LdSM: Logarithm-depth Streaming Multi-label Decision Trees

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Abstract

We consider multi-label classification where the goal is to annotate each data point with the most relevant subset of labels from an extremely large label set. Efficient annotation can be achieved with balanced tree predictors, i.e. trees with logarithmic-depth in the label complexity, whose leaves correspond to labels. Designing prediction mechanism with such trees for real data applications is non-trivial as it needs to accommodate sending examples to multiple leaves while at the same time sustain high prediction accuracy. In this paper we develop the LdSM algorithm for the construction and training of multi-label decision trees, where in every node of the tree we optimize a novel objective function that favors balanced splits, maintains high class purity of children nodes, and allows sending examples to multiple directions but with a penalty that prevents tree over-growth. Each node of the tree is trained once the previous one is completed leading to a streaming approach for training. We analyze the proposed method theoretically and show that minimizing the objective leads to pure and balanced data splits. Furthermore, we prove that optimizing it results in the monotonic decrease of the error with every split. Experimental results on benchmark data sets demonstrate that our approach achieves high prediction accuracy with logarithmic-depth trees and position LdSM as a competitive tool among existing state-of-the-art tree-based approaches in terms of the statistical performance and prediction time.

1 Introduction

Plethora of modern machine learning approaches are concerned with performing multi-label predictions, as is the case in recommendation or ranking systems. In multi-label setting we receive examples $x \in \mathcal{X} \subseteq \mathbb{R}^d$, with labels $y \subseteq \mathcal{Y} \equiv \{1, 2, \ldots, K\}$, where each data point $x$ is assigned a subset of labels $y$ from an extremely large label set $\mathcal{Y}$. This provides a generalization of the multi-class problem [1-4], where each data point instead corresponds to a single mutually exclusive label $\mathcal{Y}$. Employing the label hierarchy, commonly represented as a tree with leaves corresponding to labels, potentially allows for faster prediction when the hierarchy is balanced and thus the tree depth is of size $O(\log_M K)$ for $M$-ary tree, and enables overcoming the intractability problem of common baselines, such as one-against-all (OAA) [6] that requires evaluating $K$ classifiers per example. Tree-based predictors are therefore commonly used, but since the label hierarchy is unavailable most of the times, it has to be learned from the data.

The performance of the multi-label tree-based system heavily hinges on the structure of the tree [7,8]. Some approaches [9,10] assume arbitrary label hierarchy that is not learned. For example, PLT [9] considers a sparse probability estimates for F-measure maximization conditioned on the label tree. Majority of techniques however carefully design a splitting criterion that is recursively applied in every node of the tree to partition the data. These criteria differ between commonly-used tree-based

\[1\] It is non-trivial to extend multi-class trees to the multi-label setting [5] as their training and prediction mechanism is not suitable for the setting when an example is equipped with more than one label.
multi-label classification approaches. Multi-label Random Forest (MLRF) \cite{11} uses information theoretic losses, specifically the class entropy or the Gini index, to obtain label hierarchy. Sparse gradient boosted decision trees (GBDT-S) build a regression tree that fits the residuals from the previous trees and uses the multi-label hinge or squared loss. FastXML \cite{13}, PFastreXML \cite{8}, and SwiftXML \cite{14} (the last one focuses on the prediction task with partially revealed labels) constitute a family of methods that rely on ranking losses. FastXML learns a hierarchy over the feature space, rather than the label space, relying on the intuition that in each region of the feature space only a small subset of labels is active. The node objective function there promotes generalizability via standard regression loss and rank-prioritization via normalized Discounted Cumulative Gain (nDCG) ensuring that relevant positive labels for each point are predicted with high ranks. PFastreXML improves upon FastXML by replacing the nDCG loss with its propensity scored variant (the same is used in SwiftXML) which is unbiased to the missing classes and assigns higher rewards for accurate tail label predictions. None of the above techniques use balancing term in their objective.

There also exist methods that construct tree classifiers by optimizing clustering loss in nodes. Hierarchical \(k\)-means underlies CRAFTML \cite{15} and older approaches to multi-label classification such as LPSR \cite{16} and HOMER \cite{17}. This is also the case for Parabel \cite{5} and Bonsai \cite{18}, though these are hybrid techniques that combine tree approach with OAA classifier. Multi-label classification has also been addressed with other extensions of OAA \cite{19–24}, deep learning \cite{25–27} and learning embedding \cite{28–39} approaches. These and previously mentioned hybrid algorithm constitute a different family of approaches than purely tree-based techniques that our method belongs to and thus are not directly relevant to our work.

