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 tagging of text documents (Dekel and Shamir, 2010), content annotation for multimedia search (Deng et al., 2011), and different types of recommendation, including webpages-to-ads (Beygelzimer et al., 2009), ads-to-bid-words (Agrawal et al., 2013; Prabhu and Varma, 2014), users-to-items (Weston et al., 2013; Zhuo et al., 2020), queries-to-items (Medini et al., 2019), or items-to-queries (Chang et al., 2020). 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 efficiently, we consider a class of label tree algorithms that use a hierarchical structure of classifiers to reduce the computational complexity of training and prediction. The tree nodes contain classifiers that direct the test examples from the root down to the leaf nodes, where each leaf corresponds to one label. 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 and Bengio, 2005), implemented, for example, in fastText (Joulin et al., 2016), and conditional probability estimation tree (CPET) (Beygelzimer et al., 2009). The generalization of this idea to multi-label classification 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 some of the above algorithms use incremental procedures to train node classifiers, only CPET allows for extending the model with new labels, but it only works for multi-class classification. For all the other algorithms, a label tree needs to be given before training of the node classifiers.

In this paper, we introduce *online probabilistic label*

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trees (OPLTs), an algorithm for multi-class and multi-label problems, which 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 CPET (Beygelzimer et al., 2009), but the mechanism used there has been generalized to multi-label data. Also, 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). We rely, however, 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 tree structure 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. We refer to an algorithm satisfying this requirement as a *proper* online PLT. If the incremental tree can be built efficiently, then we additionally say that the algorithm is also *efficient*. These properties are important as a proper and efficient online PLT algorithm possesses similar guarantees as PLTs 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 addresses 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 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-class 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.

Some other existing extreme classification approaches can be tried to be used in the fully online setting, but the adaptation is not straightforward and there does not exist any such algorithm. For example, the efficient OVR approaches (e.g., DiSMEC (Babbar and Schölkopf, 2017), PPDSparse (Yen et al., 2017), ProXML (Babbar and Schölkopf, 2019)) work only in the batch mode. Interestingly, one way of obtaining a fully online OVR is to use OPLT with a 1-level tree. Popular decision-tree-based approaches, such as FastXML (Prabhu and Varma, 2014), also work in the batch mode. An exception is LOMTree (Choromanska and Langford, 2015)), which is an online algorithm. It can be adapted to the fully online setting, but as shown in (Sun et al., 2019) its performance is worse than the one of CMT. Recently, the idea of soft trees, closely related to the hierarchical mixture of experts (Jordan and Jacobs, 1994), has gained increasing attention in the deep learning community (Frosst and Hinton, 2017; Kontschieder et al., 2015; Hehn et al., 2020). However, it has been used neither in the extreme nor in the fully online setting.

The paper is organized as follows. In Section 2, we define the problem of extreme multi-label classification (XMLC). Section 3 recalls the PLT model. Section 4 introduces the OPLT algorithm, defines the desired properties and shows that the introduced algorithm satisfies them. Section 5 presents experimental results. The last section concludes the paper.

2 Extreme multi-label classification

Let $\mathcal{X}$ denote an instance space and $\mathcal{L}$ be a finite set of m labels. We assume that an instance $\boldsymbol{x} \in \mathcal{X}$ is associated with a subset of labels $\mathcal{L}_{\boldsymbol{x}} \subseteq \mathcal{L}$ (the subset can be empty); this subset is often called the set of relevant or positive labels, while the complement $\mathcal{L} \backslash \mathcal{L}_{\boldsymbol{x}}$ is considered as irrelevant or negative for $\boldsymbol{x}$. We identify the set $\mathcal{L}_{\boldsymbol{x}}$ of relevant labels with the binary vector $\boldsymbol{y} = (y_1, y_2, \ldots, y_m)$, in which $y_j = 1 \Leftrightarrow j \in \mathcal{L}_{\boldsymbol{x}}$. By $\mathcal{Y} = \{0,1\}^m$ we denote the set of all possible label vectors. We assume that observations $(\boldsymbol{x}, \boldsymbol{y})$ are generated independently and identically according to a probability distribution $\mathbf{P}(\boldsymbol{x}, \boldsymbol{y})$ 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 $\|\boldsymbol{y}\|_1 = 1$ ($\|\cdot\|$ denotes a vector norm). In case of XMLC, we assume m to be a large number but the size of the set of relevant labels $\mathcal{L}_{\boldsymbol{x}}$ is usually much smaller than m, that is $|\mathcal{L}_{\boldsymbol{x}}| \ll m$.

