Decision Machines: Interpreting Decision Tree as a Model Combination Method

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Abstract

Based on decision trees, it is efficient to handle tabular data. Conventional decision tree growth methods often result in suboptimal trees because of their greedy nature. Their inherent structure limits the options of hardware to implement decision trees in parallel. Here is a compact representation of binary decision trees to overcome these deficiencies. We explicitly formulate the dependence of prediction on binary tests for binary decision trees and construct a function to guide the input sample from the root to the appropriate leaf node. And based on this formulation we introduce a new interpretation of binary decision trees. Then we approximate this formulation via continuous functions. Finally we interpret decision tree as a model combination method. And we propose the selection-prediction scheme to unify a few learning methods.

1 Introduction

The conventional decision tree induction is to recursively partition the training set. During the tree induction, the training set is divided into smaller and smaller subsets according to the test functions of minimum split criteria until a stopping criterion is reached. As a result, it can be represented graphically as a tree and we call the terminal subsets leaf nodes. The terminal/leaf nodes take the mode of its ground truth set as the prediction value. It is greedy and data-driven. However, the trained decision tree is always implemented as a collection of ‘if-else-then’ sentences in computer. In another word, it is rule-based, which makes it friendly for us to understand and interpret. In contrast, this implementation is unfriendly for computers to execute. The duality, greedy data-driven training and hard-coded rule-based implementation, does not occur in other supervised machine learning such as deep learning methods.

To overcome the duality, there are some end-to-end training schemes for decision trees such as [36, 24, 43, 16] instead of the greedy training methods. Additionally we can vectorize the implementation of decision trees such as QuickScorer[11, 28, 30, 31] and RapidScorer[44]. These advances drive us to take
the advantages of non-greedy training and efficient vectorized implementation in purpose of boosting all the tree-based algorithms.

It is a long history to find more compact and clearer representation of decision trees [8]. In the section 2 of [14], there is an equivalent model of recursive partitioning in in the form of an expansion in a set of basis functions (as products of different step functions) by replacing the geometrical concepts of regions and splitting with the arithmetic notions of adding and multiplying. And it is to transform each tree into a well-known polynomial form in [25]. There are also some schemes to translate the decision trees into neural networks such as [20, 41, 2]. Guang-He Lee and Tommi S. Jaakkola [27] induce oblique decision trees from the derivatives of neural models. New representation form of the decision trees would bring or require new optimization and implementation methods for decision trees.

Here we show the possibility to reuse the deep learning tool kits to implement the decision trees. Our main contributions are:

- an algorithm to represent binary trees in analytic form;
- a new interpretation of binary decision trees in the error correcting output codes framework;
- an approximation of binary decision trees for non-greedy induction in the from of attention mechanism;
- a novel learning scheme to unify decision trees, mixture models and attention mechanism.

The rest is organized as follows: section 2 introduces the new conversion and interpretation; section 3 extends decision trees to differentiable trees and connects the binary trees with artificial neural network. Finally, section 4 summarizes future trend and presents our conclusions.

2 Logical Decision Machines

As mentioned before, the decision trees take the mode of the ground truth within each terminal/leaf node as the output prediction. In another word, it is the terminal/leaf node which the input samples eventually reach that determines the prediction rather than the non-terminal nodes. Note that the nature of decision tree prediction is tree traversal thus it is possible to vectorize the prediction if we can navigate the input samples to appropriate terminal/leaf nodes.

The input sample follows a path from the root to the appropriate terminal/leaf node, which we call the decision path to the leaf node.

Each decision path is equivalent to a sequence of test in decision tree.

We call the above fact the zeroth law of decision trees and it is so intuitive and obvious that we do not need a word to prove it.
2.1 Construction of Logical Decision Machines

Based on the fact (2), we will show how to represent the binary decision trees in the analytic form. The core idea is that true path is maximum likelihood path over all possible decision paths given an input. In the rest of section, we will show how to convert the given decision trees to analytic mappings.

We start with the following example.

Figure 1: A Binary Decision Tree

For example, if a sample arrives at the leaf node $v_3$ in 1, it must traverse the first, the second, the fourth and the fifth non-terminal nodes and it must pass the first and the second tests and fail the fourth and the fifth tests. Additionally, it does not take the third test for the leaf node $v_3$. In another word, it is not necessary for the leaf node $v_3$ to know the results of the third test. There are only 2 results for each test while 3 types of signal for the terminal/leaf nodes as below

1. $-1$ to represent the passed tests;
2. $+1$ to represent the failed tests;
3. $0$ to represent the absent tests.

For example, it is best to use $(-1, -1, 0, +1, +1)$ to represent the leaf node $v_3$ in 1.

