A SHORT NOTE ON THE DECISION TREE BASED NEURAL TURING MACHINE

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ABSTRACT

Turing machine and decision tree have developed independently for a long time. With the recent development of differentiable models, there is an intersection between them. Neural turing machine (NTM) opens door for the memory network. It use differentiable attention mechanism to read/write external memory bank. Differentiable forest brings differentiable properties to classical decision tree. In this short note, we show the deep connection between these two models. That is: differentiable forest is a special case of NTM. Differentiable forest is actually decision tree based neural turing machine. Based on this deep connection, we propose a response augmented differentiable forest (RaDF). The controller of RaDF is differentiable forest, the external memory of RaDF are response vectors which would be read/write by leaf nodes.

1 Introduction

Neural Turing Machine (NTM) [1-4] enhance classical turing machine with differentiable attention mechanism to visit datas/programs in the external memory bank. NTM has different names in different papers, for example, memory augmented neural networks (MANN), reservoir memory machines, differentiable neural computer... These names reveal the interesting aspects of NTM model in different ways. With external “artificial” working memory, NTM would have strong capacity to store and retrieve pieces of information just like human being. Some experiments in [1] verified its defectiveness over famous LSTMs models. Since the pioneering work of [1], NTM has been deeply studied and applied to many applications, including machine translation, recommendation systems, slam, reinforcement learning, object tracking, video understanding, Graph Networks, etc [5-15]. All the controller in these works are neural networks. Our work is the first proposition of differentiable decision tree based NTM.

Differentiable decision tree [16,17] brings differentiable properties to classical decision tree. Compared with widely used deep neural networks, tree model still has some advantages. Its structure is very simple, easy to use and explain the decision process. Especially for tabular data, gradient boosted decision trees (GBDT) [18] models usually have better accuracy than deep networks, which is verified by many Kaggle competitions and real applications. But the classical tree-based models lack of differentiability, which is the key disadvantage compare to the deep neural networks. Now the differentiable trees also have full differentiability. So we could train it with many powerful gradient-based optimization algorithms (SGD, Adam,...). We could use batch training to reduce memory usage greatly. And we could use the end-to-end learning to reduce many preprocess works. The differential operation would search in a larger continuous space, so it can find more accurate solutions. The experiments on some large datasets showed differentiable forest model has higher accuracy than best GBDT libs (LightGBM, Catboost, and XGBoost) [19].

In recent years, different research teams [16,17,20-25] have proposed different models and algorithms to implement the differentiability. [16] is a pioneering work in the differentiable decision tree model. They present a stochastic routing algorithm to learn the split parameters via back propagation. The tree-enhanced network gets higher accuracy than GoogleNet [26], which was the best model at the time of its publication. [17] introduces neural oblivious decision ensembles (NODE) in the framework of deep learning. The core unit of NODE is oblivious decision tree, which uses the same feature and decision threshold in all internal nodes of the same depth. There is no such limitation in our algorithm. As described in section ??, each internal node in our model could have independent feature and
At each time step $t$, the response augmented differential forest $\text{RaDF}$ would be optimized end-to-end with stochastic gradient descent algorithm. Just like the classic Turing machine, NTM is a recurrent machine with two main modules, the first is the controller and update its state. The main innovation of NTM is its attention mechanism which would update the weights of each read/write operation.

### 2 Differentiable forest based neural turing machine

In this section, we would first give the main structure/algorithm of differentiable forest and NTM, then reveal the essential connection between them. That is, differentiable forest is also neural turing machine with specific controller and attention mechanism. To our knowledge, this is the first proposition of differentiable forest based NTM.

#### 2.1 Neural Turing Machine

Just like the classic Turing machine, NTM is a recurrent machine with two main modules, the first is the controller and the second is external memory bank $M$. The external memory bank $M$ is usually defined as $N \times W$ matrix, which contains $N$ cells (memory locations) and the size of each cell $M^t$ is $W$. The controller would read and write $M$ to update its state. The main innovation of NTM is its attention mechanism which would update the weights of each read/write operation.

At each time step $t$, NTM would update the weight $w_i^t$ of each cell. Then the read operation would get $r_i$ and write operation would update each cell $M^t$ as:

$$ r_t = \sum_{i=1}^{N} w_i^t M_i^t $$

where $e_t$ is additional erase vector and $a_t$ is add vector. For more detail of practical robust implementation of NTM, please see [3].

#### 2.2 Response augmented differential forest (RaDF)

The response augmented differential forest $\text{RaDF}(T, Q)$ has two main modules. The first is controller $T$ which has $K$ differentiable decision trees $[T_1, T_2, \cdots, T_K]$; the second is external memory bank $Q$. Each cell of $Q$ is actually response corresponding to some leaf nodes [19]. The controller $T$ would read a write response bank $Q$. Each leaf node is just the head in the NTM to read/write response bank $Q$. So the response augmented differential forest $\text{DF}(T, R)$ is just a specific NTM.