The approach we propose in this paper belongs to the family of purely tree-based methods. It partitions tree nodes based on joint optimization in the feature and label space. The node split is based on a new objective function that explores the correlation between both spaces by conditioning the learning of feature space partitioning with data label information. The objective applies to trees of arbitrary width. It explicitly enforces class purity of children nodes (i.e. points within a partition are likely to have similar labels whereas points across partitions are likely to have different labels), but at the same time, when necessary, allows sending examples to multiple children nodes. Multi-way assignment of examples is however penalized to better control tree accuracy. Finally, the objective encourages balanced partitions to ensure efficient prediction. The objective function comes with theoretical analysis. We show that optimizing the objective improves the purity and balancedness of the data splits in isolation, i.e. when respectively the balancedness and purity is fixed, and prove that when it is perfectly optimized in every tree node it leads to zero-error multi-label classification, i.e. \(R@ = 1\) \cite{40} for any \(r\). Furthermore, we show that minimizing the objective is causing the monotonic decrease of the error with every split. The resulting tree construction-and-training algorithm, that we call LdSM, results in Logarithmic-depth trees that are trained in a streaming fashion, i.e. node-by-node,\(^2\) and achieve competitive performance to other state-of-the-art tree-based approaches, being accurate and efficient at prediction, on large multi-label classification problems.

The paper is organized as follows: Section \(\square\) presents the objective function, Section \(\square\) provides theoretical results, Section \(\square\) shows the algorithm for tree construction and training and explains how to perform testing using the tree, Section \(\square\) reports empirical results on benchmark multi-label data sets, and finally Section \(\square\) concludes the paper. Supplementary material contains proofs of theorems from Section \(\square\) and additional experimental results.

2 Objective function

We next explain the design of the objective function for the tree of arbitrary width \(M\), i.e. tree where each node has \(M\) children. In the Supplement we show a special case of a binary tree. Below we consider an arbitrary non-leaf node of the tree and thus omit node index in the notation.

In our setting, each node of the tree contains \(M\) binary classifiers \(h_j\), where \(j = 1, 2, \ldots, M\). \(h_j \in \mathcal{H}\), where \(\mathcal{H}\) is the hypothesis class with linear regressors. Consider an arbitrary non-leaf node and let \(\pi_i\),

\(^2\)When training each node we stream multiple times through the data before moving to the next node. After we move, we never go back to the previously trained ones. Thus we assume the data set is finite (but can be very large). This differs from the online setting. For distinction between streaming and online settings see \cite{41}.\)
We aim to minimize the objective
\[ \beta \]
where the multiplicative normalizing factor is an inverse of the average number of labels per example containing label \( i \) in their label set (Note that \( \sum_{i=1}^{K} \pi_i = 1 \)). The node regressors are trained in such a way that \( h_j(x) \geq 0.5 \) means that the example \( x \) is sent to the \( j \)th subtree of a node (thus sending example to more than one child is possible). To prevent examples from sticking inside the node, in case when \( h_j(x) < 0.5 \) the example is sent to the child node corresponding to the highest margin, i.e. \( (\arg \max_{j=1,2,\ldots,M} h_j(x)) \) child node. Let \( P_j = P(h_j(x) > 0.5) \) be the probability that the example \( x \) reaches child \( j \in \{1, 2, \ldots, M\} \) and let \( P_j^* = P(h_j(x) > 0.5 | i) \) denote the conditional probability of these event when the example belongs to class \( i \). Note that i) \( \sum_{j=1}^{M} P_j \geq 1 \), ii) for any \( i = 1, 2, \ldots, K \), \( \sum_{j=1}^{M} P_j^i \geq 1 \), and iii) \( P_j = \sum_{i=1}^{K} \pi_i P_j^i \). The node splitting criterion is defined as follows

\[
J := \sum_{j=1}^{M} \sum_{i=j+1}^{M} |P_j - P_i| - \lambda_1 \sum_{i=1}^{K} \sum_{j=1}^{M} \pi_i |P_j^i - P_i^i| + \lambda_2 \left( \sum_{j=1}^{M} P_j - 1 \right),
\]

where \( \lambda_1 \), and \( \lambda_2 \) are non-negative hyper-parameters. The balancing term guards an even split of examples between children nodes and is minimized for the perfectly balanced split when \( P_1 = P_2 = \ldots = P_M \). The class integrity term ensures that examples belonging to the same class are not split between children nodes. This term is maximized when \( |M| \) or \( \frac{|M|}{2} \) probabilities from among \( P_1, P_2, \ldots, P_M \) are equal to 1 and the remaining ones are equal to 0 for any \( i = 1, 2, \ldots, K \). Thus at maximum, given any class \( i \), the examples containing this class in their label set are not split between children, but they are instead simultaneously all sent to \( \frac{M}{2} \) or \( \frac{M}{K} \) children. The third term in the objective aims at compensating this multi-way assignment of examples. The multi-way penalty prevents sending examples to multiple directions too often. It is maximized when \( \forall j \in 1, 2, \ldots, M \) \( P_j = 1 \) and minimized when \( \sum_{j=1}^{M} P_j = 1 \). Thus the purity term, defined as the sum of the class integrity term and the multi-way penalty, is minimized for the perfectly pure split when no example is sent to more than one children (in other words, this is when for any \( i = 1, 2, \ldots, K \), \( P_j^i = 1 \) for one particular setting of \( j \) and \( P_j^i = 0 \) for all other \( j \)s).