Based on the fact (2), each leaf corresponds to a ternary row vector, so-called template vector of the leaf node, where the positive ones ($+1$) indicate the tests its travelers must pass; the negative ones ($-1$) indicate the tests its travelers must fail; the zeroes ($0$) indicate the tests its travelers are absent. Template
matrix $B$ of the binary decision tree consists of the template vectors of the leaf
todes as its row vectors. Here the travelers of the leaf node $n$ is referred to
the input samples which eventually reach the node $n$. The template vectors are
distinct from each other because each decision path is unique in the decision
trees.

For simplicity, we firstly consider the numerical variables to test. In decision
trees, it is only to test if the numerical variables is no greater than some given
specific threshold as shown in (1). The results of all tests are boolean, i.e., true
or false. We want to replace the test procedure with analytical representation.
The ad hoc choice is the $\text{sgn}(x)$ while it returns 0 when $x = 0$, which contradicts
with our boolean result. We can observe that the signum function $\text{sgn}(x)$ is the
subgradient of the absolute value function $|x|$ when $x \neq 0$ in $\mathbb{R}$, i.e.,

$$\text{sgn}(x) = \partial|x| = \begin{cases} -1 & \text{if } x < 0 \\ 1 & \text{if } x > 0 \end{cases}.$$  

Additionally, 0 belongs to subgradient of absolute value function at 0. Thus the
$\text{sgn}(x)$ is a special type of subgradient of absolute value function. In order to
represent the results of passed tests as $-1$s, we take $-1$ to substitute 0 in $\text{sgn}(x)$
when $x = 0$. Note that it is still a special type of subgradient of absolute value
function so we define a $\text{sgn}(x)$ in our context

$$\text{sgn}(x) = \begin{cases} -1 & \text{if } x \leq 0 \\ 1 & \text{if } x > 0 \end{cases}. \quad (1)$$

Now suppose that we want to predict the response value of the input $x$, the
input $x$ takes a series of successive tests as a path from the root to the terminal
node. If two inputs reach different leaf nodes, they must take different paths,
where there is at least one different results of the tests. It is the results of all
tests rather than the orders of tests that determine the prediction value of the
decision trees for a specific input. The travelers of a leaf node must share a
common sequence of tests and the corresponding results of these tests.

If the input takes all the tests and obtains all the results, it is supposed to
follow the ‘maximum likelihood path’. The key step is to match the test result
vector $h \in \mathbb{H}$ with the template vector $b^T \in \mathbb{H}$, where $\mathbb{H} = \{\pm 1, 0\}^{L-1}$. We
must take two numbers into consideration: (1) the total number of the nonzero
elements in template vector $b$ associated with the leaf node and (2) the total
number of test results $h_i$ which agree with the template vector $b$. We need to
count the number of agreements. Here if $h_i = b_i$, we say they match with each
other, i.e., the input sample and the leaf node achieve consensus on the $i$th test.
If these numbers are equal, it means the input would follow the corresponding
path of the template vector $b$ to the leaf node. In another word, the input
samples take all the tests and meet the requirements of the template vector. If
the template vector match with the result vector in all non-zero position, this
template vector corresponds to the maximum likelihood path. Otherwise, the
template vector does not correspond to the maximum likelihood path of the
input.
The inner product $\langle h, b^T \rangle = b \cdot h$, as a common measure of similarity, does not take the number of the tests into consideration while the cosine similarity
\[
\frac{b \cdot h}{\|b\|_2 \|h\|_2},
\]
takes the distances of both vectors into consideration. We modify the cosine similarity into so-called logical similarity
\[
LS(b, h) = \frac{b \cdot h}{\|b\|_1}. \tag{2}
\]

Here note that the $\ell_1$ norm is equal to the $\ell_0$ norm for $h \in \{\pm 1\}^{L-1}, b \in \{\pm 1, 0\}^{L-1}$. This logical similarity is limited in $[-1, 1]$ as the cosine similarity. And
\[
\frac{a \cdot b}{\|a\|_1 \|b\|_1} = \frac{\|a\|_2^2}{\|b\|_2^2} = 1 \text{ for any } b \in \mathbb{H} \text{ and } \alpha > 0; \quad \frac{a \cdot b}{\|b\|_1} = -\frac{\|b\|_2}{\|b\|_1} = -1 \text{ for any } b \in \mathbb{H} \text{ and } \alpha < 0.
\]
In contrast to symmetric distance, it is asymmetric, i.e., $LS(b, h) \neq LS(h, b)$.

In order to find the maximum likelihood path, it is necessary to compute the ‘likelihood’ of all possible paths. In another word, we need to compute the logical similarities between the result vector $h$ and the template vectors associated with the leaf nodes. Then we can find the maximum likelihood path of the input and output the prediction value.

