Online probabilistic label trees

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Abstract

We introduce online probabilistic label trees (OPLTs), an algorithm that trains a label tree classifier in a fully online manner, without any prior knowledge about the number of training instances, their features and labels. OPLTs are characterized by low time and space complexity as well as strong theoretical guarantees. They can be used for online multi-label and multi-class classification, including the very challenging scenarios of one- or few-shot learning. We demonstrate the attractiveness of OPLTs in a wide empirical study on several instances of the tasks mentioned above.

1. Introduction

In modern machine learning applications, the label space can be enormous, containing even millions of different labels. Problems of such scale are often referred to as extreme classification. Some notable examples of such problems are content annotation for multimedia search (Deng et al., 2011), tagging of text documents (Dekel & Shamir, 2010), online advertising (Beygelzimer et al., 2009; Agrawal et al., 2013), recommendation of bid words for online ads (Prabhu & Varma, 2014), and content recommendation (Weston et al., 2013). In these practical applications, learning algorithms run in rapidly changing environments. Hence, the space of labels and features might grow over time, as new data points arrive. Retraining the model from scratch every time a new label is observed is computationally expensive, requires storing all previous data points, and introduces long retention before the model can predict new labels. Therefore, it is desirable for algorithms operating in such a setting to work in an incremental fashion, efficiently adapting to the growing label and feature space.

To tackle extreme classification problems in an efficient way, we consider a class of label tree algorithms that use a hierarchical structure of classifiers to reduce the computational complexity of training and prediction. Each leaf in a label tree corresponds to one and only one label. The nodes of the tree contain classifiers that direct the test examples from the root down to the leaf nodes. We focus on a subclass of label tree algorithms that uses probabilistic classifiers. Examples of such algorithms for multi-class classification include hierarchical softmax (HSM) (Morin & Bengio, 2005), implemented for example in FASTText (Joulin et al., 2016), and conditional probability estimation trees (Beygelzimer et al., 2009). For multi-label classification this idea is known under the name of probabilistic label trees (PLTs) (Jasinska et al., 2016), and has been recently implemented in several state-of-the-art algorithms: PARABEL (Prabhu et al., 2018), EXTREMEText (Wydmuch et al., 2018), Bonsai Tree (Khandagale et al., 2019), and ATTENTIONXML (You et al., 2019). While EXTREMEText and ATTENTIONXML use incremental learning algorithms, none of them allows for extending the model with new labels. In all the above algorithm, a label tree is given before training of the node classifiers.

In this paper, we introduce online probabilistic label trees (OPLTs), an algorithm that trains a label tree classifier in a fully online manner. This means that the algorithm does not require any prior knowledge about the number of training instances, their features and labels. The tree is updated every time a new label arrives with a new example, in a similar manner as in conditional probability estimation trees (Beygelzimer et al., 2009), but the mechanism used there has been generalized to multi-label data. Similar to labels, new features are added when they are observed. This can be achieved by feature hashing (Weinberger et al., 2009) as in the popular Vowpal Wabbit package (Langford et al., 2007). This technique was successfully applied in other tree-based classifiers, like LOMTREE (Choromanska & Langford, 2015) or RECALL TREETREE (Daumé et al., 2017). We rely here on a different technique based on recent advances in the implementation of hash maps, namely the Robin Hood hashing (Celis et al., 1985).

We require the model trained by OPLT to be equivalent to a
model trained as a label tree would be known from the very beginning. In other words, the node classifiers should be exactly the same as the ones trained on the same sequence of training data using the same incremental learning algorithm, but with the tree produced by OPLT given as an input parameter before training them.

Thanks to this requirement, OPLTs posses similar guarantees as PLT in terms of computational complexity (Busa-Fekete et al., 2019) and statistical performance (Wydmuch et al., 2018).

To our best knowledge, the only algorithm that also addressed the problem of fully online learning in the extreme multi-class and multi-label setting is the recently introduced contextual memory tree (CMT) (Sun et al., 2019) which is a specific online key-value structure that can be applied to a wide spectrum of online problems. More precisely, CMT is an online algorithm that stores observed examples in the near-balanced binary tree structure that grows with each new example. The problem of mapping keys to values is converted into a collection of classification problems in the tree nodes, which predict which sub-tree contains the best value corresponding to the key. CMT has been empirically proven to be useful for the few-shot learning setting in extreme multi-classification, where it has been used directly as a classifier, and for extreme multi-label classification problems, where it has been used to augment an online one-versus-rest (OVR) algorithm. In the experimental study, we compare OPLT with its offline counterparts and CMT on both extreme multi-label classification and few-shot multi-class classification tasks.

2. Problem statement

Let \( \mathcal{X} \) denote an instance space, and let \( \mathcal{L} = [m] \) be a finite set of \( m \) class labels. We assume that an instance \( x \in \mathcal{X} \) is associated with a subset of labels \( \mathcal{L}_x \subseteq \mathcal{L} \) (the subset can be empty); this subset is often called the set of relevant or positive labels, while the complement \( \mathcal{L} \setminus \mathcal{L}_x \) is considered as irrelevant or negative for \( x \). We identify the set \( \mathcal{L}_x \) of relevant labels with the binary vector \( y = (y_1, y_2, \ldots, y_m) \), in which \( y_j = 1 \iff j \in \mathcal{L}_x \). By \( \mathcal{Y} = \{0, 1\}^m \) we denote the set of all possible label vectors. We assume that observations \( (x, y) \) are generated independently and identically according to a probability distribution \( P(x, y) \) defined on \( \mathcal{X} \times \mathcal{Y} \). Notice that the above definition of multi-label classification includes multi-class classification as a special case in which \( \|y\|_1 = 1 \). In case of extreme multi-label classification (XMLC) we assume \( m \) to be a large number (for example \( \geq 10^5 \)), but the size of the set of relevant labels \( \mathcal{L}_x \) is usually much smaller than \( m \), that is \( |\mathcal{L}_x| < m \). We use \( [n] \) to denote the set of integers from 1 to \( n \), and \( \|x\|_1 \) to denote the \( L_1 \) norm of \( x \).

3. Probabilistic label trees

We recall the definition of probabilistic label trees (PLTs), introduced in (Jasinska et al., 2016). PLTs follow a label-tree approach to efficiently solve the problem of estimation of the marginal probabilities of labels in multi-label problems. They reduce the original problem to a set of binary problems organized in the form of a rooted, leaf-labeled tree with \( m \) leaves. We denote a single tree by \( T \), a root node by \( r_T \), and the set of leaves by \( L_T \). The leaf \( l_j \in L_T \) corresponds to the label \( j \in \mathcal{L} \). The set of leaves of a (sub)tree rooted in node \( v \) is denoted by \( L_v \). The set of labels corresponding to all leaf nodes in \( L_v \) is denoted by \( \mathcal{L}_v \). The parent node of \( v \) is denoted by \( pa(v) \), and the set of child nodes by \( \text{Ch}(v) \). The path from node \( v \) to the root is denoted by \( \text{Path}(v) \). The length of the path, that is, the number of nodes on the path, is denoted by \( \text{len}_v \). The set of all nodes is denoted by \( V_T \). The degree of a node \( v \in V_T \), being the number of its children, is denoted by \( \text{deg}_v = |\text{Ch}(v)| \).

