

XBNet : An Extremely Boosted Neural Network

Tushar Sarkar

KJ Somaiya College of Engineering, Mumbai
tushar.sarkar@somaiya.edu

Abstract. Neural networks have proved to be very robust at processing unstructured data like images, text, videos, and audio. However, it has been observed that their performance is not up to the mark in tabular data; hence tree-based models are preferred in such scenarios. A popular model for tabular data is boosted trees, a highly efficacious and extensively used machine learning method, and it also provides good interpretability compared to neural networks. In this paper, we describe a novel architecture XBNet, which tries to combine tree-based models with that of neural networks to create a robust architecture trained by using a novel optimization technique, Boosted Gradient Descent for Tabular Data which increases its interpretability and performance.

Keywords: XBNet, Boosted Gradient Descent, XGBoost, Neural networks, Entropy

1 Introduction

The need and use for data keep increasing day by day in our current world, and its impact on people's daily lives is motivating data-driven decisions in many sectors of the industry. The applications of these approaches are spam/ham detectors that are commonly used in emails, anti-virus systems that prevent unnecessary spamming of emails and protect our data and our computers from potential viruses. It is used in the marketing industry as advertising systems learn to correlate the correct advertisements with the users who are looking for items in those contexts.[9] Fraud is prevented by top companies by using such systems that monitor all the activity and detect any vitriolic activity and alert people to prevent it promptly; anomaly detection techniques help banks to check to prevent fraudulent transactions.[18] The reason behind the success of these applications is the following: utility of statistical models that maps complex data dependencies between disparate entities Furthermore, the scalability of these architectures enables them to learn the relationships even in complex data sources. Even in the algorithms that are commonly used in dealing with tabular data, gradient tree boosting, [5] is an approach that outshines others in several use cases. Deep neural networks [10] have shown noteworthy success with unstructured data like images, text, videos, and audio.[7] [4] [10] [13]. For the above domains of problems, we try to precisely encode the information hidden in them into a vector space that forms the basis of our understanding and

helps tackle the problem. Tabular data is the only data type where there is a minimum success with this approach. Though it is the most common data type in the actual world of data science, which comprises any continuous and discrete features,[3] deep learning for tabular data remains dormant, as ensemble methods built on decision trees continue to perform better on such data. We propose a new architecture for tabular data, XBNet, which attempts to combine gradient boosted tree with feed-forward neural networks to give rise to a new approach of robust architectures. XBNet inputs raw tabular data and is trained using an optimization technique Boosted Gradient Descent which is initialized with the feature importance of a gradient boosted tree, and it updates the weights of each layer in the neural network in two steps:

- (1) Update weights by gradient descent.
- (2) Update weights by using feature importance, [8] of a gradient boosted tree in every intermediate layer.

2 Related Work

Tree-based models and their variants like AdaBoost, [6] Random Forest and XGBoost, etc like are widely used in classification and regression problems. They repeatedly split the input vector space and allot scores to the final node. Tree-based models not only boost the performance in tabular data they also increase the interpretability, [12] of the system which increases its usability in business scenarios. It is also frequently seen that ensemble techniques like Random Forest, [14] [1] and XGBoost, [2] are used in most of the winning solutions in the case of tabular data. These models perform better than neural networks at several classification and regression problems. Some works have advanced to amalgamate neural networks and tree-based models like decision trees. An approach in this direction was Neural Decision Forests [16]. Another interesting approach is DNDT which stands for Deep Neural Decision tree. DNDTs have a unique architecture, where a particular set of weights maps to a distinct decision tree.[19] Our proposed architecture XBNet is another step in that field and it differs from the previous methods in many approaches. The optimization technique acts as an extension of the Gradient Descent [17] technique with the help of tree-based models. In this approach, trees are trained in every layer of the architecture and their feature importance is used along with the weights determined by gradient descent for adjusting the weights of those layers respectively.