In summary, we can reorganize the binary decision trees as following
\[
h = \text{sgn}(Sx - t)), \quad p = \text{diag}(\|B_1\|_1, \cdots, \|B_L\|_1)^{-1}Bh, \tag{3}
v[i] = v[\text{arg max } p],
\]
where $\text{diag}(\cdot)$ maps a vector to a diagonal matrix; the vector $x$ and $t$ are real vectors in $\mathbb{R}^n$; the matrix $S$ is the selection matrix of the decision tree in $\mathbb{R}^{(L-1) \times n}$; the element-wise transformation $\text{sgn}$ is the sign or signum function; the matrix $B$ is the template matrix of the decision tree in $\{\pm 1, 0\}^{L \times (L-1)}$; the vector $B_i$ is the $i$th row of the matrix $B$ for $i = 1, 2, \cdots, L$; $\| \cdot \|_1$ is the $\ell_1$ norm of real vector, i.e. the sum of absolute values; the integer $L$ is the total number of terminal/leaf nodes; the function $\text{arg max}(x)$ returns the first index of maximums in the vector $x$, i.e., $i = \text{arg max}(\tilde{v}) = \min\{j \mid \tilde{v}_j = \max(\tilde{v})\}$; the output $v[i]$ is the $i$th component of vector $v$ for $i = 1, 2, \cdots, L$. In a compact form, the equation is re-expressed as
\[
i = \text{arg max}(\tilde{B} \text{sgn}(\tilde{S}\tilde{x})),
T(x) = v[i], \tag{4}
\]
where $\tilde{B} = \text{diag}(\|B_1\|_1, \cdots, \|B_L\|_1)^{-1}B$; the augmented matrix $\tilde{S} = [S \tilde{b}] \in \mathbb{R}^{L \times (n+1)}$; the augmented vector $\tilde{x} = (x^T - 1)^T \in \mathbb{R}^{n+1}$. We call the new expression of binary decision trees logical decision machines. Note that $\text{max}(\tilde{B} \text{sgn}(\tilde{S}\tilde{x})) = 1$ and each row is a unit vector in $\tilde{B}$.

And we can embed the class labels into row vectors to make a value matrix $V$. We can define the decision trees in a compact form:
\[
c = \text{arg max}_{h \in \Delta} \left\langle h, \tilde{B} \text{sgn}(\tilde{S}\tilde{x}) \right\rangle, \quad T(x) = Vc, \tag{5}
\]
where $\Delta$ is the probability simplex defined as $\Delta = \{ h \mid h > 0, h^T \mathbf{1} = 1 \}$; $c$ is a one-hot vector with the element 1 in the position of maxima, i.e., $c = \text{one-hot}[\arg \max_i z]$; each column of $V$ is the class label embedding vector associated with some terminal leaf for classification.

In order to extend our procedure for categorical variables, we need more tricks. The direct one is to use dummy or indicator variable as used in many cases. The indirect one is to embed the categorical values to real numbers such as the hashing function. The only test of categorical variable is to judge if it is equal to some value. And categorical variables are always discrete and of finite values. For example, assume that the categorical variable is embedded in the finite number set $E = \{ e_1, \ldots, e_m \} \subset \mathbb{R}$, we need a function $I$ so that $\sgn(I(x)) = -1$ if $x = e$ and $\sgn(I(x)) = 1$ if $x \neq e$ where $e \in E$. Inspired by [37], we consider the Lagrange polynomial $L(x; e_i) = \prod_{e_j \neq e_i} x - e_j e_i - e_j$ for $e_i \in E$.

Thus we define $I(x) = 1 - L(x; e_i)$ and get

$$I(x) = 1 - L(x; e_i) = \begin{cases} 0 & \text{if } x = e_i \\ 1 & \text{if } x \neq e_i \end{cases}.$$ And we can use this technique to deal with each categorical variable in decision trees.

### 2.2 An Example of Binary Decision Trees

Suppose the input variable $x$ has 4 numerical features and the trained decision tree is as shown in the figure [4] we will take a specific example to show how logical decision machine (4) works.

The threshold vector is $t = (1, 4, 3, 2, 5)^T$. The value vector is categorical or numerical, such as $v = (v_1, v_2, v_3, v_4, v_5)^T$. The selection matrix $S$ and bit-vector matrix $B$ is

$$S = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} -1 & -1 & 0 & -1 & 0 \\ -1 & -1 & 0 & +1 & -1 \\ -1 & -1 & 0 & +1 & +1 \\ -1 & +1 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 & 0 \\ +1 & 0 & +1 & 0 & 0 \end{pmatrix},$$

respectively.

Suppose input vector $x = (2, 1, 2, 2)^T$, its prediction is $v_5$ according to the figure [4]. The computation procedure is as following

$$\tilde{h} = Sx - t = \begin{pmatrix} 1 \\ -3 \\ -1 \\ -1 \\ -3 \end{pmatrix}, \quad h = \sigma(\tilde{h}) = \begin{pmatrix} +1 \\ -1 \\ -1 \\ -1 \end{pmatrix},$$
\[
b = \text{diag}(\|B_1\|^{-1}_1, \cdots, \|B_L\|^{-1}_1)B \text{sgn}(h) = \begin{pmatrix}
\frac{1}{3} \\
0 \\
-\frac{1}{2} \\
0 \\
1 \\
0
\end{pmatrix},
\]

\[
i = \text{arg max}(b) = 5, v[i] = v_5,
\]

thus then the output is given by

\[
T(x) = v[\text{arg max}(B \text{sgn}(Sx - t))] = v_5.
\]

Here we do not specify the data types of the elements in the value vector. For regression, the value vector \( v \) is numerical; for classification, it is categorical\(^1\).