For a dataset with N samples $X = \{x\}$ and its target $Y = \{y\}$. Each $x$ has M attributes, $x = [x_1, x_2, \cdots, x_M]^T$. The $\text{RaDF}(T, Q)$ would learn $K$ differentiable decision trees $[T_1, T_2, \cdots, T_K]$ and the response bank $Q$ to minimize the loss between the target $y$ and prediction $\hat{y}$.

$$ \hat{y} = \frac{1}{K} \sum_{h=1}^{K} T_h (x) $$

Figure 1(a) shows the simplest case of RaDF. The controller is just a simple decision tree(one root node, two leaf nodes). All leaf nodes in the controller would read/write corresponding response in the external memory. For each input $x$, the gating function $g$ at root node would generate probabilities for both leaf nodes. Formula 3 gives the general definition of gating function $g$ with learn-able parameters $A$ and threshold $b$. $\sigma$ would map $Ax - b$ to probability between [0,1], for example, the sigmoid function.

$$ g(A, x, b) = \sigma (Ax - b) \tag{3} $$

So as shown in Figure 1(b), The sample $x$ would be directed to each nodal $j$ with probability $p_j$. And finally, the input $x$ would reach all leaves. For a tree with depth $d$, we represent the path as $n_1, n_2, \cdots, n_d$, where $n_1$ is the root node.
and \( n_d \) is the leaf node \( j \). \( p_j \) is just the product of the probabilities of all nodes in this path:

\[
p_j = \prod_{n \in \{n_1, \ldots, n_d\}} g_n
\]

(4)

In the model of classical decision tree, the gating function \( g \) is just the heav-side function, either left or right. So for each sample \( x \), only one leaf node is activated in the classical decision tree, while in RaDF model, all leaf nodes are activated (with probability \( p_j \)) to read/write response bank \( Q \).

![Diagram of decision tree with response](image1)

In the model of classical decision tree, the gating function \( g \) is just the heav-side function, either left or right. So for each sample \( x \), only one leaf node is activated in the classical decision tree, while in RaDF model, all leaf nodes are activated (with probability \( p_j \)) to read/write response bank \( Q \).

The read operation of leaf node \( j \) would return a response vector \( q_j = (q_{j_1}, q_{j_2}, \cdots, q_{j_F})^T \). Then the output of tree \( h \) is just the probability average of these responses.

\[
Q_h(x) = \sum_{j \text{ is leaf of } h} p_j q_j
\]

(5)

A single tree is a very weak learner, so we should merge many trees to get higher accuracy, just like the random forest or other ensemble learning method. The final prediction \( y \) is weighted summary of all trees. In the simplest case, the weight is always \( 1/K \), \( \hat{y} \) is just the average result.

\[
\hat{y}(x) = \frac{1}{K} \sum_{h=1}^{K} Q_h(x)
\]

(6)

Let \( \Theta \) represents all parameters \((A, b, Q)\), then the final loss would be represented by the general form of formula 7

\[
L(\Theta : x, y) = \frac{1}{K} \sum_{h=1}^{K} L_h(\Theta : x, y) = \frac{1}{K} \sum_{h=1}^{K} L_h(A, b, Q : x, y)
\]

(7)

where \( L : \mathbb{R}^F \rightarrow \mathbb{R} \) is a function that maps vector to object value. In the case of classification problem, the classical function of \( L \) is cross-entropy. For regression problem, \( L \) maybe mse, mae, huber loss or others. To minimize the loss in formula 7, we use stochastic gradient descent (SGD) method to train this model.

### 2.3 Algorithm of response augmented differentiable forest

As a specified case of nTM, RaDF would also be trained by SGD just like neural network. The main difference in the implementation is the update process of controller.

Based on the general loss function defined in formula 8, we use stochastic gradient descent method \[27, 28\] to reduce the loss. As formula 8 shows, update all parameters \( \Theta \) batch by batch:

\[
\Theta^{t+1} = \Theta^t - \eta \sum_{(x, y) \in B} \frac{\partial L}{\partial \Theta}(\Theta^t; x, y)
\]

(8)
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where $\mathcal{B}$ is the current batch, $\eta$ is the learning rate, $(x, y)$ is the sample in current batch.

The detailed algorithm is as follows:

Algorithm 1 Implementation of response augmented differentiable forest

**Input:** input training, validation and test dataset

**Output:** learned model: response bank $Q$ in external memory and threshold values $b$

1: Init feature weight matrix $A$
2: Init response bank $Q$ at external memory. Each leaf node has its response stored in one cell of $Q$.
3: Init threshold values $b$
4: Init time step $t = 0$
5: while not converge do
6:     for each batch do
7:         Calculate gating value at each internal node
8:         $g(A, x, b) = \sigma(Ax - b)$
9:         Calculate probability at each leaf node
10:        $p_j = \prod_{n \in \{n_1, \ldots, n_d\}} g_n$
11:        Read response bank $Q$, update prediction of each tree
12:        $\hat{y}_h(x) = \sum_{j \text{ is leaf}} p_j Q_j$
13:        Calculate the loss $L$
14:        Backpropagate to get the gradient
15:        $(\delta A, \delta b, \delta Q) \leftarrow \delta L$
16:        Update weight of each response cell $w^t_i$
17:        Update response bank $Q$ with erase vector $e_t$ and add vector $a_t$
18:        $Q^t_i = Q^t_{i-1} [1 - w^t_i e_t] + w^t_i a_t$
19:        Update the parameters: $A$, $b$
20:    Evaluate loss at validation dataset
21:    $t = t + 1$
22: return learned model

3 Conclusion

In this short note, we revealed the deep connection between differentiable forest and neural turing machine. Based on the detailed analysis of both models, the Response augmented differential forest (RaDF) is actually a special case of NTM. The controller of RaDF is differentiable forest, the external memory cells of RaDF are response vectors which would be read/write by leaf nodes. This novel discovery will deepen the understanding of both two models and inspire some new algorithms. We give a detailed training algorithm of RaDF. We will give more detailed experiments in later papers.

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