3 Methodology

3.1 Feature importance

The feature importance of the gradient boosted tree which plays a great role in our architecture as well as training, is determined based on information gain [15] of the features of the tree, that is a way of determining which attribute in a

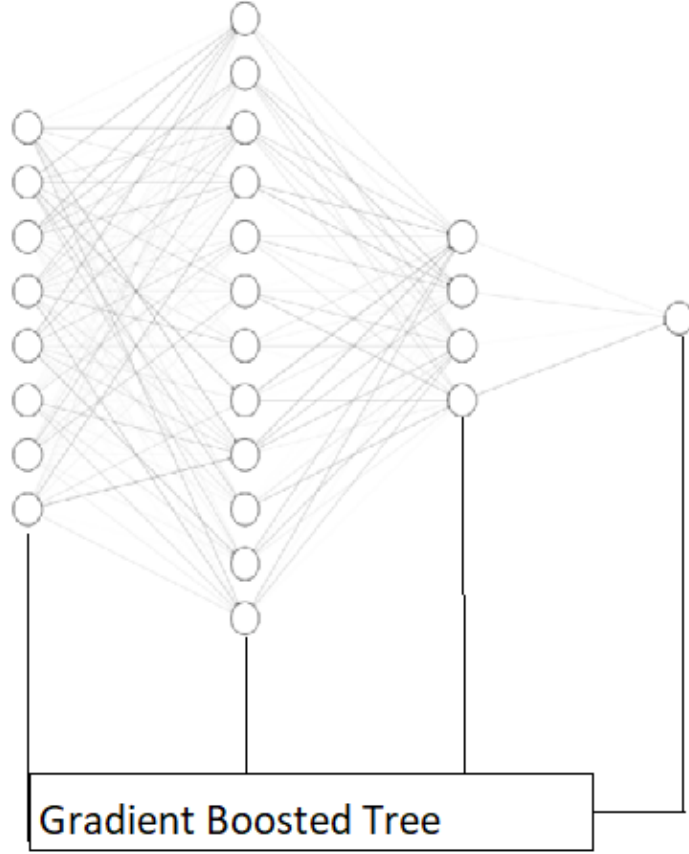


Fig. 1. This shows how this entire feed forward neural network is connected to the tree with respect to our model

given set of feature vectors is most useful for distinguishing between the classes to be learned which in turn is dependent on entropy[11] that is a common way of measuring impurity. Impurity measures the homogeneity of the target variable at every node.

Let \mathcal{P} be a probability distribution such that

$$\mathcal{P} = (p_1, p_2, \dots, p_n)$$

where p_i is the probability of a data point that belongs to a subset d_i of dataset \mathcal{D}

Entropy can be defined as:

$$Entropy(\mathcal{P}) = \sum_{i=1}^n -p_i \log_2(p_i)$$

$$InformationGain = Entropy_{beforeSplit} - Entropy_{afterSplit}$$

The information gain calculated is then used to determine the feature importance of the boosted tree which is used in Boosted Gradient Descent.

3.2 Gradient Descent

Gradient Descent is an optimization technique for finding the minima of the required differentiable loss function. Gradient descent is employed to determine the optimum values of a function's parameters that minimize the given loss function. Given below is the algorithm for gradient descent where $g(x)$ is the activation function, m is the mini-batch; $A^{[l]}$ is the output of the l th layer with is activated with an activation function and $z^{[l]}$ is the output of the l th layer before applying the activation function, $\hat{y}^{(i)}, y^{(i)}$ are the predicted and actual values respectively..

Algorithm 1: Basic Gradient Descent approach

Result: Cost function is minimized using Gradient Descent

Initialize w, α ;

for $t = 1, 2, \dots, m$ **do**

 Forward propagation on X^t ;

$$z^{[l]} = w^{[l]} A^{[l-1]} + b^{[l]};$$

$$A^{[l]} = g^{[l]}(z^{[l]});$$

 Compute cost $J =$

$$\frac{1}{m} \sum \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m} \sum (||w^{[l]}||_f^2)$$

 ;

 Backward propagation on J^t ;

$$w^{[l]} = w^{[l]} - \alpha \nabla w^{[l]};$$

$$b^{[l]} = b^{[l]} - \alpha \nabla b^{[l]};$$

end

Our optimization strategy will add another step to the traditional gradient descent approach to boost the performance.