### 2.3 Template Matrix

The matrix \( B \) in (4) is called template matrix which consists of the template vectors of the leaf nodes as its row vectors. This matrix is related with the structure of decision tree. The sibling leaves share the same parent and ancestor nodes thus their template vectors share the same zero elements and the results of tests except the one corresponding to their parent node. From the computation perspective, the difference of sibling template vectors is parallel to certain unit vector(one-hot vector).

The number of non-zeroes in template vector is equal to the depth of the corresponding leaf node to the root plus 1. And the depth of binary tree is equal to the \( \infty \)-norm of the template matrix plus 1. And the following theorem is obvious.

The sum of the binary tree depth is equal to the trace of the \( BB^T \) plus the number of leaf nodes.

Based on the fact that only the sibling terminal nodes share all the tests and the only different result is returned by their parent node, We observe some facts on the template vector: (1) the template vectors associated with sibling terminal nodes are linearly independent even they share the same elements except the one corresponding to their parent node. (2) the sibling template vectors are independent of other template vectors according to the nonzero elements associated with their parent node in the sibling column vectors, which we cannot combine the zero elements in other vectors to generate. The common elements in two template vector correspond to the common ancients of leaf nodes associated with these vectors.

Another observation is that the root node will test all samples so that its corresponding results are not zero in all template vectors. In another word, there is an column vector without any 0 in the template matrix. The column vector corresponds to the results, which a nonterminal node returns for all template vectors.

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\(^1\)See more differences of classification trees and regression trees in [29].
vectors. For example, the first column of $B$ in the above subsection corresponds to the test associated with the root node, which means the test is true for the first four leaves and false for the last two ones. Thus it implies that the first four leaves belongs to left subtree of the root node and the last two ones belong to the right subtree of the root node. Every test will produce two results so each column must have at least one $1$ and $-1$. In another word, each test must be involved with at least two decision path. The number of nonzero elements in the column vectors is the number of decision path associated with the corresponding non-terminal node. The $-1$ ($1$) of row vector means that leaf is in the left(right) subtree of the corresponding non-terminal node.

Note that the template matrix $B$ is of full column rank in the above subsection. In another word, the rank of template matrix is equal to the number of nonterminal nodes. We conjecture that

The template matrix $B$ is of full column rank for any binary decision tree.

It is to say that we can use basic column operation to preserve an unique element in each column, which are in different row. Note that it is equivalent to prove the terminal nodes can be separated by the vertical line across the non-terminal nodes. In another word, each terminal node is constrained in the cell fenced on the right and left sides.

Based on these observation, it is not too difficult to recover the kinship of all nodes in binary decision methods when the template matrix is given.

Additionally, we can find the subtree is associated with the submatrix of the template matrix. For example, we can find the template matrix of the left subtree in 1 as following

$$
\begin{pmatrix}
-1 & -1 & 0 \\
-1 & +1 & -1 \\
-1 & +1 & +1 \\
+1 & 0 & 0
\end{pmatrix}
$$

2.4 Theoretical Interpretation

Now we prove the correctness of the conversion algorithms (3).

Theorem 1 The conversion algorithms (3) is correct.

Proof 2.1 We only need to prove that (1) the true path always obtains the maximum logical similarity; (2) the maximum is unique in the vector $p$ in the equation (3). Here the true path refers to the path which the input sample really follows from the root to the exit leaf node.

The logical similarity $\text{LS}(b, h)$ get the maximum if and only if $(b-h)^T b = 0$ for $b, h \in \{\pm 1, 0\}$ $L^{-1}$. The true path of the input $x$ is the path which $x$ follow from the root node to the exit leaf thus the binary test in the true path will return the same results as in the true template vector $b(x)$. Note that the elements 0es in the template vector will ignore the tests absent in its decision path so it is
not necessary for the input samples to take the same results of all tests if they reach the same leaf. In another word, the true template vector $b(x)$ coincide the non-zero element with the result vector $h$ at the same position, So the logical similarity between them is equal to 1, i.e. $LS(b(x), h) = \max(B \text{sgn}(S_y)) = 1$.

Every decision node returns the unique result: if it is true, the $-1$ is returned; if it is false, the $1$ is returned. And we modified the original sgn function to \[1\] in order to meet this requirement. And the uniqueness of the maxima of vector $p$ is because of the facts that only the true path share the same results of all binary test in its path. If the template vector is not the corresponding vector of the maximum likelihood path, then at least one result in this path conflicts with the result in the result vector $p$.