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 marginal probabilities of labels in

Algorithm 1 IPLT.Train($T, A_{\text{online}}, \mathcal{D}$)

```
1: H_T = ∅                                                          ▷ Initialize a set of node probabilistic classifiers
2: for v ∈ V_T do η̂(v) = NewClassifier(), H_T = H_T ∪ {η̂(v)}       ▷ Initialize binary classifier for each node in the tree
3: for i = 1 → n do                                                 ▷ For each observation in the training sequence
4:     (P, N) = AssignToNodes(T, x_i, L_{x_i})                      ▷ Compute its positive and negative nodes
5:     for v ∈ P do A_online.Update(η̂(v), (x_i, 1))                 ▷ Update all positive nodes with a positive update with x
6:     for v ∈ N do A_online.Update(η̂(v), (x_i, 0))                 ▷ Update all negative nodes with a negative update with x
7: return H_T                                                       ▷ Return the set of node probabilistic classifiers
```

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 $\mathrm{pa}(v)$, and the set of child nodes by $\mathrm{Ch}(v)$. The path from node v to the root is denoted by $\mathrm{Path}(v)$. The length of the path is the number of nodes on the path, which is denoted by 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 $\deg_v = |\mathrm{Ch}(v)|$.

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

$$z_v = [\![\textstyle\sum_{\ell_j \in L_v} y_j \geq 1]\!] \,. \tag{1}$$

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

$$\eta_v(\boldsymbol{x}) = \mathbf{P}(z_v = 1\,|\,\boldsymbol{x}) = \prod_{v' \in \mathrm{Path}(v)} \eta(\boldsymbol{x}, v') \,, \tag{2}$$

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

$$\eta_{l_j}(\boldsymbol{x}) = \eta_j(\boldsymbol{x}) \,, \quad \text{for } l_j \in L_T \,. \tag{3}$$

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

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

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

$$|\eta_j(\boldsymbol{x}) - \hat{\eta}_j(\boldsymbol{x})| \leq \sum_{v' \in \mathrm{Path}(l_j)} \eta_{\mathrm{pa}(v')}(\boldsymbol{x})\, |\eta(\boldsymbol{x}, v') - \hat{\eta}(\boldsymbol{x}, v')| \,,$$

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

Prediction for a test example $\boldsymbol{x}$ relies on searching the tree. For metrics such as precision@k, the optimal strategy is to predict k labels with the highest marginal probability $\eta_j(\boldsymbol{x})$. To this end, the prediction procedure traverses the tree using the uniform-cost search to obtain the top k estimates $\hat{\eta}_j(\boldsymbol{x})$ (see Appendix B for the pseudocode).

4 Online probabilistic label trees

A PLT model can be trained incrementally, on observations from $\mathcal{D} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i)\}_{i=1}^n$, using an incremental learning algorithm A_{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 AssignToNodes procedure (see Appendix A for the pseudocode and description). The positive nodes are those for which the current training example is treated as positive (i.e, $(\boldsymbol{x}, z_v = 1)$), while the negative nodes are those for which the example is treated as negative (i.e., $(\boldsymbol{x}, z_v = 0)$). 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; Khandagale et al., 2019). In all such algorithms, the tree is built prior to the learning of node classifiers.

Algorithm 2 OPLT.Init()

1: $r_T = \text{NewNode}()$, $V_T = \{r_T\}$ ▷ Create the root of the tree
2: $\hat{\eta}(r_T) = \text{NewClassifier}()$, $H_T = \{\hat{\eta}_T(r_T)\}$ ▷ Initialize a new classifier in the root
3: $\hat{\theta}(r_T) = \text{NewClassifier}()$, $\Theta_T = \{\theta(r_T)\}$ ▷ Initialize an auxiliary classifier in the root

Algorithm 3 OPLT.Train($\mathcal{S}, A_{\text{online}}, A_{\text{policy}}$)