We aim to minimize the objective \( J \) to obtain high quality partitions. We next show theoretical properties of the objective introduced in Equation [1] in Section 3.

### 3 Theoretical results

In this section we analyze the properties of the objective and its influence on the purity and balancedness of node splits. Next we show its connection to the multi-label error.

#### 3.1 General properties of the objective and its relation to node partitions

Lemma [1] below provides the basic mathematical understanding of the objective \( J \).

**Lemma 1.** For any hypotheses \( h_j \in \mathcal{H} \), where \( j = 1, 2, \ldots, M \), and sufficiently large \( \lambda_2 \), i.e. \( (M - 3 < \frac{\lambda_2}{\lambda_1}) \), the objective \( J \) defined in Equation [1] satisfies \( J \in [-\lambda_1 (M - 1), \lambda_2 (M - 1)] \) and it is minimized if and only if the split is perfectly balanced and perfectly pure.

Let \( J^* \) denote the lowest possible value of the objective \( J \), i.e. \( J^* = -\lambda_1 (M - 1) \).

Next we study how the objective promotes building nodes that are as balanced and pure as possible given the data. We first introduce useful definitions.

**Definition 1.** (Balancedness) The node split is \( \beta \)-balanced if the following holds

\[
\max_{j \in \{1, 2, \ldots, M\}} \left| P_j - \frac{\sum_{i=1}^{M} P_i}{M} \right| = \beta, \quad \text{where } \beta \in \left[ 0, 1 - \frac{1}{M} \right].
\]

We call \( \beta \) a balancedness factor. Note that a split is perfectly balanced if and only if \( \beta = 0 \).
We call $\alpha$ a *purity factor*. Note that a split is perfectly pure if and only if $\alpha = 0$.

Next lemmas show that in isolation, when either the purity or balancedness of the split is fixed, decreasing the value of the objective leads to recovering more balanced or pure split, respectively.

**Lemma 2.** *If a node split has a fixed purity term $\alpha$, with corresponding $J_p^{\alpha}$ then $\beta \leq J - J_p^{\alpha}$.***

**Lemma 3.** *If a node split has a fixed balanced term $\beta$, with corresponding $J^B_{\text{balance}}$ and assuming that the following condition holds: $\lambda_1(M-1) + J^B_{\text{balance}} \geq \lambda_2 \geq \lambda_1 \frac{M-1}{2}$, then $\alpha \leq (J - J^B_{\text{balance}} + \lambda_2) \frac{2}{M(2\lambda_2 - \lambda_1(M-1))}$ (4)

### 3.2 Relation of the objective to the multi-label error

We next prove that when the objective $J$ is perfectly minimized in every node of the tree then this tree achieves zero multi-label classification error. Assume each example has $R$ labels. Denote $t(x)$ to be a fixed target function with domain $X$, which assigns the data point $x$ to its set of labels. We consider the $r$-level multi-label error of the tree $T$, where $r = 1, 2, \ldots, R$.

$$\epsilon_r(T) = \frac{1}{R} \sum_{i=1}^{K} P(i \in t(x), i \notin y_r(x)) = 1 - R@r, \quad (5)$$

where $y_r(x)$ denotes the label set consisting of top $r$ labels assigned to $x$ by the tree, $t(x)$ is the true label set and $R@r$ denotes the $r$-level multi-label recall. The following theorem holds:

**Theorem 1.** *Assume each example has $R$ labels. When the objective function $J$ from Equation 1 is perfectly minimized in every node of the tree, i.e. $J = J^*_r$, then the resulting multi-label tree achieves zero $r$-level multi-label error, as given by Equation 5 for any $r = 1, 2, \ldots, R$.***

We next analyze the behavior of the recall error under weak learning assumption.

**Assumption 3.1.** *For any distribution $P$ over the data, at each node $n$ of the tree $T$ there exist a partition such that \[ \sum_{i=1}^{K} \sum_{j=1}^{M} \sum_{l=1}^{M} \pi_i |P^l_j - P^l_i| \geq \gamma, \text{ where } \gamma \in (0, 1). \]

The above definition essentially assumes that in every node of the tree we are able to recover a partition with the corresponding class integrity term bounded away from zero. Since the value of this term ranges in $[0, 1]$, such assumption is indeed very “weak”. Also, specifically note that it is enough that for one class $i$ the following holds: $|P^j_i - P^l_i|$ to satisfy the assumption.

**Theorem 2.** *Under the Weak Hypothesis Assumption 3.1 the recall error is monotonically decreasing with every split of the tree.***

The weak hypothesis assumption considers class integrity term, a component of our objective. Interestingly, such weak condition suffices to ensure the monotonic decrease of the error.