PLT uses tree \( T \) to factorize conditional probabilities of labels, \( \eta_j(x) = P(y_j = 1|x) = P(j \in \mathcal{L}_x|x) \). To this end let us define for every \( y \) a corresponding vector \( z \) of length \( |V_T| \), whose coordinates, indexed by \( v \in V_T \), are given by:

\[
    z_v = \left[ \sum_{l_j \in L_v} y_j \geq 1 \right].
\]

(1)

In other words, the element \( z_v \) of \( z \), corresponding to the node \( v \in V_T \), is set to one iff \( y \) contains at least one label corresponding to a node in \( L_v \). With the above definition, it holds for any node \( v \in V_T \) that:

\[
    \eta_v(x) = P(z_v = 1|x) = \prod_{v' \in \text{Path}(v)} \eta(x, v'),
\]

(2)

where \( \eta(x, v) = P(z_v = 1|z_{pa(v)} = 1, x) \) for non-root nodes, and \( \eta(x, v) = P(z_v = 1|x) \) for the root (see, e.g., Jasinska et al. 2016). Notice that for leaf nodes we get the conditional probabilities of values, i.e.,

\[
    \eta_{l_j}(x) = \eta_j(x), \text{ for } l_j \in L_T.
\]

(3)

For a given \( T \) it suffices to estimate \( \eta(x, v) \), for \( v \in V_T \) to train a PLT. To this end one usually uses a function class \( H : \mathbb{R}^d \rightarrow [0, 1] \) which contains probabilistic classifiers of choice, for example, logistic regression. We assign a classifier from \( H \) to each node of the tree \( T \). We index this set of classifiers by the elements of \( V_T \) as \( H = \{\hat{\eta}(v) | v \in V_T\} \). Training is performed usually on a dataset \( D = \{(x_i, y_i)\}_{i=1}^n \) consisting of \( n \) tuples of feature vector \( x_i \in \mathbb{R}^d \) and label vector \( y_i \in \{0, 1\}^m \). Because of factorization (2), node classifiers can be trained as independent tasks.

The quality of the estimates \( \hat{\eta}_j(x), j \in \mathcal{L} \), can be expressed in terms of the \( L_1 \)-estimation error in each node classifier, i.e., by \( |\eta(x, v) - \hat{\eta}_j(x, v)| \). PLTs obey the following bound (Wydmuch et al., 2018).
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Algorithm 1 IPLT.Train(T, Aonline, D)

1: \( H_T = \emptyset \) \hspace{1cm} \triangleright \text{Initialize a set of node probabilistic classifiers}
2: \textbf{for} each node \( v \in V_T \text{ do } } \hat{y}(v) = \text{NEWCLASSIFIER}(), \ H_T = H_T \cup \{ \hat{y}(v) \} \hspace{1cm} \triangleright \text{Initialize binary classifier for each node in the tree.}
3: \textbf{for } i = 1 \rightarrow n \textbf{ do}
4: \hspace{0.5cm} (P, N) = ASSIGNTONODES(T, x_i, L_{x_i}) \hspace{1cm} \triangleright \text{Compute its positive and negative nodes}
5: \hspace{0.5cm} \textbf{for } v \in P \textbf{ do } A_{\text{online}}. \text{UPDATE}(\hat{y}(v), (x_i, 1)) \hspace{1cm} \triangleright \text{Update all positive nodes with a positive update with } x_i.
6: \hspace{0.5cm} \textbf{for } v \in N \textbf{ do } A_{\text{online}}. \text{UPDATE}(\hat{y}(v), (x_i, 0)) \hspace{1cm} \triangleright \text{Update all negative nodes with a negative update with } x_i.
7: \textbf{return} H_T \hspace{1cm} \triangleright \text{Return the set of node probabilistic classifiers}

\textbf{Theorem 1.} \text{For any tree } T \text{ and } P(y|x) \text{ the following holds for } v \in V_T:

\[ |\eta_j(x) - \hat{y}_j(x)| \leq \sum_{v' \in \text{Path}(l_j)} \eta_{pa(v')}(x) |\eta(x, v') - \hat{y}(x, v')|, \]

where for the root node \( \eta_{pa(r_T)}(x) = 1 \).

Prediction for a test example \( x \) relies on searching the tree. For metrics such as precision@\( k \), the optimal strategy is to predict \( k \) labels with the highest marginal probability \( \eta_j(x) \).

To this end, the prediction procedure traverses the tree using the uniform-cost or beam search computing the top \( k \) estimates \( \hat{y}_j(x) \). We present the pseudocode of such an algorithm in Appendix B.

\section{4. Online probabilistic label trees}

A PLT model can be trained incrementally, on observations from \( D = \{(x_i, y_i)\}_{i=1}^{\infty} \), using an incremental learning algorithm \( A_{\text{online}} \) for updating the tree nodes. Such incremental PLT (IPLT) is given in Algorithm 1. In each iteration, it first identifies the set of positive and negative nodes using the \text{ASSIGNTONODES} procedure (see Appendix C for the pseudocode). The positive nodes are those for which the current training example is treated as positive (i.e., \( (x, z_v = 1) \)), while the negative nodes are those for which the example is treated as negative (i.e., \( (x, z_v = 0) \)).

Next, IPLT appropriately updates classifiers in the identified nodes. Unfortunately, the incremental training in IPLT requires the tree structure \( T \) to be given in advance.

To construct a tree at least the number \( m \) of labels needs to be known. More advanced tree construction procedures exploit additional information like feature values or label co-occurrence (Prabhu et al., 2018). In all such algorithms, the tree is built prior to the learning of node classifiers. Here, we analyze a different scenario in which an algorithm operates on a possibly infinite sequence of training instances, and the tree is constructed online, simultaneously with incremental training of node classifiers, without any prior knowledge of the set of labels or training data.

Let us denote a sequence of observations by \( S = \{(x_1, L_{x_1})\} \) and a subsequence consisting of the first \( t \) instances by \( S_t \). We use here \( L_{x_i} \) instead of \( y_i \) as the number of labels \( m \), which is also the length of \( y_i \), increases over time in this online scenario.\footnote{The same applies to \( x_i \), as the number of features also increases. However, we keep the vector notation in this case, as it does not impact the description of the algorithm.}

Furthermore, let the set of labels observed in \( S_t \) be denoted by \( L_t \), with \( L_0 = \emptyset \).

An online algorithm returns at step \( t \) a tree structure \( T_t \) constructed over labels in \( L_t \) and a set of node classifiers \( H_t \). Notice that the tree structure and the set of classifiers change in each iteration in which one or more new labels are observed. Below we discuss two properties that are desired for such online algorithms, defined in relation to the IPLT algorithm given above.

\textbf{Definition 1 (A proper online PLT algorithm).} \text{Let } T_t \text{ and } H_t \text{ be respectively a tree structure and a set of node classifiers trained on a sequence } S_t \text{ using an online algorithm } A. \text{ We say that } A \text{ is a proper online PLT algorithm, when for any } S \text{ and } t \text{ we have that}

\begin{itemize}
  \item \( l_j \in L_{T_t} \iff j \in L_t \), i.e., leaves of \( T_t \) correspond to all labels observed in \( S_t \),
  \item and \( H_t \) is exactly the same as \( H = \text{IPLT.Train}(T_t, A_{\text{online}}, S_t) \), i.e., node classifiers from \( H_t \) are the same as the ones trained incrementally by Algorithm 1 on \( D = S_t \) and tree \( T_t \) given as input parameter.
\end{itemize}

In other words, we require that whatever the tree the online algorithm produces, the node classifiers should be trained in the same way as if the tree was known from the very beginning of training. Thanks to that we can control the quality of each node classifier, as we are not missing any update. Since the result of a proper online PLT is the same as of IPLT, the same statistical guarantees apply to both of them.

