classification problems in HEP. While some researchers have shown that ensemble methods such as boosting is better, others have sworn that neural networks is better. Our results show that there is practically no difference between the two techniques in terms of accuracy. However, the difference in throughput is more pronounced and it makes sense to use neural networks over ensemble methods. The basic classifiers, as expected did not show a very good accuracy with the exception of decision tree classifiers. The accuracy achieved using decision tree classifier is only marginally less than neural network, but the achieved throughput is an order of magnitude better. This makes the decision tree classifier an attractive alternative. Another important note is that the achieved ROC Area of 0.91 is better than state-of-the-art techniques [3] by over 2%.

6. CONCLUSION

We explored a number of different classification techniques for the purpose of classifying events occurring within the large Hadron collider based on kinematic properties of certain particles. Our best classifier outperforms the state-of-the-art by 2%. Our results also showed that there is practically no difference in accuracy between neural networks and ensemble methods. However, the neural networks outperforms ensemble methods in terms of throughput making it the better choice. But, our results show that a simple tree-based technique could prove to be a reasonable alternative for practical purposes.

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APPENDIX

The source code of the implementations is available in github: `https://github.com/vickyavb/Data-Analysis`