### 4 Algorithm

In this section we present the algorithm for simultaneous tree construction and training. We then discuss how to assign labels to the test example. The tree construction and training algorithm is split into four sub-algorithms that we refer to as Algorithm 1 (top-level procedure), 2, 3, and 4. The tree construction is performed in a top-down node-by-node fashion. As can be seen in Algorithm 1 we select a node to be expanded into children nodes based on the priority computed as the difference of the sum and maximum value of the bins of the label histogram in the node. The intuition behind the node priority is that we want to split nodes that are reached by many examples from different classes, where at least two classes have significant mass. High priority is attained by these nodes that were visited by examples with many different labels. When the node is selected for expansion, we train its regressors according to Algorithm 2. Specifically, we optimize the objective function for each example reaching the considered node (see Algorithm 3). In Algorithm 3 we search over all possible ways of sending an example to $M$ directions (including multi-way cases) and we choose the set of
Algorithm 1 BuildTree

% v.I denotes the list of indices of examples reaching node v
Input: · maximum # of nodes: $T_{\text{max}}$;
· tree width: $M$;
· # of training epochs: $E$;
· training data $(x_1, y_1), \ldots, (x_N, y_N)$
% $y_i$: all labels of the $i^{th}$ example

procedure UpdateHist ($LHist$, $y$)
    for $i \in v.I$ do
        $LHist[i] \leftarrow 1$
    end for
    $v.I \leftarrow \{1, 2, \ldots, N\}$;
    $v.LHist \leftarrow \emptyset$
    for $i \in v.I$ do
        % add $y_i$ to histogram
        $v.LHist \leftarrow \emptyset$
        UpdateHist ($v.LHist$, $y_i$)
    end for
    $t \leftarrow 1$
    $Q.push(v.root, 0)$ % initialize priority queue $Q$
    while $Q \neq \emptyset$ and $t < T_{\text{max}}$ do
        $v \leftarrow Q.pop()$
        TrainRegressors ($v$)
        $ch \leftarrow \text{CreateChildren ($v$)}$
        for $m \in ch$ do
            priority $\leftarrow$
            $\sum_{k \in \text{ch}[m], LHist[k]} ch[m].LHist[k]$ $-$
            $\max_{k \in \text{ch}[m], LHist[k]} ch[m].LHist[k]$
            $Q.push(ch[m], \text{priority})$
        end for
        $t \leftarrow t + M$
    end while
    return $v.root$

Algorithm 2 TrainRegressors ($v$)

% $y_i.size()$ denotes the size of vector $y_i$
$v.C_v \leftarrow 0$; $v.I_v \leftarrow \emptyset$; $v.isLeaf \leftarrow \text{false}$
for $m = 1 \ldots M$ do
    $v.w_m \leftarrow \text{random weights}$; $v.P_m \leftarrow 0$
    for $i = 1 \ldots K$ do
        $v.P_i \leftarrow 0$
    end for
end for
for $e = 1 \ldots E$ do
    for $i \in v.I$ do
        for $k \in y_i$ do
            % $v.C_v[k]++$
        end for
        $\hat{y} \leftarrow \text{OptimizeObjective ($v$)}$
        for $m = 1 \ldots M$ do
            $\text{Train } v.w_m\text{ with example } (x_i, \hat{y}[m])$
        end for
        $\text{sent} \leftarrow \text{false}$
    end for
    for $m \in 1 \ldots M$ do
        if $v.w_m x_i > 0.5$ then
            % example $(x_i, y_i)$ goes to child $m$
            $v.ch[m].I_v \leftarrow 0$
            $v.ch[m].LHist \leftarrow \emptyset$
            $v.ch[m].isLeaf \leftarrow \text{true}$
        end if
    end for
end for

Algorithm 3 OptimizeObjective ($v$)

$J_{\text{opt}} \leftarrow +\infty$
for $m = 1 \ldots 2^M - 1$ do
    if $s \land 2^{(m-1)}$ then
        $P_m \leftarrow \frac{v.C_v - y_i.size()}{v.C_v} - y_i.size()$
        for $k \in y_i$ do
            $p_k \leftarrow \frac{v.C_v(k) - 1)v.P_{m}^{k} + 1}{v.C_v}$
        end for
    else
        $P_m \leftarrow \frac{v.C_v - y_i.size()}{v.C_v} - y_i.size()$
        for $k \in y_i$ do
            $p_k \leftarrow \frac{v.C_v(k) - 1)v.P_{m}^{k}}{v.C_v}$
        end for
    end if
end for
% objective computation
$B \leftarrow \sum_{j=1}^{M} \sum_{i=j+1}^{M} |P_j - P_l|$
$CI \leftarrow \sum_{i=1}^{K} \sum_{j=1}^{M} \sum_{i=j+1}^{M} \frac{v.C_v(i)}{v.C_v} |P_j - P_l|$
$MWP \leftarrow \left| \sum_{j=1}^{M} P_j - 1 \right|
$J \leftarrow B - \lambda_1 CI + \lambda_2 MWP$
if $J < J_{\text{opt}}$ then
    $J_{\text{opt}} \leftarrow J$
    for $m = 1 \ldots M$ do
        $\hat{y}[m] \leftarrow s \land 2^{(m-1)}$
    end for
end if
end for