The above definition can be satisfied by a naive algorithm that stores all observations seen so far, use them in each iteration to build a tree and train node classifiers with the IPLT algorithm. This approach is costly in terms of both memory, used for storing \( S_t \), and time, as all computations are run from scratch in each iteration. Therefore, we also demand an online algorithm to be space and time efficient in the following sense.
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Definition 2 (An efficient online PLT algorithm). Let \( T_t \) and \( H_t \) be respectively a tree structure and a set of node classifiers trained on a sequence \( S_t \) using an online algorithm \( A \). Let \( C_s \) and \( C_l \) be the space and time training cost of IPLT trained on sequence \( S_t \) and tree \( T_t \). An online algorithm is an efficient online PLT algorithm when for any \( S \) and \( t \) we have its space and time complexity to be in constant factor of \( C_s \) and \( C_l \), respectively.

In this definition we abstract from the actual implementation of IPLT. In other words, the complexity of an efficient online PLT algorithm depends directly on design choices for IPLT. The space complexity is upperbounded by \( 2m - 1 \) (i.e., the maximum number of node models), but it also depends on the chosen type of node models and the way of storing them. Let us also notice that the definition implies that the update of a tree structure has to be in a constant factor of the training cost of a single instance.

4.1. Online tree building and training of node classifiers

Below we describe an online PLT algorithm that, as we show in subsection 4.3, satisfies both properties defined above. It is similar to the conditional probability estimation tree (CPET) (Beygelzimer et al., 2009), introduced for multi-class problems and binary trees, but extends it to multi-label problems and trees of any shape. We refer to this algorithm as OPLT.

The pseudocode is presented in Algorithms 2-6. In a nutshell, OPLT proceeds observations from \( S \) sequentially, updating node classifiers. For new incoming labels, it creates new nodes according to a chosen tree building policy which is responsible for the main logic of the algorithm.

Each new node \( v \) is associated with two classifiers, a regular one \( \eta(v) \in H_T \), and an auxiliary one \( \theta(v) \in \Theta_T \), where \( H_T \) and \( \Theta_T \) denote the corresponding sets of node classifiers. The task of the auxiliary classifiers is to accumulate positives updates. The algorithm uses them later to initialize classifiers in new nodes added to a tree. They can be removed if a given node will not be used anymore to extend the tree. A particular criterion for removing an auxiliary classifier depends, however, on a tree building policy.

OPLT.Train, outlined in Algorithm 2, administrates the entire process. It first initializes a tree with a root node \( v_r \). Only creates the corresponding classifiers, \( \eta(v_r) \) and \( \theta(v_r) \). Notice that the root has both classifiers initialized from the very beginning without a label assigned to it. Thanks to this, the algorithm can properly estimate the probability of \( P(y = 0 \mid x) \). Observations from \( S \) are proceeded sequentially in the main loop of OPLT.Train. If a new observation contains one or more new labels, then the tree structure is appropriately extended by calling UpdateTree. The node classifiers are updated in UpdateClassifiers. After each iteration \( t \), the algorithm sends \( H_T \) along with the tree structure \( T \), respectively as \( H_t \) and \( T_t \), to be used outside the algorithm for prediction tasks. We assume that tree \( T \) along with sets of its all nodes \( V_T \) and leaves \( L_T \), as well as sets of classifiers \( H_T \) and \( \Theta_T \), are accessible to all the algorithms discussed below.

Algorithm 3, UpdateTree, builds the tree structure. It iterates over all new labels from \( L_x \). If there were no labels in the sequence \( S \) before, the first new label taken from \( L_x \) is assigned to the root node. Otherwise, the tree needs to be extended by one or two nodes according to a selected tree building policy. One of these nodes is a leaf to which the new label will be assigned. There are in general three variants of performing this step illustrated in Figure 1. The first one relies on selecting an internal node \( v \) whose number of children is lower than the accepted maximum, and adding to it a child node \( v'' \) with the new label assigned to it. In the second one, two new child nodes, \( v' \) and \( v'' \), are added to a selected internal node \( v \). Node \( v' \) becomes a new parent of child nodes of the selected node \( v \), i.e., the subtree of \( v \) is moved down by one level. Node \( v'' \) is a leaf with the new label assigned to it. The third variant is a modification of the second one. The difference is that the selected node \( v \) is a leaf node. Therefore there are no children nodes to be moved to \( v' \), but label of \( v \) is reassigned to \( v' \). The \( A_{policy} \) method encodes the tree building policy, i.e., it decides which of the three variants to follow and selects the node \( v \). The additional node \( v' \) is inserted by the InsertNode method. Finally, a leaf node is added by the AddLeaf method. We discuss the three methods in more detail below.

\( A_{policy} \) returns the selected node \( v \) and a Boolean variable \( insert \), which indicates whether an additional node \( v' \) has to be added to the tree. For the first variant, \( v \) is an internal node, and \( insert \) is set to false. For the second variant, \( v \) is an internal node, and \( insert \) is set to true. For the third variant, \( v \) is a leaf node, and \( insert \) is set to true. In general, the policy can be as simple as selecting a random node or a node based on the current tree size to construct a complete tree. It can also be much more complex, guided in general by \( x \), current label \( j \), and set \( L_x \) of all labels of \( x \). Nevertheless, as mentioned before, the complexity of this step should be at most proportional to the complexity of updating the node classifiers for one label, i.e., it should be proportional to the depth of the tree. We propose two such policies later in the next subsection.

The InsertNode and AddLeaf procedures involve specific operations concerning initialization of classifiers in the new nodes. InsertNode is given in Algorithm 4. It inserts a new node \( v' \) as a child of the selected node \( v \). If \( v \) is a leaf, then its label is reassigned to the new node. Otherwise, all children of \( v \) become the children of \( v' \). In both
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Algorithm 2 OPLT.TRAIN($\mathcal{S}, A_{\text{online}}, A_{\text{policy}}$)

1: $r_T = \text{NEWNODE}(), V_T = \{r_T\}$  
2: $\hat{\eta}(r_T) = \text{NEWCLASSIFIER}(), H_T = \{\hat{\eta}(r_T)\}$  
3: $\theta(r_T) = \text{NEWCLASSIFIER}(), \Theta_T = \{\theta(r_T)\}$  
4: for $(x_t, L_{x_t}) \in S$ do  
5: if $L_{x_t} \setminus L_{t-1} \neq \emptyset$ then $\text{UPDATETREE}(x_t, L_{x_t}, A_{\text{policy}})$  
6: $\text{UPDATECLASSIFIERS}(x_t, L_{x_t}, A_{\text{online}})$  
7: send $H_t, T_t = H_T, V_T$  

$\triangleright$ Create the root of the tree  
$\triangleright$ Initialize a new classifier in the root  
$\triangleright$ Initialize an auxiliary classifier in the root  
$\triangleright$ For each observation in $S$  
$\triangleright$ If the observation contains new labels, add them to the tree  
$\triangleright$ Update the classifiers  
$\triangleright$ Send the node classifiers and the tree structure.