The correctness of our procedure is based on above facts.

We call this template matching interpretation of decision trees\[4\] because it is to select the prediction value based on similarity between template vectors of leaf nodes and the tests results of input samples.

In one hand, if two input samples arrive at the same terminal node, they must take the same path, i.e., they must take the same sequence of tests and get the same results. In notation, if two input sample $x, y$ arrive at the same terminal node, then $\arg \max(B \text{sgn}(Sx)) = \arg \max(B \text{sgn}(Sy))$. In another hand, if the samples take all the tests and share the same maximum similarity decision path, they must reach the same leaf associated with maximum likelihood path. In notation, if $B_s \text{sgn}(Sx) = B_s \text{sgn}(Sy) = 1$, then two input sample $x, y$ arrive at the same terminal node $i$.

And according to the proof of \[1\] we can reformulate the \[4\] as following
\[
 h = \tilde{B} \text{sgn}(\tilde{S}x), \\
 T(x) = \sum_{i=1}^{L} \delta(1 - h_i)v[i], \tag{6}
\]
where $\delta(x) = \begin{cases} 
 1 & \text{if } x = 0 \\
 0 & \text{otherwise}.
\end{cases}$

Based on \[6\] we can rewrite the additive models such as \[7\] \[9\] in analytic form
\[
 F(x) = \sum_{i=1}^{N} w_i T_i(x) \tag{7}
\]
where $w_i \in \mathbb{R}$ and the tree $T_i$ is formulated as \[6\]. There is another representation of additive trees via block matrix. For example, suppose we have two decision trees $T(x)$ and $T_s(x)$ as following
\[
 h = \tilde{B} \text{sgn}(\tilde{S}x), T(x) = \sum_{i=1}^{L} \delta(1 - h_i)v[i], \\
 h^* = \tilde{B}_s \text{sgn}(\tilde{S}_s x), T_s(x) = \sum_{i=1}^{L_s} \delta(1 - h^*_i)v^*[i],
\]
then we can add them as following
\[ h = (B \text{sgn}[S\tilde{x}]), \]
\[ T_s(x) = \frac{1}{2} \sum_{i=1}^{L} \delta(1 - h_i)v[i] + \frac{1}{2} \sum_{i=1+L}^{L+L_s} \delta(1 - \tilde{h}_i)v^*[i - L], \]
where
\[ S = \begin{pmatrix} \tilde{S} \\ \tilde{S}_s \end{pmatrix} \]
and
\[ B = \begin{pmatrix} \tilde{B} & 0 \\ 0 & \tilde{B}_s \end{pmatrix}. \]

It is also similar to the error correcting output codes (ECOC)[12, 23] framework, which is a powerful tool to deal with multi-class categorization problems. The basic idea of ternary ECOC is to associate each class \( r \) with a row of a coding matrix \( M \in \{-1, 0, +1\}^{k \times \ell} \). We briefly introduce ECOC in the algorithms(2.4).

**Algorithm 1** Ternary Error Correcting Output Codes

1. Train the binary classifier \( f_s \) for each column \( s = 1, \cdots, \ell \).
2. For training classifier \( s \), example labeled \( y \) is mapped to \( M(y, s) \). Omit examples for which \( M(y, s) = 0 \).
3. Given test example \( x \), choose the row \( y \) of \( M \) that is “closest” to binary predictions \( (f_1(x), \ldots, f_\ell(x)) \) according to some distance (e.g. modified Hamming).

The bitvector corresponds to the error-correcting code \( h \) and the bitvector matrix \( B \) corresponds to the error-correcting code matrix \( M \). All intermediate nodes are associated with binary test, which are parameterized by \( S \) and \( t \). And each binary test corresponds to one dichotomizer. In fact, there is a ternary variant of the error-correcting output codes such as [11]. The main difference between [2.4] and [4] is that the row in the code matrix \( M \) corresponds to a specific class while the row in the template matrix \( B \) corresponds to a specific leaf which is attached with label. In one hand, we can consider our method as another coding strategy of ternary error-correcting output codes. In another hand, the coding strategy such as [13] will help to find new induction methods of decision tree.

Their main difference is that each class is attached with a single codeword in ECOC while each class may be associated with multiple leaves in decision trees.
3 Analytical Decision Machines

The operator arg max(·) and sng make the decision trees different from the differentiable models such as deep neural networks.