Algorithm 4 CreateChildren ($v$)

for $m \in 1 \ldots M$ do
    $v.ch[m].I_v \leftarrow 0$
end for
$v.ch[m].LHist \leftarrow \emptyset$
$v.ch[m].isLeaf \leftarrow \text{true}$
end for
for $i \in v.I$ do
    if $v.w_i x_i > 0.5$ then
        $\text{UpdateHist (v.ch[m], LHist, y_i)}$
        $v.ch[m].I_v \leftarrow 0$
        $v.ch[m].LHist \leftarrow \emptyset$
        $v.ch[m].isLeaf \leftarrow \text{true}$
    end if
end for
if not sent then
    $m \leftarrow \arg \max_{m \in \{1, 2, \ldots, M\}} v.w_m x_i$
end if
end for
return $v.ch$
Algorithm 5 Predict ($x, R$)
\[
\text{procedure GetLeaves}(v)\\
\text{if } v.\text{isLeaf} \text{ then}\\
\quad \text{leafList.push}(v)\\
\text{else}\\
\quad \text{for } m \in 1 \ldots M \text{ do}\\
\qquad \text{if } v.w_m^T x > 0.5 \text{ then}\\
\quad\quad \text{GetLeaves}(v_m)\\
\quad\quad \text{sent } \leftarrow \text{true}\\
\quad\quad \text{end if}\\
\quad\text{end for}\\
\text{if } \text{not } \text{sent} \text{ then}\\
\quad m \leftarrow \arg\max_{m \in \{1, 2, \ldots, M\}} v.w_m^T x\\
\quad \text{GetLeaves}(v_m)\\
\quad \text{end if}\\
\text{end if}\\
\]
\[
\text{leafList } \leftarrow \emptyset \text{ } \% \text{ list of leaves reached by example } x\\
\text{GetLeaves}(v_{\text{root}})\\
\text{hist } \leftarrow \emptyset\\
\text{for } v_l \in \text{leafList} \text{ do}\\
\quad \text{sum } \leftarrow \sum_{k \in v_l.\text{hist}} v_l.\text{hist}[k]\\
\text{for } k \in v_l.\text{hist} \text{ do}\\
\quad \text{hist}[k] += v_l.\text{hist}[k]/\text{sum}\\
\text{end for}\\
\text{end for}\\
\text{labels } \leftarrow \text{select } R \text{ top entries from hist}\\
\text{return labels}\\
\]

For the explanation of these evaluation metrics, LPSR, FastXML, PFastXML, PLT, GBDT-S, and CRAFTML (comparison with OAA-based and hybrid schemes are deferred to the Supplement as their underlying mechanism is fundamentally different from ours). The performance of the competitors was obtained from the corresponding papers introducing these techniques and multi-label repository [40]. The data sizes are reported in Table 1 ($D$ is the data dimensionality). The experimental setup is described in the Supplement.

In Table 1 we compare the precisions $P@1$, $P@3$, and $P@5$ and nDCG scores $N@1$, $N@3$, $N@5$ (see [40]).

In Table 2 we provide per-example prediction time (training time is deferred to the Supplement) on different data sets for LdSM and competitor methods. The table demonstrates that LdSM can perform efficient multi-label prediction. Figure 2 shows that the depth of trees constructed with LdSM are $O(\log_{log_{2M}} K)$, specifically they lie in the interval $[\log_{2M} K, 3\log_{2M} K]$ for Mediamill, Bibtex and Delicious-200k data sets and $[\log_{2M} K, 2\log_{2M} K]$ for Delicious, AmazonCat-13k, Wiki10-31k, WikiLSHTC-325k and Amazon-670k data sets.

Next we discuss the results captured in Figure 1. Note that additional figures related to this study can be found in the Supplement. In the top left plot we report the behavior of precision and nDCG score as the size of the LdSM ensemble grows. Clearly the most rapid improvement in precision is achieved when increasing the ensemble size to 10 trees (across different data sets this was found to be between 5 and 10, except Bibtex (case $M = 2$), for which it was 20). After that, the increase of $P@1$, $P@3$, $P@5$, $N@1$, $N@3$, and $N@5$ saturates and we obtain less than 2% improvement when increasing the ensemble further to 50. The same can be observed for nDCG score. The right top plot captures how the precision and nDCG score depend on the number of nodes in the tree and the
depth of the deepest tree in the ensemble. As we increase the maximum allowed number of nodes ($T_{\text{max}}$) in the LdSM algorithm, it recovers $O(\log M(T_{\text{max}}))$-depth trees. One can observe the general tendency that increasing the number of nodes $\phi$ times, results in increasing the tree depth by less than $2\log M(\phi)$. We also observed that increasing the number of nodes/tree depth for most data sets leads to the improvement in precisions $P_{@1}$, $P_{@3}$, and $P_{@5}$ and nDCG scores $N_{@1}$, $N_{@3}$, and $N_{@5}$ by less than 3%, suggesting that often shallower trees already achieve acceptable performance. The bottom two plots in Figure 1 demonstrate that single LdSM tree outperforms single FastXML tree. The same property holds for ensembles.