1: **for** $(\boldsymbol{x}_t, \mathcal{L}_{\boldsymbol{x}_t}) \in \mathcal{S}$ **do** ▷ For each observation in $\mathcal{S}$
2: **if** $\mathcal{L}_{\boldsymbol{x}_t} \setminus \mathcal{L}_{t-1} \neq \emptyset$ **then** UpdateTree($\boldsymbol{x}_t, \mathcal{L}_{\boldsymbol{x}_t}, A_{\text{policy}}$) ▷ If the obser. contains new labels, add them to the tree
3: UpdateClassifiers($\boldsymbol{x}_t, \mathcal{L}_{\boldsymbol{x}_t}, A_{\text{online}}$) ▷ Update the classifiers
4: **send** $H_t, T_t = H_T, V_T$ ▷ Send the node classifiers and the tree structure

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 $\mathcal{S} = \{(\boldsymbol{x}_i, \mathcal{L}_{\boldsymbol{x}_i})\}_{i=1}^{\infty}$ and a subsequence consisting of the first t instances by $\mathcal{S}_t$. We use here $\mathcal{L}_{\boldsymbol{x}_i}$ instead of $\boldsymbol{y}_i$ as the number of labels m, which is also the length of $\boldsymbol{y}_i$, increases over time in this online scenario.[1] Furthermore, let the set of labels observed in $\mathcal{S}_t$ be denoted by $\mathcal{L}_t$, with $\mathcal{L}_0 = \emptyset$. An online algorithm returns at step t a tree structure T_t constructed over labels in $\mathcal{L}_t$ 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.

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

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

In other words, we require that whatever 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 model produced by 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, uses them in each iteration to build a tree and train node classifiers with the IPLT algorithm from scratch. This approach is costly. Therefore, we also demand an online algorithm to be space and time-efficient in the following sense.

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 $\mathcal{S}_t$ using an online algorithm B. Let C_s and C_t be the space and time training cost of IPLT trained on sequence $\mathcal{S}_t$ 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_t, 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 upper bounded 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 CPET (Beygelzimer et al., 2009), 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 2-7. In a nutshell, OPLT proceeds observations from $\mathcal{S}$ se-

[1] The same applies to $\boldsymbol{x}_i$ as the number of features also increases. However, we keep the vector notation in this case, as it does not impact the algorithm's description.

Algorithm 4 OPLT.UPDATETREE($\boldsymbol{x}, \mathcal{L}_{\boldsymbol{x}}, A_{\text{policy}}$)

for $j \in \mathcal{L}_{\boldsymbol{x}} \setminus \mathcal{L}_{t-1}$ **do** ▷ For each new label in the observation
  if $\mathcal{L}_T = \emptyset$ **then** LABEL(r_T) $= j$ ▷ If no labels have been seen so far, assign label j to the root node
  else ▷ If there are already labels in the tree
    v, *insert* $= A_{\text{policy}}(\boldsymbol{x}, j, \mathcal{L}_{\boldsymbol{x}})$ ▷ Select a variant of extending the tree
    if *insert* **then** INSERTNODE(v) ▷ Insert an additional node if needed
    ADDLEAF(j, v) ▷ Add a new leaf for label j

Algorithm 5 OPLT.INSERTNODE(v)

$v' =$ NEWNODE(), $V_T = V_T \cup \{v'\}$ ▷ Create a new node and add it to the tree nodes
if ISLEAF(v) **then** LABEL(v') = LABEL(v), LABEL(v) = NULL ▷ If node v is a leaf reassign label of v to v'
else ▷ Otherwise
  $\mathrm{Ch}(v') = \mathrm{Ch}(v)$ ▷ All children of v become children of v'
  for $v_{\text{ch}} \in \mathrm{Ch}(v')$ **do** $\mathrm{pa}(v_{\text{ch}}) = v'$ ▷ And v' becomes their parent
$\mathrm{Ch}(v) = \{v'\}$, $\mathrm{pa}(v') = v$ ▷ The new node v' becomes the only child of v
$\hat{\eta}(v') = \mathrm{COPY}(\hat{\theta}(v))$, $H_T = H_T \cup \{\hat{\eta}(v')\}$ ▷ Create a classifier
$\hat{\theta}(v') = \mathrm{COPY}(\hat{\theta}(v))$, $\Theta_T = \Theta_T \cup \{\hat{\theta}(v')\}$ ▷ And an auxiliary classifier

quentially, 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 $\hat{\eta}(v) \in H_T$, and an *auxiliary* one $\hat{\theta}(v) \in \Theta_T$, where H_T and Θ_T denote the corresponding sets of node classifiers. The task of the auxiliary classifiers is to accumulate positive updates. The algorithm uses them later to initialize classifiers associated with 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.