In [36], the sign/signum function is formulated as following:

\[
\text{sgn}(\tilde{h}) = \arg \max_{\hat{h} \in \mathbb{H}} \left< h, \hat{h} \right> \quad \forall \hat{h} \in \mathbb{R}^{L-1}
\]

where \( \mathbb{H} = \{1, -1, 0\}^{L-1} \). And it is obvious that \( \text{sgn}(\tilde{h})_i = \frac{(\tilde{h})_i}{|(\tilde{h})_i|} \) except \((\tilde{h})_i = 0 \)

where the number \( \text{sgn}(\tilde{h})_i \) is the \( i \)th component of the real vector \( \tilde{h} \) and \( |(\tilde{h})_i| \)

is the absolute value of \( \tilde{h} \). However, it is not compatible with our definition in (1). For example, suppose \( \tilde{h} = (1, -1, 0)^T \), we will obtain

\[
\arg \max_{\hat{h} \in \mathbb{H}} \left< h, \hat{h} \right> = \{(1, -1, 0)^T, (1, -1, 1)^T, (1, -1, -1)^T \}
\]

where the maximizers are not unique and only the \((1, -1, 0)^T\) is our expected result. And we formulate the sign/signum function as solution to the following minimization problem

\[
\text{sgn}(\tilde{h}) = \arg \min_{\hat{h} \in [-1, 1]^{L-1}} \left< h, \hat{h} \right> \quad \text{subject to} \quad |\hat{h}| = \left< h, \hat{h} \right>, \forall \hat{h} \in \mathbb{R}^{L-1}.
\]

And we can formulate the decision tree in 3-splitting way as following

\[
T(x) = Vc, \\
\text{subject to } c = \arg \max_{h \in \Delta} \left< h, \hat{B}z \right>, \\
z = \text{sgn}(S\tilde{x}).
\]

Here \( \Delta \) is the probability simplex and \( \mathbb{H} = \{\pm 1, 0\}^{L-1} \). Other notations are explained in [5].

We formulate the dependence of prediction on binary tests explicitly

\[
T(x) = v f((\hat{B}\text{sgn}(S\tilde{x})))
\]

where the mapping \( f : \mathbb{R}^L \mapsto \mathbb{H} \) maps its maximum component to 1 and other components to 0. The only non-zero of \( f(\cdot) \) is at the index of the selected leaf. And we can obtain the upper bound on empirical loss in [36] and use the non-greedy methods therein to train the decision trees.

3.1 Construction of Analytical Decision Machines

Inspired by the soft decision tree [17], a node redirects instances to its children with some confidence calculated by a scoring function. In another word, we substitute the sgn with some differentiable functions as the following formula.

\[
i = \arg \max(\hat{B}\sigma(\tilde{S}\tilde{x})) , \quad T(x) = v[i],
\]

\footnote{As convention, the sign/signum function maps the 0 to 1 in artificial neural network community while the sign function is defined to be 0 at the original point in mathematics.}

\[
11
\]
where σ is monotonic, \(-σ(x) = σ(-x)\) and \(\lim_{x \to \infty} σ(x) = 1\). Note that we can translate any cumulative density function to the scoring function such as the hyperbolic tangent function \(σ(x) = \frac{1}{1 + \exp(-2x)} - 1\).

Saturated linear function \(σ\), an alternative to sign/signum function, is defined as following

\[
\sigma(x) = \begin{cases} 
1, & \text{if } x > \epsilon \\
\frac{1}{2}x, & \text{if } -\epsilon \leq x \leq \epsilon \\
-1, & \text{if } x < -\epsilon
\end{cases}
\]

and we can obtain

\[
\arg \max (\tilde{B} \text{sgn}(\tilde{S}x)) = \arg \max (\tilde{B} σ(\tilde{S}x))
\]

if each component does not belong to the gap interval \((-\epsilon, \epsilon)\). Here \(\epsilon\) is conventionally set to be 1 as in [6]. The gap interval \((-\epsilon, \epsilon)\) makes (10) difficult to deal with the categorical attributes. And \(\max(\tilde{B} σ(\tilde{S}x)) \leq 1\) so that we cannot extend [6] directly.

Note that in [4] the prediction phase can be regarded as an inner product

\[
v[i] = \sum_{n=1}^{L} v[n] δ_{in}
\]

where \(δ_{in} = 1\) if \(i = n\) otherwise \(δ_{in} = 0\). The operator \(\arg \max\) is equivalent to choose an one-hot vector, and such a vector is only non-zero at the index of the selected leaf. Here we do not specify the data type or any requirement on the value vector \(v\). The element \(v[i]\) can be anything such as function. Usually it is numerical for regression and categorical/discrete for classification.

In order to make (10) differentiable, we apply softmax to approximate the one-hot vector:

\[
T(x) = \sum_{i=1}^{L} e_i v_i.
\]

(11)

Here \((e_1, \cdots, e_L)^T = \text{softmax}(\frac{\tilde{B} σ(Sx-b)}{τ})\); the hyperparameter \(τ > 0\) is the temperature parameter. In another word we use the softmax function as an alternative to the navigation function in [36]. Additionally, there are a few alternatives of softmax such as [13, 21, 26].