Algorithm 3 OPLT.UPDATETREE($x, L_x, A_{\text{policy}}$)

1: for $j \in L_x \setminus L_{x-1}$ do  
2: if $L_T$ is $\emptyset$ then $\text{LABEL}(r_T) = j$  
3: else  
4: $v^\prime, \text{insert} = A_{\text{policy}}(x, j, L_x)$  
5: if $\text{insert}$ then $\text{INSERTNODE}(v^\prime)$  
6: $\text{ADDLEAF}(j, v^\prime)$

$\triangleright$ For each new label in the observation  
$\triangleright$ If no labels have been seen so far, assign label $j$ to the root node  
$\triangleright$ If there are already labels in the tree.  
$\triangleright$ Select a variant of extending the tree  
$\triangleright$ Insert an additional node if needed,  
$\triangleright$ Add a new leaf for label $j$.

cases, $v'$ becomes the only child of $v$. Figure 1 illustrates inserting $v'$ as either a child of an internal node (c) or a leaf node (d). Since, the node classifier of $v'$ aims at estimating $\hat{\eta}(x, v')$, defined as $P(z_{v'} = 1 | z_{pa(v')} = 1, x)$, its both classifiers, $\hat{\eta}(v')$ and $\hat{\theta}(v')$, are initialized as copies (by calling the COPY function) of the auxiliary classifier $\hat{\theta}(v)$ of the parent node $v$. Recall that the task of auxiliary classifiers is to accumulate all positive updates in nodes, so the conditioning $z_{pa(v')} = 1$ is satisfied in that way.

Algorithm 5 outlines the AddLeaf procedure. It adds a new leaf node $v''$ for label $j$ as a child of node $v$. The classifier $\hat{\eta}(v'')$ is created as an “inverse” of the auxiliary classifier $\hat{\theta}(v)$ from node $v$. More precisely, the INVERSECLASSIFIER procedure creates a wrapper inverting the behavior of the base classifier. It predicts $1 - \hat{\eta}$, where $\hat{\eta}$ is the prediction of the base classifier, and flips the updates, i.e., positive updates become negative and negative updates become positive. Finally, the auxiliary classifier $\hat{\theta}(v'')$ of the new leaf node is initialized.

The final step in the main loop of OPLT.TRAIN updates the node classifiers. The regular classifiers, $\hat{\eta}(v) \in H_T$, are updated exactly as in IPLT.TRAIN given in Algorithm 1. The auxiliary classifiers, $\theta(v) \in \Theta_T$, are updated only in positive nodes according to their definition and purpose.

4.2. Random and best-greedy policy

We discuss two policies $A_{\text{policy}}$ for OPLT that can be treated as non-trivial generalization of the policy used in CPET to the multi-label setting. CPET builds a binary balanced tree by expanding leaf nodes, which corresponds to the use of the third variant of tree extension only. In this way, it gradually moves away labels that initially were placed close to each other. Particularly, labels of the first observed examples will finally end in leaves at the opposite sides of the tree. This may result in lowering the predictive performance and increasing training and prediction times. To address these issues, we introduce a solution, inspired by (Prabhu et al., 2018; Wydmuch et al., 2018), in which pre-leaf nodes, i.e., parents of leaf nodes, can be of much higher arity than the other internal nodes. In general, we guarantee that arity of each pre-leaf node is upperbounded by $b_{\text{max}}$, while all other internal nodes by $b$, where $b_{\text{max}} \geq b$.

Both policies, presented jointly in Algorithm 7, start with selecting one of the pre-leaves. The first policy traverses a tree from top to bottom by randomly selecting child nodes. The second policy, in turn, selects a child node using a trade-off between the balancedness of the tree and fit of $x$, i.e., the value of $\hat{\eta}(x)$:

$$\text{score}_x = (1 - \alpha)\hat{\eta}_p(x) + \alpha \frac{1}{|L_T|} \log \left( \frac{|L_{T_{\text{pa}(v)}}|}{|\text{Ch}(\text{pa}(v))|} \right)$$

where $\alpha$ is the trade-off parameter. It is worth to notice that both policies work in logarithmic time of the number of internal nodes. Moreover, we run this selection procedure only once for the current observation, regardless of the number of new labels. If the selected node $v$ has fewer leaves than $b_{\text{max}}$, both policies follow the first variant of the tree extension, i.e., they add a new child node with the new label assigned to node $v$. Otherwise, the policies follow the second variant, in which additionally, a new internal node is added as a child of $v$ with all its children inherited. In case, the selected node has only one leaf node among its children, which only happens after assigning a new label according to the second variant, the policy changes the selected node $v$ to the previously added leaf node.
The original CPET algorithm needs to maintain auxiliary classifiers in all leaf nodes, which would be very inefficient for trees with a higher degree of pre-leaf nodes.

4.3. Theoretical analysis of OPLT

The OPLT algorithm has been designed to satisfy the properness and efficiency property. The theorem below states this fact formally.

**Theorem 2.** OPLT is an proper and efficient online PLT algorithm.

We present the proof in Appendix A. To show the properness, it uses induction for both the outer and inner loop of the algorithm, where the outer loop iterates over observations \( (x_t, L_{x_t}) \), while the inner loop over new labels in \( L_x \). The key elements to prove this property are the use of the auxiliary classifiers and the analysis of the three variants of the tree structure extension. The efficiency is proved by noticing that the algorithm creates up to two new nodes per new label, each node having at most two classifiers. Therefore, the number of updates is no more than twice the number of updates in IPLT. Moreover, any node selection policy in which cost is proportional to the cost of updating IPLT classifiers for a single label meets the efficiency requirement. Notably, the policies presented above satisfy this constraint.

5. Experiments

In this section, we empirically compare OPLT and CMT on two tasks, extreme multi-label classification and few-shot multi-class classification. We implemented OPLT in C++. We use online logistic regression for node classifiers with the AdaGrad (Duchi et al., 2011) updates. For CMT, we use a Vowpal Wabbit (Langford et al., 2007) implementation, provided by courtesy of its authors. It uses linear models also incrementally updated by an Adagrad, but all model weights are stored in one large continuous array using the hashing trick. It requires, however, at least some prior knowledge about size of the feature space since the size of the array must be determined beforehand, which can be hard in a fully online setting. To address the problem of unknown features space, we store weights in OPLT in an easily extendable dictionary. To ensure good performance, we use the modern implementation of hash maps based on Robin Hood Hashing (Celis et al., 1985). It allows for very efficient insert and find operations. Since for sparse data the model sparsity increases with the depth of a tree, this solution might be much more efficient in terms of used memory than the hashing trick and does not negatively impact predictive performance.

For all experiments, we use the same hyper-parameters in OPLT. We set learning rate to 1, Adagrad’s \( \alpha \) to 0.01, the tree balancing parameter \( \alpha \) to 0.5. The only difference is the degree of pre-leaf nodes which we set to 100 in the ex-
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**Algorithm 5** OPLT\.ADDLEAF\((j, v)\)

1: \(v'' = NEW\text{NODE}(j, V_T = V_T \cup \{v''\})\)
2: \(Ch(v) = Ch(v) \cup \{v''\}, \forall v', v'', \text{LABEL}(v') = j\)
3: \(\hat{\eta}(v'') = I\text{NVERSECLASSIFIER}(\tilde{\theta}(v)), H_T = H_T \cup \{\hat{\eta}(v'')\}\)
4: \(\tilde{\theta}(v'') = N\text{EWCLASSIFIER}(\cdot), \Theta_T = \Theta_T \cup \{\tilde{\theta}(v'')\}\)
5: \(\triangleright\text{Add this node to children of } v \text{ and assign label } j \text{ to the node } v''\)
6: \(\triangleright\text{Initialize a classifier for } v''\)