In Figure 2 we show how the objective function is optimized as we move from the root deeper into the tree. Intuitively root faces the most difficult optimization task as it sees the entire data set and consequently the objective function there is optimized more weakly, i.e. to a higher level, than in case of nodes lying deeper in the tree. As we move closer to the leaves, the convergence is faster due to the “cleaner” nature of the data received by the nodes there (less label variety).

6 Conclusions

This paper develops a new decision tree algorithm, that we call LdSM, for multi-label classification problem. The technical contributions of this work include: a novel objective function and its corresponding theoretical analysis and a resulting novel algorithm for tree construction and training that we evaluate empirically. We find experimentally that LdSM is competitive to the state-of-the-art multi-label tree-based approaches, performs efficient prediction, and achieves high multi-label accuracy with logarithmic-depth trees. This new method is therefore suitable for applications involving large label spaces.
Table 1: Precisions: $P@1$, $P@3$, and $P@5$ (%) and nDCG scores: $N@1$, $N@3$, and $N@5$ (%) obtained by different methods on common multi-label data sets.

| Algorithm | Delicious-200k | Mediamill | Bibtex | Bibtex | Bibtex | Bibtex | Bibtex |
|-----------|----------------|-----------|--------|--------|--------|--------|--------|
|           | $P@1$ | $P@3$ | $P@5$ | $N@1$ | $N@3$ | $N@5$ | $P@1$ | $P@3$ | $P@5$ | $N@1$ | $N@3$ | $N@5$ |
| LPSR      | 85.37 | 65.78 | 49.97 | 85.37 | 74.06 | 69.34 | 62.11 | 36.65 | 26.53 | 62.11 | 36.50 | 38.23 |
| PLT       | -     | -     | -     | -     | -     | -     | -     | -     | -     | -     | -     | -     |
| GBDT-S    | 84.23 | 67.85 | -     | 84.22 | 75.41 | 72.37 | 63.42 | 39.23 | 28.86 | 63.42 | 59.51 | 61.70 |
| CRAFTML   | 85.86 | 69.01 | 54.65 | -     | -     | -     | 63.46 | 39.22 | 29.14 | 63.46 | 59.61 | 62.12 |
| FastXML   | 84.22 | 67.33 | 53.04 | 84.22 | 75.41 | 72.37 | 63.42 | 39.23 | 28.86 | 63.42 | 59.51 | 61.70 |
| PFastreXML| 83.98 | 67.37 | 53.02 | 83.98 | 75.31 | 72.21 | 63.46 | 39.22 | 29.14 | 63.46 | 59.61 | 62.12 |
| LdSM      | 90.64 | 73.60 | 58.62 | 90.64 | 82.14 | 79.23 | 64.60 | 37.90 | 29.25 | 64.60 | 60.37 | 62.73 |
| LdSM      | 71.91 | 65.34 | 60.24 | 71.91 | 66.90 | 63.09 | 93.87 | 75.41 | 57.86 | 93.87 | 85.06 | 80.63 |
| LdSM      | 83.74 | 71.74 | 61.51 | 83.74 | 74.60 | 66.77 | 44.90 | 40.58 | 38.22 | 44.90 | 41.62 | 39.80 |
| LdSM      | 55.00 | 34.57 | 25.29 | 55.00 | 48.32 | 47.80 | 42.17 | 37.60 | 34.09 | 42.17 | 39.83 | 38.22 |

Table 2: Prediction time [ms] per example (LPSR and PLT are NA).

| Algorithm       | GBDT-S | CRAFTML | FastXML | PFastreXML | LdSM |
|-----------------|--------|---------|---------|------------|------|
| Mediamill       | 0.05   | NA      | 0.37    | 0.05       |      |
| Bibtex          | NA     | 0.64    | 0.73    | 0.013      |      |
| Delicious       | 0.04   | NA      | NA      | 0.017      |      |
| AmazonCat-13k   | NA     | 5.12    | 1.21    | 3.44       |      |
| Wiki10-31k      | 0.20   | NA      | 1.38    | NA         |      |
| Delicious-200k  | 0.14   | 8.67    | 2.87    | 4.64       |      |
| WikiLSHTC-325k  | NA     | 7.67    | 1.02    | 2.77       |      |
| Amazon-670k     | NA     | 5.02    | 1.48    | 1.98       | 3.04 |

Figure 3: The behavior of the LdSM objective function $J$ during training at different levels in the tree for an exemplary LdSM tree. Delicious data set. Tree depth is 20 and $M$ was set to $M = 2$. $J_{min}$ and $J_{max}$ denote respectively the minimum and maximum value of $J$. 