We can regard the representation formulae (11) as the smooth version of (6) if we rewrite (11) as following

\[
\tilde{p} = \text{softmax}(\frac{\tilde{B} σ(Sx-b)}{τ}),
\]

\[
T(x) = \sum_{i=1}^{L} p_i v[i].
\]

(12)

Here \(e_i > 0\) and \(\sum_{i=1}^{L} e_i = 1\).
3.2 Connection with Attention Mechanism

We compute the similarities between the hidden vector $\sigma(Sx - b)$ and all template vectors

$$\tilde{B}\sigma(Sx - b) = \text{diag}(\|B_1\|_1, \cdots, \|B_L\|_1)^{-1}B\sigma(Sx - b)$$

$$= \left( \frac{B_1h}{\|B_1\|_1}, \cdots, \frac{B_Lh}{\|B_L\|_1} \right)^T$$

$$= (LS(B_1, h), \cdots, LS(B_L, h))^T$$

where $L$ is the number of the leaves; $h = \sigma(Sx - b)$. Here $LS(\cdot, \cdot)$ is the logical similarity defined in [2].

And we find that the decision tree (4) is in the form of hard attention mechanism [42]. Generally, the ECOC 2.4 takes the form of hard attention mechanism, although the code matrix of ECOC is to design via training diverse classifiers and code matrix is usually binary or ternary.

And we can reformulate the equation 11 in the terms of soft attention mechanism [40, 34]

$$h = \sigma(\tilde{S}\tilde{x}),$$

$$T(x) = \text{Attention}(B, h, v).$$

Here we adapt the scaled dot-product attention to the logical similarity

$$\text{Attention}(B, h, v) = v \text{softmax}(\tilde{B}\sigma(\tilde{S}\tilde{x})).$$

The first layer is a common fully connected layer with special activation function. In the terms of attention mechanism, the hidden vector $h$ is the query, and template vectors $\{B_1, \cdots, B_L\}$ are the keys. Additionally $v$ is the value vector. And it is key-value attention. In this setting, it is exactly a shallow neural network with attention mechanism.

The expression (13) describe the logical decision trees (5) if we set $\sigma = \text{sgn}$ and substitute the attention with the hard attention [39]. The logical decision machines [2] are the exact translation of decision trees while soft attention mechanism [13] is an approximation and generalization framework of decision trees. All the operators are common in deep learning such as matrix multiplication and softmax. We call those models ‘analytic decision machines’ because we describe the decision tree in the analytic way. Analytic decision machines are continuous so it is not suitable to the categorical features/attributes. And we can take advantages of the mature software infrastructure to implement decision machines at large scale. As a cost, we cannot interpret the analytic decision machines in the ECOC framework.

The representation (13) is ‘mixed-precision’ because only $B$ is 0-1 valued and the rest are real.

---

3In a vanilla binary decision tree, the selection matrix is also 0-1 valued. Here we focus on oblique/multivariate decision trees.
The work [40] inspires diverse variants of attention mechanism via modifying softmax such as [32, 46, 35, 33, 10]. So that we can use these variants to replace the softmax in [11]. Note that we use softmax to approximate the one-hot vector so we prefer the sparse alternatives to softmax. And a generalized attention equation is proposed in [22] for any similarity function as following

$$\text{Attention}(q, K, V) = \sum_{i=1}^{n} \frac{\text{sim}(K_i, q)}{\sum_{i=1}^{n} \text{sim}(K_i, q)} V_i. \quad (14)$$

Thus we say that the decision machines belong to generalized attention mechanism.

### 3.3 Extension of Decision Machines

The large scale piece-wise linear model or mixed logistic regression in [15] is also interpreted as generalized attention mechanism:

$$f(x) = \langle g(Mx), \text{softmax}(Wx) \rangle = \sum_{i=1}^{m} \frac{\exp(\langle W^T_j, x \rangle)}{\sum_{j=1}^{m} \exp(\langle W^T_j, x \rangle)} g_i(x) \quad (15)$$

where $g = \sigma(Mx)$, $g_i = \sigma(M_i x)$ and $\sigma$ is the element-wise sigmoid function. And $\langle W^T_j, x \rangle$ is the inner product. Here the value term, query term and key term is $g$, $x$, $W$, respectively. Note that the value term $h$ is the generalized linear model with the respect to the input $x$.

And its counterpart of decision trees is the generalized linear model trees in [38] where each leaf is associated with a generalized linear model rather than a constant. In the framework of [4], we can formulate the generalized linear model trees as following

$$i = \arg \max (\tilde{B} \text{sgn}(\tilde{S}x)), \quad T(x) = g_i(x), \quad (16)$$

where $g_i$ is a generalized linear model. And we can approximate the (16) in the framework of analytic decision machines [11]

$$T(x) = \sum_{j} \frac{\exp(\tilde{B}_j \sigma(Sx - b))}{\sum_i \exp(\tilde{B}_j \sigma(Sx - b))} g_j(x) \quad (17)$$

where $g_j(x)$ is the generalized linear model associated with the leaf $j$ and $\sigma$ is the modified sign function [11].