**Algorithm 6** OPLT\.UPDATE\(CLASSIFIERS(\mathcal{X}, \mathcal{L}_x, A_{\text{online}})\)

1: \((P, N) = ASSIGN\text{TONODES}(T, x, \mathcal{L}_x)\)
2: for \(v \in P\) do
3: \(A_{\text{online}}.U\text{UPDATE}(\hat{\eta}(v), (x, 1))\)
4: if \(\tilde{\theta}(v) \in \Theta\) then \(A_{\text{online}}.U\text{UPDATE}(\tilde{\theta}(v), (x, 1))\)
5: for \(v \in N\) do \(A_{\text{online}}.U\text{UPDATE}(\hat{\eta}(v), (x, 0))\)
6: \(\triangleright\text{Compute its positive and negative nodes}\)
7: \(\triangleright\text{For all positive nodes}\)
8: \(\triangleright\text{If auxiliary classifier exists, update it with a positive update with } x.\)
9: \(\triangleright\text{Update all negative nodes with a negative update with } x.\)

---

**Table 1.** Datasets used for experiments on extreme multi-label classification task and few-shot multi-classification task. Notation: \(N\) – number of samples, \(m\) – number of labels, \(d\) – number of features, \(S\) – shot

| Dataset    | 1186239 | 306782 | 13330 | 203882 |
|------------|---------|--------|-------|--------|
| AmazonCat  | 14146   | 6616   | 30938 | 101938 |
| Wiki10     | 1778351 | 587084 | 325056| 161789 |
| WikiLSHTC  | 490449  | 153025 | 670091| 135909 |
| Amazon     | 97200   | 10800 | 1001  | 129    |
| WikiPara   | 10000   | 10000 | 10000 | 188084 |

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**5.1. Extreme multi-label classification**

In the extreme multi-label classification setting we compare performance in terms of precision at \(\{1, 5\}\) and running times of training and test procedures on four benchmark datasets: AmazonCat, Wiki10, WikiLSHTC and Amazon, taken from the XML repository.\(^2\) Statistics of these datasets are included in Table 1. In this setting, CMT has been originally used to augment an online one-versus-rest (OVR) algorithm. In other words, it can be treated as a specific index that enables fast prediction and speeds up training by performing a kind of negative sampling. In addition to OPLT and CMT, we also report results of IPLT and PARABEL (Prabhù et al., 2018). IPLT is implemented similarly to OPLT, but uses a tree structure built in offline mode. PARABEL is, in turn, a fully batch variant of IPLT. Not only the tree structure is built offline, but also node classifiers are trained as batch logistic regression using the LIBLINEAR library (Fan et al., 2008). We use here its variant which uses a single tree. Both IPLT and PARABEL are used with the same tree building algorithm which is based on a specific hierarchical 2-means clustering of labels (Prabhù et al., 2018). No additional data processing was used for these experiments. Results of the comparison are presented in Table 2. Unfortunately, CMT does not scale very well neither in the number of labels nor in the number of examples, resulting in much higher memory usage for massive datasets. Therefore, we managed to obtain results only for Wiki10 and AmazonCat datasets using all available 64GB of memory. OPLT with BEST- Greedy extension policy achieves results as good as PARABEL and IPLT on AmazonCat and Wiki10 datasets just after one pass over the training data. For larger datasets OPLT obtains worse results than its offline counterparts, especially on WikiLSHTC dataset. It is easy to notice that the BEST-Greedy policy outperforms the RANDOM policy, but it is worse than trees build with hierarchical 2-means clustering. OPLT trained only on one pass over training data outperforms significantly CMT trained on three passes on almost all datasets. In terms of training times OPLT is slower IPLT due to worse tree structure that requires updating of larger The prediction times seem to be the fastest for PARABEL, but this algorithm is only efficient when the test batches are sufficiently large as it needs to decompress node models during prediction.

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**5.2. Batch few-shot multi-class classification**

In the second experiment we compare OPLT with CMT on three few-shot learning multi-classification datasets: ALOI (Geusebroek et al., 2005) and the 3-shot and 5-shot versions of WikiPara. Statistics of these datasets are also included in Table 1. CMT has been proven...
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Algorithm 7 Random and Best-greedy $A_{\text{policy}}(x, j, \mathcal{L}_x)$

1: if $\text{RunFirstFor}(x)$ then \hfill $\triangleright$ If run for the first time for first time for the current observation $x$
2: \hspace{2em} $v = r_x$. \hfill $\triangleright$ Set current node $v$ to root node
3: \hspace{2em} while $\text{Ch}(v) \not\subseteq L_T \land \text{Ch}(v) = b$ do \hfill $\triangleright$ While children of the current node are not only leaf nodes and arity is equal to $b$
4: \hspace{4em} if RANDOM policy then $v = \text{SelectRandomly}(\text{Ch}(v))$ \hfill $\triangleright$ In the case of RANDOM policy randomly choose child node
5: \hspace{4em} else if $\text{Best-greedy policy then}$ \hfill $\triangleright$ In the case of BEST-GREEDY policy
6: \hspace{6em} $v = \arg \max_{x \in \text{Ch}(v)} (1 - \alpha) \eta(x) + \alpha |L_{T_{x,v}}|^{-1} (\log |L_{T_{x,v}}| - \log |\text{Ch}(v)|)$ \hfill $\triangleright$ Select child node with the best score
7: \hspace{4em} else \hfill $\triangleright$ If the same $x$ is observed as the last time
8: \hspace{6em} $v = \text{GetSelectedNode}()$ \hfill $\triangleright$ Select the node used previously
9: \hspace{2em} if $|\text{Ch}(v) \cap L_T| = 1$ then $v = v' \in \text{Ch}(v) : v' \in L_T$ \hfill $\triangleright$ If node $v$ has only one leaf change the selected node to this leaf
10: \hspace{2em} $\text{SaveSelectedNode}(v)$ \hfill $\triangleright$ Save the selected node $v$
11: \text{return} $(v, |\text{Ch}(v)| = b_{\text{max}} \lor v \subseteq L_T)$ \hfill $\triangleright$ Return selected node, if number of $v$'s children reached max. or $v$ is leaf, insert new node.

Table 2. Precision at $\{1, 5\}$ and prediction CPU time of PARABEL, PLT, CMT, OPLT for extreme multi-label classification tasks. Notation: $P@k$ – precision at $k$-position, $T$ – CPU time, $N$ – number of samples in test set, $R$ – RANDOM policy, $B$ – BEST-GREEDY policy, $p$ – number of passes over train dataset.

| Algorithm     | AmazonCat | Wiki10 | WikILSHTC | AmazonCat | Wiki10 | WikILSHTC |
|---------------|-----------|--------|-----------|-----------|--------|-----------|
| PARABEL       |           |        |           |           |        |           |
| $p = 1$       | 92.64     | 63.81  | 10.4ms    | 83.94     | 62.98  | 4.3ms     |
|               | 93.09     | 67.77  | 0.84ms    | 85.17     | 65.46  | 24.6ms    |
| $p = 3$       | 93.12     | 63.73  | 0.82ms    | 85.63     | 65.55  | 74.1ms    |
| CMT           | 87.51     | 53.99  | 0.35ms    | 80.59     | 53.85  | 10.3ms    |
| $p = 1$       | 89.43     | 54.23  | 2.67ms    | 78.86     | 55.25  | 35.1ms    |
| $p = 3$       | 92.45     | 62.64  | 2.77ms    | 84.05     | 64.16  | 30.1ms    |
| OPLT ($R$, $p = 1$) | 92.65 | 62.83  | 3.55ms    | 84.77     | 64.20  | 31.4ms    |
| OPLT ($B$, $p = 1$) | 92.65 | 62.83  | 3.55ms    | 84.77     | 64.20  | 31.4ms    |
| OPLT ($R$, $p = 3$) |        |        |           | 46.42     | 22.85  | 204.5ms   |
| OPLT ($B$, $p = 3$) |        |        |           | 53.89     | 26.24  | 181.1ms   |