8
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Logarithm-depth Streaming Multi-label Decision Trees  
(Supplementary material)

Abstract

This Supplement presents additional details in support of the full article. These include the proofs of the theoretical statements from the main body of the paper and additional theoretical results. We also provide the description of the experimental setup. The Supplement also contains additional experiments and figures to provide further empirical support for the proposed methodology.

7 Objective function: binary case

In the binary case the objective simplifies to the following form:

\[ J := |P_R - P_L| - \lambda_1 \sum_{i=1}^{k} \pi_i |P^i_R - P^i_L| + \lambda_2 |P_R + P_L - 1|, \tag{6} \]

where \( P_R \) and \( P^i_R \) (\( P_L \) and \( P^i_L \)) denote the probabilities that the example reaches right (left) child, marginally and conditional on class \( i \) respectively.

In case of the binary tree, each node is equipped with two linear classifiers, \( h_R \) and \( h_L \).

8 Theoretical proofs

Lemma 4. (Binary tree) For any hypotheses \( h_R, h_L \in H \), the objective \( J \) defined in Equation 6 satisfies \( J \in [-\lambda_1, \lambda_2] \) and it is minimized if and only if the split is perfectly balanced and perfectly pure.

Proof of Lemma 4. We rewrite the objective using the total law of probability:

\[ J = \left| \sum_{i=1}^{k} \pi_i (P^i_R - P^i_L) \right| - \lambda_1 \sum_{i=1}^{k} \pi_i |P^i_R - P^i_L| + \lambda_2 \sum_{i=1}^{k} \pi_i (P^i_R + P^i_L - 1) \tag{7} \]

where \( P^i_R, P^i_L \in [0, 1] \) for all \( i = 1, 2, \ldots, K \). The objective admits optimum on the extremes of the \([0, 1]\) interval. Therefore, we define the following:

\[ L_1 = \{ i : i \in \{1, \ldots, K \}, P^i_R = 1 \& P^i_L = 1 \}, \quad L_2 = \{ i : i \in \{1, \ldots, K \}, P^i_R = 0 \& P^i_L = 0 \} \]

\[ L_3 = \{ i : i \in \{1, \ldots, K \}, P^i_R = 1 \& P^i_L = 0 \}, \quad L_4 = \{ i : i \in \{1, \ldots, K \}, P^i_R = 0 \& P^i_L = 1 \} \tag{8} \]

By substituting the above in the objective we have:

\[ J = \left| \sum_{i \in L_3} \pi_i - \sum_{i \in L_4} \pi_i \right| - \lambda_1 \sum_{i \in (L_3 \cup L_4)} \pi_i + \lambda_2 \sum_{i \in (L_3 \cup L_4)} \pi_i + \sum_{i \in L_1} 2\pi_i - 1 \tag{9} \]

We send each example either to the right, left or both directions:

\[ \sum_{i \in (L_1 \cup L_3 \cup L_4)} \pi_i = \sum_{i \in L_1} \pi_i + \sum_{i \in L_3} \pi_i + \sum_{i \in L_4} \pi_i = \sum_{i \in L_1} \pi_i + \sum_{i \in L_3} \pi_i + \sum_{i \in L_4} \pi_i = 1 \]
Thus we can further write

\[
J = \left| 1 - \sum_{i \in L_1} \pi_i - 2 \sum_{i \in L_4} \pi_i \right| - \lambda_1 \left( 1 - \sum_{i \in L_1} \pi_i \right) + \lambda_2 \sum_{i \in L_1} \pi_i
\]  

(12)

For ease of notation, we define \(a := \sum_{i \in L_4} \pi_i, \quad a' := \sum_{i \in L_3} \pi_i\), and \(b := \sum_{i \in L_1} \pi_i\). Therefore

\[
J = |1 - b - 2a| - \lambda_1 (1 - b) + \lambda_2 b = |b + 2a' - 1| - \lambda_1 (1 - b) + \lambda_2 b,
\]  

(13)

where \(a, b \in [0, 1]\). Since we are interested in bounding \(J\), we consider the values of \(a\) and \(b\) at the extremes of \([0, 1]\) interval:

if \(a = 1\) then \(b = 0 \rightarrow J = 1 - \lambda_1\),  
if \(b = 1\) then \(a = 0 \rightarrow J = \lambda_2\)

(14)

if \(a = 0\) then \(\begin{cases} b = 0 \quad (a' = 1) & \rightarrow J = 1 - \lambda_1 \\ b = 1 & \rightarrow J = \lambda_2 \end{cases}\)

(15)

if \(b = 0\) then \(\begin{cases} a = 0 \quad (a' = 1) & \rightarrow J = 1 - \lambda_1 \\ a = 1 & \rightarrow J = 1 - \lambda_1 \\ a = 0.5 & \rightarrow J = -\lambda_1 \end{cases}\)

(16)

Therefore \(J \in [-\lambda_1, \lambda_2]\).