Both methods (17) and (15) share the selection and prediction procedure. Its belief is that distinct partition corresponds to different models and each model only approximates the global true model in a local region. In the selection stage, we compute weights for different models via softmax regression. Then the prediction models vote for the final result with the weights in the selection.
stage. They are conditional aggregation and mixture models. In the term of (14), they choose different similarities in the selection stage.

If the model $g_i$ is the Gaussian distribution function, then we derive the mixture density network [3].

Combining the advantages of these methods, we derive the selection-prediction model

$$T(x) = \sum_{i=1}^{n} \frac{\text{sim}(W_j, f(x))}{\sum_{j=1}^{n} \text{sim}(W_j, f(x))} g_i(x),$$

where $g_i$ is the prediction formula and the similarity function $\text{sim}(\cdot, \cdot)$ is always non-negative. Clearly it is a weighted linear combination of diverse models. And for different tasks, we can find the proper prediction formula $g_i$ for the samples clustered at the leaf $i$.

Based on above equation, we can unify ECOC[2.4], generalized attention[14], mixed logistic model (15), decision machines[16], mixture density network [3]. As an example, we can rewrite the logical decision machine

$$h = B \text{sgn}(\tilde{S}\tilde{x}),$$

$$T(x) = \sum_{i=1}^{L} \frac{\delta(1 - h_i)}{\sum_{j=1}^{L} \delta(1 - h_j)} v[i],$$

where the notations share with the 6. Here the $\text{sim}(\cdot, \cdot)$ is defined in implicit way: $\text{sim}(x, B_i) = \delta(1 - B_i \text{sgn}(\tilde{S}\tilde{x}))$.

And we can use other similarity function $\text{sim}(\cdot, \cdot)$ as an alternative to the Dirac delta function. For example, we can extend the (15) in the selection-prediction framework

$$y(x) = \sum_{i=1}^{n} \frac{\exp(-\frac{\|x-W_i\|^2}{\tau})}{\sum_{j=1}^{n} \exp(-\frac{\|x-W_j\|^2}{\tau})} g_i(x)$$

where $\tau > 0$ and $g(\cdot)$ is a generalized linear model or generalized additive model.

### 3.4 Decision Machines as Mixtures of Experts

Decision trees are viewed as a model combination method [4] in a descriptive way. Here we clarify this statement in an analytic way. In fact, ECOC is always as an ensemble methods to combine classifiers. In the term of model combination, the logical decision machine is exactly the model selection; the analytic decision machine belongs to the model averaging. In the perspective of model selection, we define the logical similarity[2] as the model selection criteria in (4). We encode the partitioning or the sequential decision in the selection matrix. And the extension of decision machines above are a weighted sum of different models. The extended scheme [18] is a mixtures-of-experts, which is closer to model averaging than the hierarchical mixtures of experts [19][5].

Here we derive the mixtures of experts [15] as an extension of decision trees. In fact they have the common basic idea – divide-and-conquer principle. The
model averaging is the generalization of the mixtures-of-experts. Generally model averaging is to aimed to handle the uncertainty of models while decision machines are originally designed as an analytic representation form of decision trees.

So the formulation 18 is a simple framework to unify decision machines, attention mechanism, model averaging and model selection. We can invent different scheme to mix the models by taking different similarity function. The component \( g_i(\cdot) \) in 18 is designed according to the learning tasks. This interpretation of decision trees helps us to extend it to learn more tasks other than regression and classification. And it also helps us to combine the ensemble learning methods.

4 Discussion and Conclusion

We represent the binary decision tree in an analytic form (3), (4). We illustrate this representation with a concrete example and explore some intrinsic properties in theory. Then we prove the equivalence of binary decision trees and two-layer networks with sign activation function 1. As a byproduct we find that binary decision tree share the implementation approach with the ECOC framework. Based on the proof of 1 we represent the additive trees in analytic form (7). By explicitly formulating the decision tree, we can obtain the upper bound on empirical loss proved in 30.

In order to make decision trees continuous we modify the logical decision machines (3), (4) via softening the \( \text{sgn} \) and \( \text{arg max} \) in (3). And we find that the analytic decision machines (10) (11) are related with generalized attention mechanism 14. And in the term of attention mathematics, we extend the value terms into generalized linear/additive models. We propose the selection-prediction scheme (15) to unify analytic decision machines (13), generalized attention mechanism 14, mixed logistic regression 15 and mixture density network 3.

It is hard for the analytic decision trees to deal with the categorical attribute and missing or incomplete data.

The future trends are to find more robust and efficient implementation of decision trees. As shown the analytic form of decision trees may help to apply regularization techniques and mixed integer programming to tree construction. It also provides some insights on the interpretation of deep learning models.

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