3.3 Training and Optimization using Boosted Gradient Descent

Now we combine the above subsections to create our architecture and optimizer. Our architecture creates a Sequential structure of layers with the first and last being the input and output layers respectively. The weights of the first layer are not initialized randomly but it is the feature importance of a gradient boosted tree which is trained at the time of initialization of the model. Apart from this the architecture also contains a gradient boosted tree that is connected to each layer. At the time of training the model, the data that is fed completes a forward and backward propagation, and the weights of all the layers get updated according to gradient descent once and then instead of going to the next epoch of training it goes through all the layers again and updates its weights again based on the feature importance of the gradient boosted tree that is trained on the layers respectively. The number of layers of the neural network on which the tree should be trained is a hyperparameter. Further, the trees are trained on the hidden layers during the forward propagation of the feed-forward neural network and their feature importance is stored which is updated after the backward pass. So in this approach, the feature importance also plays the role of adjusting the weight which boosts the performance of the architecture. To ensure that the contribution of the weights provided by the feature importance and the weights of gradient descent is in the same order the feature importance is scaled down to the same power as that of the weights of the gradient descent algorithm. This is necessary because after some epochs the feature importance remains in the same order by virtue of its definition but the weights provided by gradient descent decreases by several orders. Only one gradient boosted tree is initialized inside the architecture as all the layers will have different inputs after epoch and therefore the same tree is used for each layer and each epoch and the feature importance are stored before training the tree on the next layer which saves space while providing the required result. Here is the algorithm for training XBNet; $g(x)$ is the activation function, m is the mini-batch; $A^{[l]}$ is the output of the l th layer with is activated with an activation function and $z^{[l]}$ is the output of the l th layer before applying the activation function, tree is a gradient boosted tree, $f^{[l]}$ is the feature importance of the hidden layers, $\hat{y}^{(i)}, y^{(i)}$ are the predicted and actual values respectively.

3.4 Prediction

During testing, there is no requirement of using the gradient boosted tree as the purpose of the feature importance of the tree is to only ensure the precise updation of weights to improve the performance of the network which is done while training the model. Hence the prediction speed only depends on the number of layers as there is no contribution of trees while predicting.

4 Results

We evaluate our model on the Breast Cancer Dataset and we create several models with different number of layers, number of nodes, activation functions,

Algorithm 2: Training Algorithm for XBNet using Boosted Gradient Descent

Result: Cost function is minimized using Boosted Gradient Descent

Initialize $w, b, \alpha, \text{tree}$;

$w^{[1]} = \text{tree.train}(X, y).\text{importance}$;

for $t = 1, 2, \dots, m$ **do**

 Forward propagation on X^t ;

$z^{[l]} = w^{[l]} A^{[l-1]} + b^{[l]}$;

$A^{[l]} = g^{[l]}(z^{[l]})$;

$f^{[l]} = \text{tree.train}(A^{[l]}, y^{(i)}).\text{importance}$;

 Compute cost $J =$

$$\frac{1}{m} \sum \mathcal{L}(\hat{y}^{(i)}, y^{(i)}) + \frac{\lambda}{2m} \sum (||w^{[l]}||_f^2$$

;

 Backward propagation on J^t ;

$w^{[l]} = w^{[l]} - \alpha \nabla w^{[l]}$;

$f^{[l]} = f^{[l]} \times 10^{\log(\min(w^{[l]}))}$;

$w^{[l]} = w^{[l]} + f^{[l]}$;

$b^{[l]} = b^{[l]} - \alpha \nabla b^{[l]}$;

end

and different number of boosted layers i.e number of hidden layers on which tree is trained. Here is a summary of the results:

- (1) When a model with 2 layers having 16,1 nodes respectively whose 1st layer is boosted with a default xgboost tree with no hyperparameter tuning is trained on 100 epochs it yields a loss of 0.12 on the training data and a loss of 0.08 on the validation data when BCE loss criterion was used as the loss function.
- (2) When a model with 2 layers having 8,1 nodes respectively whose 1st layer is boosted with a default xgboost tree with no hyperparameter tuning is trained on 100 epochs it yields a loss of 0.10 on the training data and a loss of 0.09 on the validation data when BCE loss criterion was used as the loss function.
- (3) When a model with 2 layers having 8,1 nodes respectively whose 1st as well as 2nd layer is boosted with a default xgboost tree with no hyperparameter tuning is trained on 100 epochs it yields a loss of 0.13 on the training data and a loss of 0.11 on the validation data when BCE loss criterion was used as the loss function.
- (4) When a model with 3 layers having 32,16,1 nodes respectively whose 1st layer is boosted with a default xgboost tree with no hyperparameter tuning is trained on 100 epochs it yields a loss of 21.78 on the training data and a loss of 19.45 on the validation data when BCE loss criterion was used as the loss function.