The algorithm starts with OPLT.INIT procedure, presented in Algorithm 2, that initializes a tree with only a root node v_{r_T} and corresponding classifiers, $\hat{\eta}(v_{r_T})$ and $\hat{\theta}(v_{r_T})$. 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 $\mathbf{P}(\boldsymbol{y} = \mathbf{0} \mid \boldsymbol{x})$. From now on, OPLT.TRAIN, outlined in Algorithm 3, administrates the entire process. In its main loop, observations from $\mathcal{S}$ are proceeded sequentially. 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 Θ_T, are accessible to all the algorithms discussed below.

Algorithm 4, UPDATETREE, builds the tree structure. It iterates over all new labels from $\mathcal{L}_{\boldsymbol{x}}$. If there were no labels in the sequence $\mathcal{S}$ before, the first new label taken from $\mathcal{L}_{\boldsymbol{x}}$ 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 $\boldsymbol{x}$, current label j, and set $\mathcal{L}_{\boldsymbol{x}}$ of all labels of $\boldsymbol{x}$. Nevertheless, as mentioned before, the complexity of this

Algorithm 6 OPLT.AddLeaf(j, v)

```
v'' = NewNode(), V_T = V_T ∪ {v''}                         ▷ Create a new node and add it to the tree nodes
Ch(v) = Ch(v) ∪ {v''}, pa(v'') = v, Label(v'') = j          ▷ Add this node to children of v and assign label j to the node v''
η̂(v'') = InverseClassifier(θ̂(v)), H_T = H_T ∪ {η̂(v'')}     ▷ Initialize a classifier for v''
θ̂(v'') = NewClassifier(), Θ_T = Θ_T ∪ {θ̂(v'')}             ▷ Initialize an auxiliary classifier for v''
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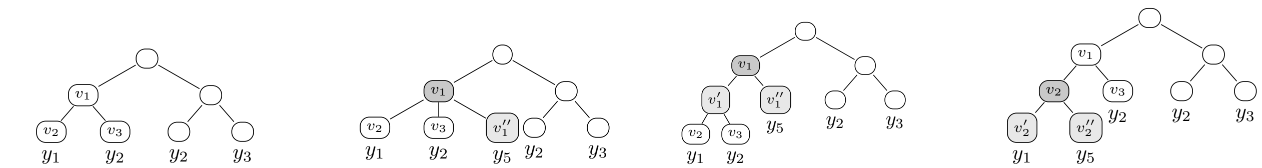

(a) Tree T_{t-1} after $t-1$ iterations.

(b) Variant 1: A leaf node v_1'' for label j added as a child of an internal node v_1.

(c) Variant 2: A leaf node v_1'' for label j and an internal node v_1' (with all children of v_1 reassigned to it) added as children of v_1.

(d) Variant 3: A leaf node v_2'' for label j and a leaf node v_2' (with a reassigned label of v_2) added as children of v_2.

Figure 1: Three variants of tree extension for a new label j.

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 in the next subsection.

The InsertNode and AddLeaf procedures involve specific operations initializing classifiers in the new nodes. InsertNode is given in Algorithm 5. 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 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 $\eta(\boldsymbol{x}, v')$, defined as $\mathbf{P}(z_{v'} = 1 \,|\, z_{\mathrm{pa}(v')} = 1, \boldsymbol{x})$, 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 $z_{\mathrm{pa}(v')} = 1$ is satisfied in that way.

Algorithm 6 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.

Notice that OPLT.Train can also be run without prior initialization with OPLT.Init if only a tree with properly trained node and auxiliary classifiers is provided. One can create such a tree using a set of already available observations $\mathcal{D}$ and then learn node and auxiliary classifiers using the same OPLT.Train algorithm. Because all labels from $\mathcal{D}$ should be present in the created tree, it is not updated by the algorithm. From now on, OPLT.Train can be used again to correctly update the tree for new observations.

4.2 Random and best-greedy policy

We discuss two policies A_{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 the tree structure extension only. As the result, it gradually moves away labels that initially have been 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 the arity of each pre-leaf node is upper bounded by $b_{\max}$, while all other internal nodes by b, where $b_{\max} \geq b$.

Both policies, presented jointly in Algorithm 8, start

Algorithm 7 OPLT.UpdateClassifiers($\boldsymbol{x}, \mathcal{L}_{\boldsymbol{x}}, A_{\text{online}}$)