Table 3. Accuracy of prediction and train and test CPU time of CMT, OPLT for few-shot multi-class classification tasks. Notation: Acc – accuracy, $T$ – CPU time, $N$ – number of samples in test set, $R$ – RANDOM policy, $B$ – BEST-GREEDY policy, $p$ – number of passes over train dataset.

| Algorithm     | ALOI | Wikipara 3-shot | Wikipara 5-shot |
|---------------|------|-----------------|-----------------|
|               | Acc  | $T_{train}$  | $T_{test}/N$   | Acc  | $T_{train}$  | $T_{test}/N$   | Acc  | $T_{train}$  | $T_{test}/N$   |
| CMT ($p = 1$) | 17.63 | 37.8s | 0.78ms | 1.89 | 6.9s | 0.31ms | 3.56 | 37.2s | 0.91ms |
| OPLT ($R$, $p = 1$) | 62.58 | 6.0s | 0.12ms | 10.01 | 6.9s | 3.64ms | 22.91 | 11.5s | 3.58ms |
| OPLT ($B$, $p = 1$) | 63.91 | 6.1s | 0.12ms | 10.01 | 6.1s | 3.14ms | 22.91 | 10.6s | 3.48ms |
| CMT ($p = 3$) | 71.98 | 207s | 0.57ms | 2.27 | 26.3s | 1.60ms | 3.96 | 96.9s | 0.66ms |
| OPLT ($R$, $p = 3$) | 66.50 | 20.3s | 0.11ms | 24.34 | 16.4s | 4.68ms | 38.67 | 27.6s | 4.67ms |
| OPLT ($B$, $p = 3$) | 67.26 | 18.1s | 0.10ms | 24.34 | 15.6s | 4.55ms | 38.67 | 27.6s | 4.52ms |

in (Sun et al., 2019) to perform better than two other logarithmic-time online multi-class classification algorithms, LOMTREE (Choromanska & Langford, 2015) and RECALL TREE (Daumé et al., 2017) on these specific datasets. We use here the same version of CMT as used in a similar experiment in the original paper (Sun et al., 2019).

Table 3 summarizes the results. On all datasets OPLT achieves better accuracy than CMT after one pass over training data. After three passes CMT outperforms OPLT on ALOI dataset, but OPLT increases its dominance on the WikiPara datasets.

6. Conclusions

In this paper, we introduced online probabilistic label trees (OPLT), an algorithm that trains a label tree classifier in a fully online manner, without any prior knowledge about the number of training instances, their features and labels. OPLT can be used for both multi-label and multi-class classification. They outperform similar CMT at the same time scaling much more efficiently on tasks with a large number of examples, features and labels.
References

Agrawal, R., Gupta, A., Prabhu, Y., and Varma, M. Multi-label learning with millions of labels: Recommending advertiser bid phrases for web pages. In 22nd International World Wide Web Conference, WWW ’13, Rio de Janeiro, Brazil, May 13-17, 2013, pp. 13–24. International World Wide Web Conferences Steering Committee / ACM, 2013.

Beygelzimer, A., Langford, J., Lifshits, Y., Sorkin, G. B., and Strehl, A. L. Conditional probability tree estimation and algorithms. In UIAI 2009, Proceedings of the Twenty-Fifth Conference on Uncertainty in Artificial Intelligence, Montreal, QC, Canada, June 18-21, 2009, pp. 51–58. AUAI Press, 2009.

Busa-Fekete, R., Dembczynski, K., Golovnev, A., Jasinska, K., Kuznetsov, M., Sviridenko, M., and Xu, C. On the computational complexity of the probabilistic label tree algorithms, 2019.

Celis, P., Larson, P.-A., and Munro, J. I. Robin hood hashing. In Proceedings of the 26th Annual Symposium on Foundations of Computer Science, SFCS ’85, pp. 281–288, USA, 1985. IEEE Computer Society. ISBN 0818608444.

Choromanska, A. and Langford, J. Logarithmic time online multiclass prediction. In Advances in Neural Information Processing Systems 28: Annual Conference on Neural Information Processing Systems 2015, December 7-12, 2015, Montreal, Quebec, Canada, pp. 55–63. AUAI Press, 2015.

Daumé, III, H., Karampatziakis, N., Langford, J., and Mineiro, P. Logarithmic time one-against-some. In Precup, D. and Teh, Y. W. (eds.), Proceedings of the 34th International Conference on Machine Learning, volume 70 of Proceedings of Machine Learning Research, pp. 923–932, International Convention Centre, Sydney, Australia, 06–11 Aug 2017. PMLR.

Dekel, O. and Shamir, O. Multiclass-multilabel classification with more classes than examples. In Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics, AISTATS 2010, Chia Laguna Resort, Sardinia, Italy, May 13-15, 2010, volume 9 of JMLR Proceedings, pp. 137–144. JMLR.org, 2010.

Deng, J., Satheesh, S., Berg, A. C., and Li, F. Fast and balanced: Efficient label tree learning for large scale object recognition. In Advances in Neural Information Processing Systems 24: 25th Annual Conference on Neural Information Processing Systems 2011. Proceedings of a meeting held 12-14 December 2011, Granada, Spain., pp. 567–575, 2011.

Duchi, J., Hazan, E., and Singer, Y. Adaptive subgradient methods for online learning and stochastic optimization. Journal of Machine Learning Research, 12(Jul): 2121–2159, 2011.

Fan, R., Chang, K., Hsieh, C., Wang, X., and Lin, C. LIBLINEAR: A library for large linear classification. Journal of Machine Learning Research, 9:1871–1874, 2008.

Geusebroek, J.-M., Burghouts, G., and Smeulders, A. The amsterdam library of object images. Int. J. Comput. Vision, 61(1):103–112, 2005. ISSN 0920-5691. doi: 10.1023/B:VISI.0000042993.50813.60.

Jasinska, K., Dembczynski, K., Busa-Fekete, R., Pfannschmidt, K., Klerx, T., and Hüllermeier, E. Extreme F-measure maximization using sparse probability estimates. In Proceedings of the 33rd International Conference on Machine Learning, ICML 2016, New York City, NY, USA, June 19-24, 2016, volume 48 of JMLR Workshop and Conference Proceedings, pp. 1435–1444. JMLR.org, 2016.

Joulin, A., Grave, E., Bojanowski, P., and Mikolov, T. Bag of tricks for efficient text classification. CoRR, abs/1607.01759, 2016.

Khandagale, S., Xiao, H., and Babbar, R. Bonsai - diverse and shallow trees for extreme multi-label classification. CoRR, abs/1904.08249, 2019.

Langford, J., Strehl, A., and Li, L. Vowpal wabbit, 2007.

Morin, F. and Bengio, Y. Hierarchical probabilistic neural network language model. In Proceedings of the Tenth International Workshop on Artificial Intelligence and Statistics, AISTATS 2005, Bridgetown, Barbados, January 6-8, 2005. Society for Artificial Intelligence and Statistics, 2005.

Prabhu, Y. and Varma, M. Fastxml: a fast, accurate and stable tree-classifier for extreme multi-label learning. In The 20th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, KDD ’14, New York, NY, USA - August 24 - 27, 2014, pp. 263–272. ACM, 2014.

Prabhu, Y., Kag, A., Harsola, S., Agrawal, R., and Varma, M. Parabel: Partitioned label trees for extreme classification with application to dynamic search advertising. In Proceedings of the 2018 World Wide Web Conference on World Wide Web, WWW 2018, Lyon, France, April 23-27, 2018, pp. 993–1002. ACM, 2018.