Results on different Datasets

Dataset	Training Accuracy	Testing Accuracy
Iris	100	100.
Breast Cancer	96.7	96.49
Diabetes	77.09	78.78
Titanic	80.25	79.85
German Credit	69.8	71.33

Training Classification metrics on Breast Cancer

Class	Precision	Recall	f1-score
0	0.96	0.98	0.97
1	0.97	0.93	0.95
micro avg	0.96	0.96	0.96
macro avg	0.96	0.96	0.96
weighted avg	0.96	0.96	0.96

Testing Classification metrics on Breast Cancer

Class	Precision	Recall	f1-score
0	0.99	0.93	0.96
1	0.89	0.98	0.93
micro avg	0.95	0.95	0.95
macro avg	0.94	0.96	0.94
weighted avg	0.95	0.95	0.95

5 Conclusion

This paper about XBNet discussed the techniques that we employed for building this architecture and described the training, optimization, and inference techniques for this model. As the need and use for data keep increasing day-by-day in our current world and its impact on the daily life of people is motivating data-driven decisions in many sectors of the industry, this paper was an effort to combine neural networks and gradient boosted trees to provide an alternative approach to the currently used techniques which will pave the way for future work using this approach. The performance, interpretability, and scalability of this architecture will make it possible for data scientists and machine learning engineers to optimally utilize the model.

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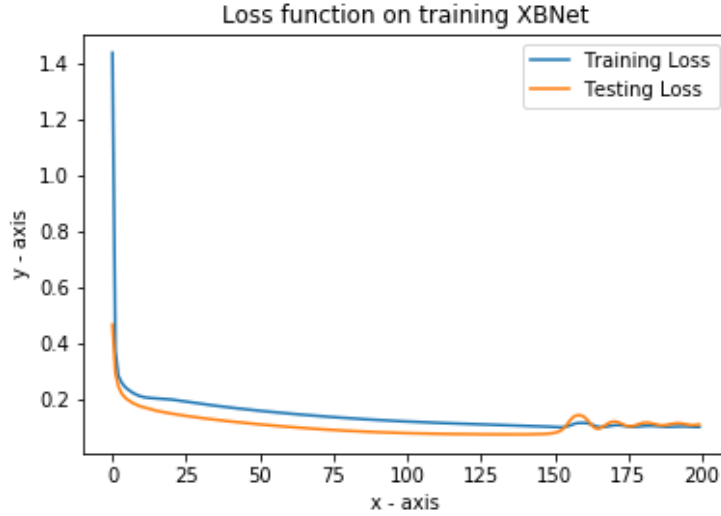


Fig. 2. BCE Loss function vs Number of epochs

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7 References

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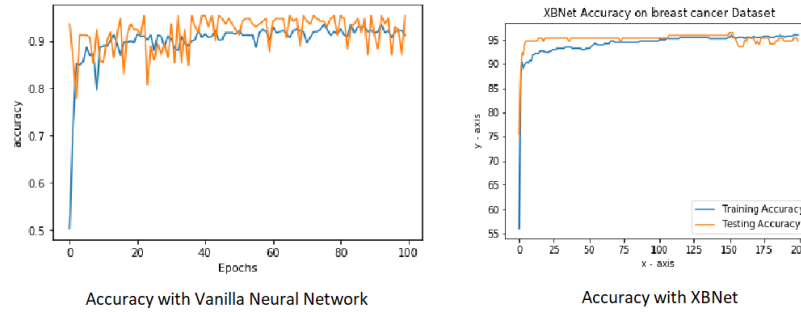


Fig. 3. Comparision of performance in Vanilla Neural Network vs XBNet

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