$(P, N) =$ AssignToNodes($T, \boldsymbol{x}, \mathcal{L}_{\boldsymbol{x}}$) ▷ Compute its positive and negative nodes
for $v \in P$ **do** ▷ For all positive nodes
  A_{online}.Update($\hat{\eta}(v), (\boldsymbol{x}, 1)$) ▷ Update classifiers with a positive update with $\boldsymbol{x}$
  if $\hat{\theta}(v) \in \Theta$ **then** A_{online}.Update($\hat{\theta}(v), (\boldsymbol{x}, 1)$) ▷ If aux. classifier exists, update it with a positive update with $\boldsymbol{x}_i$
for $v \in N$ **do** A_{online}.Update($\hat{\eta}(v), (\boldsymbol{x}, 0)$) ▷ Update all negative nodes with a negative update with $\boldsymbol{x}$

Algorithm 8 Random and Best-greedy $A_{\text{policy}}(\boldsymbol{x}, j, \mathcal{L}_{\boldsymbol{x}})$

if RunFirstFor($\boldsymbol{x}$) **then** ▷ If the algorithm is run for the first time for the current observation $\boldsymbol{x}$
  $v = r_T$ ▷ Set current node v to root node
  while $\text{Ch}(v) \nsubseteq L_T \wedge \text{Ch}(v) = b$ **do** ▷ While the node's children are not only leaf nodes and arity is equal to b
    if Random policy **then** $v =$ SelectRandomly(Ch(v)) ▷ If Random policy, randomly choose child node
    else if Best-greedy policy **then** ▷ In the case of Best-greedy policy
      $v = \arg\max_{v' \in \text{Ch}(v)} (1-\alpha)\hat{\eta}(\boldsymbol{x}, v') + \alpha |L_{v'}|^{-1} (\log |L_v| - \log |\text{Ch}(v)|)$ ▷ Select child node with the best score
else $v =$GetSelectedNode() ▷ If the same $\boldsymbol{x}$ is observed as the last time, select the node used previously
if $|\text{Ch}(v) \cap L_T| = 1$ **then** $v = v' \in \text{Ch}(v) : v' \in L_T$ ▷ If node v has only one leaf, change the selected node to this leaf
SaveSelectedNode(v) ▷ Save the selected node v
return $(v, |\text{Ch}(v)| = b_{\max} \vee v \subseteq L_T)$ ▷ Return node v, if num. of v's children reached the max. or v is a leaf, insert a new node

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 $\boldsymbol{x}$, i.e., the value of $\hat{\eta}(\boldsymbol{x}, v)$:

$$\text{score}_v = (1-\alpha)\hat{\eta}(\boldsymbol{x}, v) + \alpha \frac{1}{|L_v|} \log \frac{|L_{\text{pa}(v)}|}{|\text{Ch}(\text{pa}(v))|} \,,$$

where α is a 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_{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 adding a new label with the second variant, the policy changes the selected node v to the previously added leaf node.

The above policies have two advantages over CPET. Firstly, new labels coming with the same observation should stay close to each other in the tree. Secondly, the policies allow for efficient management of auxiliary classifiers, which basically need to reside only in pre-leaf nodes, with the exception of leaf nodes added in the second variant. The original CPET algorithm needs to maintain auxiliary classifiers in all 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 a proper and efficient online PLT algorithm.

We present the proof in Appendix C. To show the properness, it uses induction for both the outer and inner loop of the algorithm, where the outer loop iterates over observations $(\boldsymbol{x}_t, \mathcal{L}_{\boldsymbol{x}_t})$, while the inner loop over new labels in $\mathcal{L}_{\boldsymbol{x}_t}$. 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. Note that training of IPLT can be performed in logarithmic time in the number of labels under the additional assumption of using a balanced tree with constant nodes arity (Busa-Fekete et al., 2019). Because presented policies aim to build trees close to balanced, the time complexity of the OPLT training should also be close to logarithmic in the number of labels.

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++, based on recently introduced