Sun, W., Beygelzimer, A., Iii, H. D., Langford, J., and Mineiro, P. Contextual memory trees. In Chaudhuri, K. and Salakhutdinov, R. (eds.), Proceedings of
the 36th International Conference on Machine Learning, volume 97 of Proceedings of Machine Learning Research, pp. 6026–6035, Long Beach, California, USA, 09–15 Jun 2019. PMLR.

Weinberger, K. Q., Dasgupta, A., Langford, J., Smola, A. J., and Attenberg, J. Feature hashing for large scale multi-task learning. In Proceedings of the 26th Annual International Conference on Machine Learning, ICML 2009, Montreal, Quebec, Canada, June 14-18, 2009, volume 382 of ACM International Conference Proceeding Series, pp. 1113–1120. ACM, 2009.

Weston, J., Makadia, A., and Yee, H. Label partitioning for sublinear ranking. In Proceedings of the 30th International Conference on Machine Learning, ICML 2013, Atlanta, GA, USA, 16-21 June 2013, volume 28 of JMLR Workshop and Conference Proceedings, pp. 181–189. JMLR.org, 2013.

Wydmuch, M., Jasinska, K., Kuznetsov, M., Busa-Fekete, R., and Dembczynski, K. A no-regret generalization of hierarchical softmax to extreme multi-label classification. In Bengio, S., Wallach, H., Larochelle, H., Grauman, K., Cesa-Bianchi, N., and Garnett, R. (eds.), Advances in Neural Information Processing Systems 31, pp. 6355–6366. Curran Associates, Inc., 2018.

You, R., Zhang, Z., Wang, Z., Dai, S., Mamitsuka, H., and Zhu, S. Attentionxml: Label tree-based attention-aware deep model for high-performance extreme multi-label text classification. In Wallach, H., Larochelle, H., Beygelzimer, A., d Alché-Buc, F., Fox, E., and Garnett, R. (eds.), Advances in Neural Information Processing Systems 32, pp. 5812–5822. Curran Associates, Inc., 2019.
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A. The proof of the result from Section 4.3

Theorem 2 concerns two properties, properness and efficiency, of an OPLT algorithm. We first prove that the OPLT algorithm satisfies each of the property in two separate lemmas. The final proof of the theorem is then straight-forward.

**Lemma 1.** OPLT is a proper OPLT algorithm.

*Proof.* We need to show that for any $S$ and $t$ the two of the following hold. Firstly, that the set $L_{T_t}$ of leaves of tree $T_t$ built by OPLT correspond to $L_t$, the set of all labels observed in $S_t$. Secondly, that the set $H_t$ of classifiers trained by OPLT is exactly the same as $H = \text{IPLTTrain}(T_t, A_{\text{online}}, S_t)$, i.e., the set of node classifiers trained incrementally by Algorithm 1 on $D = S_t$ and tree $T_t$ given as input parameter. We will prove it by induction with the base case for $S_0$ and the induction step for $S_t$, $t \geq 1$, with the assumption that the statement holds for $S_{t-1}$.

For the base case of $S_0$, tree $T_0$ is initialized with the root node $r_T$ with no label assigned and set $H_0$ of node classifiers with a single classifier assigned to the root. As there are no observations, this classifier receives no updates. Now, notice that IPLT.Train, run on $T_0$ and $S_0$, returns exactly the same set of classifiers $H$ that contains solely the initialized root node classifier without any updates (assuming that initialization procedure is always the same). There are no labels in any sequence of 0 observations and also $T_0$ has no label assigned.

The induction step is more involved as we need to take into account the internal loop which extends the tree with new labels. Let us consider two cases. In the first one, observation $(x_t, L_{x_t})$ does not contain any new label. This means that the tree $T_{t-1}$ will not change, i.e., $T_{t-1} = T_t$. Moreover, node classifiers from $H_{t-1}$ will get the same updates for $(x_t, L_{x_t})$ as classifiers in IPLT.Train, therefore $H_t = \text{IPLTTrain}(T_t, A_{\text{online}}, S_t)$. It also holds that $l_j \in L_{t-1}$ if and only if $l_j \in L_t$, since $L_{t-1} = L_t$. In the second case, observation $(x_t, L_{x_t})$ has $m' = |L_{x_t} \setminus L_{t-1}|$ new labels. Let us make the following assumption for the UPDATE_TREE procedure, which we later prove that it indeed holds. Namely, we assume that the set $H_t'$ of classifiers after calling the UPDATE_TREE procedure is the same as the one being returned by IPLT.Train($T_t, A_{\text{online}}, S_{t-1}$), where $T_t$ is the extended tree. Moreover, leaves of $T_t$ correspond to all observed labels seen so far. If this is the case, the rest of the induction step is the same as in the first case. All updates to classifiers in $H_t'$ for $(x_t, L_{x_t})$ are the same as in IPLT.Train. Therefore $H_t = \text{IPLTTrain}(T_t, A_{\text{online}}, S_t)$.

Now, we need to show that the assumption for the UPDATE_TREE procedure holds. To this end we also use induction, this time on the number $m'$ of new labels. For the base case, we take $m' = 1$. The induction step is proved for $m' > 1$ with the assumption that the statement holds for $m' - 1$.

For $m' = 1$ we need consider two scenarios. In the first scenario, the new label is the first label in the sequence. This label will be then assigned to the root node $r_T$. So, the structure of the tree does not change, i.e., $T_{t-1} = T_t$. Furthermore, the set of classifiers also does not change, since the root classifier has already been initialized. It might be negatively updated by previous observations. Therefore, we have $H_t = \text{IPLTTrain}(T_t, A_{\text{online}}, S_{t-1})$. Furthermore, all observed labels are appropriately assigned to the leaves of $T_t$. In the second scenario, set $L_{t-1}$ is not empty. We need to consider in this scenario the three variants of tree extension illustrated in Figure 1.

In the first variant, tree $T_{t-1}$ is extended by one leaf node only without any additional ones. ADD_NODE creates a new leaf node $v''$ with the new label assigned to the tree. After this operation the tree contains all labels from $S_t$. The new leaf $v''$ is added as a child of the selected node $v$. This new node is initialized as $\hat{\eta}(v'') = \text{INVERSECLASSIFIER}((\theta(v)))$. Recall that INVERSECLASSIFIER creates a wrapper that inverts the behavior of the base classifier. It predicts $1 - \hat{\eta}$, where $\hat{\eta}$ is the prediction of the base classifier, and flips the updates, i.e., positive updates become negative and negative updates become positive. From the definition of the auxiliary classifier, we know that $\theta(v)$ has been trained on all positives updates of $\hat{\eta}(v)$. So, $\hat{\eta}(v'')$ is initialized with a state as if it was updated negatively each time $\hat{\eta}(v)$ was updated positively in sequence $S_{t-1}$. Notice that in $S_{t-1}$ there is no observation labeled with the new label. Therefore $\hat{\eta}(v'')$ is the same as if it was created and updated using IPLT.Train. There are no other operations on $T_{t-1}$, so we have that $H_t' = \text{IPLTTrain}(T_t, A_{\text{online}}, S_{t-1})$.