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

Dataset	N_{train}	N_{test}	m	d
AmazonCat	1186239	306782	13330	203882
Wiki10	14146	6616	30938	101938
WikiLSHTC	1778351	587084	325056	1617899
Amazon	490449	153025	670091	135909
ALOI	97200	10800	1001	129
WikiPara-S	$S \times 10000$	10000	10000	188084

napkinXC (Jasinska-Kobus et al., 2020).[2] We use online logistic regression to train node classifiers with the AdaGrad (Duchi et al., 2011) updates.

For CMT, we use a Vowpal Wabbit (Langford et al., 2007) implementation (also in C++), provided by courtesy of its authors. It uses linear models also incrementally updated by AdaGrad, but all model weights are stored in one large continuous array using the hashing trick. However, it requires at least some prior knowledge about the 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 of OPLT in an easily extendable hash map based on Robin Hood Hashing (Celis et al., 1985), which ensures very efficient insert and find operations. Since the model sparsity increases with the depth of a tree for sparse data, 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, fixed hyper-parameters for OPLT. We set learning rate to 1, AdaGrad's ϵ to 0.01 and the tree balancing parameter α to 0.75, since more balanced trees yield better predictive performance (see Appendix F for empirical evaluation of the impact of parameter α on precision at k, train and test times, and the tree depth). The only exception is the degree of pre-leaf nodes, which we set to 100 in the XMLC experiment, and to 10 in the few-shot multi-class classification experiment. For CMT we use hyper-parameters suggested by the authors. According to the appendix of (Sun et al., 2019), CMT achieves the best predictive performance after 3 passes over training data. For this reason, we give all algorithms the maximum of 3 such passes and report the best results (see Appendix D and E for the detailed results after 1 and 3 passes). We repeated all the experiments 5 times, each time shuffling the training set and report the mean performance. We performed all the experiments on an Intel Xeon E5-2697 v3 2.6GHz machine with 128GB of memory.

5.1 Extreme multi-label classification

In the XMLC setting, we compare performance in terms of precision at $\{1, 3, 5\}$ and the training time (see Appendix D for prediction times and propensity scored precision at $\{1, 3, 5\}$) on four benchmark datasets: AmazonCat, Wiki10, WikiLSHTC and Amazon, taken from the XMLC repository (Bhatia et al., 2016). We use the original train and test splits. 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 (Prabhu 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 PLT. Not only the tree structure, but also node classifiers are trained in the batch mode using the LIBLINEAR library (Fan et al., 2008). We use a single tree variant of this algorithm. Both IPLT and Parabel are used with the same tree building algorithm, which is based on a specific hierarchical 2-means clustering of labels (Prabhu et al., 2018). Additionally, we report the results of an OPLT with warm-start (OPLT-W) that is first trained on a sample of 10% of training examples and a tree created using hierarchical 2-means clustering on the same sample. After this initial phase, OPLT-W is trained on the remaining 90% of data using the Best-greedy policy (see Appendix G for the results of OPLT-W trained with different sizes of the warm-up sample and comparison with IPLT trained only on the same warm-up sample).

Results of the comparison are presented in Table 2. Unfortunately, CMT does not scale very well 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 128GB of memory. OPLT with both extension policies achieves results as good as Parabel and IPLT and significantly outperforms CMT on AmazonCat and Wiki10 datasets. For larger datasets OPLT with Best-greedy policy outperforms the Random policy but obtains worse results than its offline counterparts, with trees built with hierarchical 2-means clustering, especially on the WikiLSHTC dataset. OPLT-W, however, achieves results almost as good as IPLT what proves that good initial structure, even with only some labels, helps to

[2] Repository with the code and scripts to reproduce the experiments: https://github.com/mwydmuch/napkinXC

Table 2: Mean precision at $\{1, 3, 5\}$ (%) and CPU train time of Parabel, IPLT, CMT, OPLT for XMLC tasks.

	AmazonCat				Wiki10				WikiLSHTC				Amazon			
Algo.	P@1	P@3	P@5	t_{train}	P@1	P@3	P@5	t_{train}	P@1	P@3	P@5	t_{train}	P@1	P@3	P@5	t_{train}
Parabel	92.58	78.53	63.90	10.8m	84.17	72.12	63.30	4.2m	62.78	41.22	30.27	14.4m	43.13	37.94	34.00	7.2m
IPLT	93.11	78.72	63.98	34.2m	84.87	74.42	65.31	18.3m	60.80	39.58	29.24	175.1m	43.55	38.69	35.20	79.4m
CMT	89.43	70.49	54.23	168.2m	80.59	64.17	55.25	35.1m	-	-	-	-	-	-	-	-
OPLT$_R$	92.66	77.44	62.52	99.5m	84.34	73.73	64.31	30.3m	47.76	30.97	23.37	330.1m	38.42	34.33	31.32	134.2m
OPLT$_B$	92.74	77.74	62.91	84.1m	84.47	73.73	64.39	27.7m	54.69	35.32	26.31	300.0m	41.09	36.65	33.42	111.9m
OPLT-W	93.14	78.68	63.92	43.7m	85.22	74.68	64.93	28.2m	59.23	38.39	28.38	205.7m	42.21	37.60	34.25	98.3m

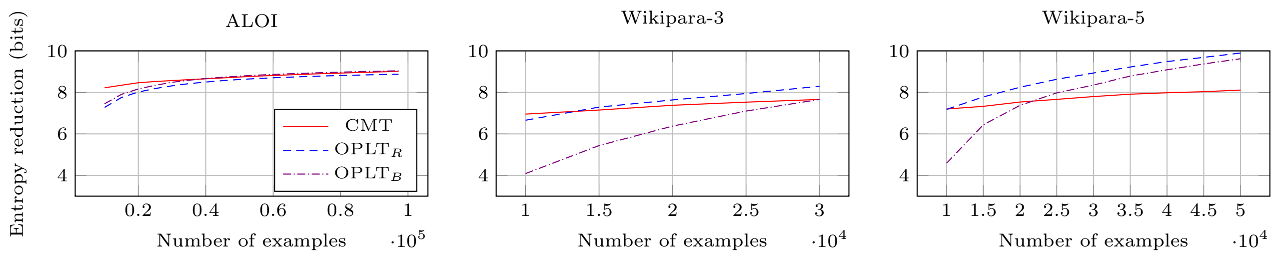

Figure 2: Online progressive performance of CMT and OPLT with respect to the number of samples on few-shot multi-class classification tasks.

Table 3: Mean accuracy of prediction (%) and train CPU time of CMT, OPLT for few-shot multi-class classification tasks.

	ALOI		Wikipara-3		Wikipara-5	
Algo.	Acc.	t_{train}	Acc.	t_{train}	Acc.	t_{train}
CMT	71.98	207.1s	3.28	63.1s	4.21	240.9s
OPLT$_R$	66.50	20.3s	27.34	16.4s	40.67	27.6s
OPLT$_B$	67.26	18.1s	24.66	15.6s	39.13	27.2s

build a good tree in an online way. In terms of training times, OPLT, as expected, is slower than IPLT due to additional auxiliary classifiers and worse tree structure, both leading to a larger number of updates.

5.2 Few-shot multi-class classification

In the second experiment, we compare OPLT with CMT on three few-shot learning multi-class datasets: ALOI (Geusebroek et al., 2005), 3 and 5-shot versions of WikiPara. Statistics of these datasets are also included in Table 1. CMT has been proven in (Sun et al., 2019) to perform better than two other logarithmic-time online multi-class algorithms, LOMTree (Choromanska and 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).

Since OPLT and CMT operate online, we compare their performance in two ways: 1) using online progressive validation (Blum et al., 1999), where each example is tested ahead of training and 2) using offline evaluation on the test set after seeing the whole training set. Figure 2 summarizes the results in terms of progressive performance. In the same fashion as in (Sun et al., 2019), we report entropy reduction of accuracy from the constant predictor, calculated as $\log_2(\text{Acc}_{\text{algo}}) - \log_2(\text{Acc}_{\text{const}})$, where Acc_{algo} and $\text{Acc}_{\text{const}}$ is mean accuracy of the evaluated algorithm and the constant predictor. In Table 3, we report results on the test datasets. In online and offline evaluation, OPLT performs similar to CMT on ALOI dataset, while it significantly dominates on the WikiPara datasets.

6 Conclusions

In this paper, we introduced online probabilistic label trees, 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 can be used for both multi-label and multi-class classification. They outperform CMT in almost all experiments, scaling at the same time much more efficiently on tasks with a large number of examples, features and labels.

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