In the second variant, tree $T_{t-1}$ is extended by internal node $v'$ and leaf node $v''$. The internal node $v'$ is added in INSERT_NODE. It becomes a parent of all child nodes of the selected node $v$ and the only child of this node. Thus, all leaves of the subtree of $v$ does not change. Since $v'$ is the root of this subtree, its classifier $\hat{\eta}(v')$ should be initialized as a copy of the auxiliary classifier $\theta(v)$, which has accumulated all updates from and only from observations with labels assigned to the leaves of this subtree. Addition of the leaf node $v''$ can be analyzed as in the first variant. Since nothing else has changed in the tree and in the node classifiers, we have that $H_t' = \text{IPLTTrain}(T_t, A_{\text{online}}, S_{t-1})$. Moreover, the tree contains the new label, so the statement holds.
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The third variant is similar to the second one. Tree $T_{i-1}$ is extended by two leaf nodes $v'$ and $v''$ being children of the selected node $v$. Insertion of leaf $v'$ is similar to insertion of node $v'$ in the second variant, with the difference that $v$ does not have any children and its label has to be reassigned to $v'$. The new classifier in $v'$ is initialized as a copy of the auxiliary classifier $\hat{\theta}(v)$, which contains all updates from and only from observations with the label assigned previously to $v$. Insertion of $v''$ is exactly the same as in the second variant. From the above, we conclude that $H_{i'} = IPLT.T_{\text{TRAIN}}(T_t, A_{\text{online}}, S_{t-1})$ and that $T_t$ contains all labels from $T_{t-1}$ and the new label. In this way we prove the base case.

The induction step is similar to the second scenario of the base case. The only difference is that we do not extend tree $T_{i-1}$, but an intermediate tree with $m' - 1$ new labels already added. Because of the induction hypothesis, the rest of the analysis of the three variants of tree extension is exactly the same. This ends the proof that the assumption for the inner loop holds. At the same time it finalizes the entire proof.

**Lemma 2.** IPLT is an efficient IPLT algorithm.

**Proof.** The IPLT maintains one additional classifier per each node in comparison to IPLT. Hence, for a single observation there is at most one update more for each positive node. Furthermore, the time and space cost of the complete tree building policy is constant per a single label, if implemented with an array list. In this case, insertion of any new node can be made in amortized constant time, and the space required by the array list is linear in the number of nodes. Concluding the above, the time and space complexity of IPLT is in constant factor of $C_t$ and $C_s$, the time and space complexity of IPLT respectively. This proves that IPLT is an efficient IPLT algorithm.

**Theorem 2.** IPLT is an proper and efficient online PLT algorithm.

**Proof.** The theorem directly follows from Lemma 1 and Lemma 2.

**B. Prediction in PLT**

Algorithm 8 outlines the prediction procedure for PLTs that returns top $k$ labels. It is based on the uniform-cost search. Alternatively, one can use beam search.

**Algorithm 8 IPLT/OPLT.PREDICTTOPLABELS($T, H, k, x$)**

1. $\hat{y} = 0$, $Q = \emptyset$, $\hat{y}$ Initialize prediction vector to all zeros and a priority queue
2. $k' = 0$, $\hat{y}$ Initialize counter of predicted labels
3. $Q$.add($((r_x, \hat{y}(x), r_x))$) $\triangleright$ Add the tree root with the corresponding estimate of probability
4. **while** $k' < k$ **do** $\triangleright$ While the number of predicted labels is less than $k$
5. **if** $v$ is a leaf **then** $\triangleright$ Pop the top element from the queue
6. $\hat{y}_v = 1$, $\triangleright$ If the node is a leaf
7. $\hat{y}_v = 1$, $\triangleright$ If the node is an internal node
8. $k' = k' + 1$, $\triangleright$ For all child nodes
9. **else** $\triangleright$ Compute $\hat{y}_v(x)$ using $\hat{y}(v') \in H$
10. **for** $v' \in \text{Ch}(v)$ **do** $\triangleright$ Add the node and the computed probability estimate
11. $\tilde{\hat{y}}_{v'}(x) = \hat{y}_v(x) \times \hat{\theta}(x, v')$ $\triangleright$ Return the prediction vector
12. $Q$.add($((v', \tilde{\hat{y}}_{v'}(x)))$)
13. **return** $\hat{y}$

**C. Training in PLT**

Training of PLTs relies on a proper assignment of training examples to nodes. Algorithm 9 outlines such a procedure for a single training example, which identifies the set of positive and negative nodes, i.e., the nodes for which the training example is treated respectively as positive (i.e., $(x, z_v = 1)$) or negative (i.e., $(x, z_v = 0)$).

Theorem 2. OPLT is an proper and efficient online PLT algorithm.

**Proof.** The theorem directly follows from Lemma 1 and Lemma 2.

**B. Prediction in PLT**

Algorithm 8 outlines the prediction procedure for PLTs that returns top $k$ labels. It is based on the uniform-cost search. Alternatively, one can use beam search.

**Algorithm 8 IPLT/OPLT.PREDICTTOPLABELS($T, H, k, x$)**

1. $\hat{y} = 0$, $Q = \emptyset$, $\hat{y}$ Initialize prediction vector to all zeros and a priority queue
2. $k' = 0$, $\hat{y}$ Initialize counter of predicted labels
3. $Q$.add($((r_x, \hat{y}(x), r_x))$) $\triangleright$ Add the tree root with the corresponding estimate of probability
4. **while** $k' < k$ **do** $\triangleright$ While the number of predicted labels is less than $k$
5. **if** $v$ is a leaf **then** $\triangleright$ Pop the top element from the queue
6. $\hat{y}_v = 1$, $\triangleright$ If the node is a leaf
7. $\hat{y}_v = 1$, $\triangleright$ If the node is an internal node
8. $k' = k' + 1$, $\triangleright$ For all child nodes
9. **else** $\triangleright$ Compute $\hat{y}_v(x)$ using $\hat{y}(v') \in H$
10. **for** $v' \in \text{Ch}(v)$ **do** $\triangleright$ Add the node and the computed probability estimate
11. $\tilde{\hat{y}}_{v'}(x) = \hat{y}_v(x) \times \hat{\theta}(x, v')$ $\triangleright$ Return the prediction vector
12. $Q$.add($((v', \tilde{\hat{y}}_{v'}(x)))$)
13. **return** $\hat{y}$

**C. Training in PLT**

Training of PLTs relies on a proper assignment of training examples to nodes. Algorithm 9 outlines such a procedure for a single training example, which identifies the set of positive and negative nodes, i.e., the nodes for which the training example is treated respectively as positive (i.e., $(x, z_v = 1)$) or negative (i.e., $(x, z_v = 0)$).
Algorithm 9 IPLT/OPLT.AssignToNodes($T, x, \mathcal{L}_x$)

1: $P = \emptyset, N = \{r_T\}$  \quad \triangleright \text{Initialize sets of positive and negative nodes}
2: for $j \in \mathcal{L}_x$ do  \quad \triangleright \text{For all labels of the training example}
3: \hspace{1em} $v = \ell_j$  \quad \triangleright \text{Set } v \text{ to a leaf corresponding to label } j
4: \hspace{1em} while $v$ not null and $v \not\in P$ do  \quad \triangleright \text{On a path to the root or the first positive node (excluded)}
5: \hspace{2em} $P = P \cup \{v\}$  \quad \triangleright \text{Assign a node to positive nodes}
6: \hspace{2em} $N = N \setminus \{v\}$  \quad \triangleright \text{Remove the node from negative nodes if added there before}
7: \hspace{1em} for $v' \in \text{Ch}(v)$ do  \quad \triangleright \text{For all its children}
8: \hspace{2em} if $v' \not\in P$ then  \quad \triangleright \text{If a child is not a positive node}
9: \hspace{3em} $N = N \cup \{v'\}$  \quad \triangleright \text{Assign it to negative nodes}
10: \hspace{1em} $v = \text{pa}(v)$  \quad \triangleright \text{Move up along the path}
11: return $(P, N)$  \quad \triangleright \text{Return a set of positive and negative nodes for the training example}