Next, we show that the perfectly balanced and pure split is attained at the minimum of the objective. The perfectly balanced split is achieved when \(P_R = P_L\) and then the balancing term in the objective becomes zero. The perfectly pure split is achieved when the class integrity term in the objective satisfies \(\sum_{i=1}^{K} \pi_i |P_R^j - P_L^j| = \sum_{i=1}^{K} \pi_i = 1\). Simultaneously, the following holds \(\sum_{i=1}^{K} \pi_i (P_R^j + P_L^j) = 1\), and therefore the multi-way penalty is zero as well. Thus, \(J = 0 - \lambda_1 + 0 = -\lambda_1\). In order to prove the opposite direction of the claim, recall that the minimum of the objective occurs for \(b = 0\) and \(a = 0.5\). Since \(a + a' + b = 1\), therefore \(a' = 0.5\). This corresponds to the perfectly pure and balanced split.

**Proof of Lemma**\[7\] \(P_j^i \in [0, 1]\) for all \(i = 1, 2, \ldots, K\) and \(j = 1, 2, \ldots, M\). The objective admits optimum on the extremes of the \([0, 1]\) interval. In the following proof we consider a different approach than in the proof of Lemma\[4\]. In order to get the minimum of the objective, we try to minimize each of its terms separately and on the top of that incorporate their correlations. For now, we assume that the first term, the balancing term, is minimized and therefore is equal to zero. We define case \(C_n\) as the scenario when for any \(i = 1, 2, \ldots, K, P_j^i = 1\) for \(n\) “directions” \((n \leq M)\), i.e. \(n\) distinct \(j\)s such that \(j \in \{1, 2, \ldots, M\}\), and \(P_j^{n'} = 0\) for the remaining \(j\)’s. The class integrity and multi-way penalty terms can then be derived as follows:

\[
J_{\text{class integrity term}|C_n} = \lambda_1 K \sum_{i=1}^{K} \sum_{j=1}^{M} \sum_{l=j+1}^{M} \pi_i |P_R^i - P_L^i| = n(M - n)
\]  

(17)

\[
J_{\text{multi-way penalty term}|C_n} = \lambda_2 \left( \sum_{j=1}^{M} P_j \right) - 1 = n - 1.
\]  

(18)

Therefore, the objective value would then become: \(J = -\lambda_1 n(M - n) + \lambda_2 (n - 1)\). We aim to have the minimum of the objective for perfectly pure split. The perfectly pure split is achieved when case \(C_1\) holds. Therefore, we need:

\[
-\lambda_1 (M - 1) < -\lambda_1 n(M - n) + \lambda_2 (n - 1) \quad \text{for} \quad n \in \{2, \ldots, M\}.
\]  

(19)

The lower-bound of the right side is achieved for \(n = 2:\)

\[
-\lambda_1 (M - 1) < -\lambda_1 2(M - 2) + \lambda_2 \quad \rightarrow \quad M - 3 < \frac{\lambda_2}{\lambda_1}
\]  

(20)

With the above condition, the minimum of the objective is equal to \(-\lambda_1 (M - 1)\). Note that our first assumption on the balancing term can still hold for all \(C_n\) cases. Therefore, we have shown that the
minimum of the objective corresponds to the perfectly pure and balanced split.
In order to get the upper-bound for \( J \), we first show that \( J_{\text{balancing term}} \leq J_{\text{class integrity term}} \) as follows:

\[
J_{\text{balancing term}} = \sum_{j=1}^{M} \sum_{l=j+1}^{M} |P_j - P_l| = \sum_{j=1}^{M} \sum_{l=j+1}^{M} \left| \sum_{i=1}^{K} \pi_i (P^j_i - P^l_i) \right|
\]

\[
\leq \sum_{j=1}^{M} \sum_{l=j+1}^{M} \sum_{i=1}^{K} |P^j_i - P^l_i| = J_{\text{class integrity term}}
\]

(21)

Therefore, the maximum of the summation of the terms is achieved when \( J_{\text{balancing term}} = J_{\text{class integrity term}} \). The maximum of the multi-way penalty term is attained when sending all examples to every direction, resulting in \( J_{\text{multi-way penalty term}} = (M - 1) \). In this case, \( J_{\text{balancing term}} = J_{\text{class integrity term}} = 0 \), and thus, \( J = \lambda_2(M - 1) \). Hence, we have \( J \in [-\lambda_1(M - 1), \lambda_2(M - 1)] \). □

Next lemma shows that in isolation, when the purity of the split is perfect, decreasing the value of the objective leads to recovering more balanced splits.

**Lemma 5.** If a node split is perfectly pure, then

\[
\beta \leq J - J^*.
\]

(23)

**Proof of Lemma**

The perfectly pure split is attained when \( P^j_i = 1 \) for only one value of \( j \), and \( P^j_i = 0 \) for the remaining \( j \)'s. This leads the class integrity term to satisfy \( \sum_{j=1}^{M} \sum_{l=j+1}^{M} \sum_{i=1}^{K} \pi_i |P^j_i - P^l_i| = (M - 1) \) and the multi-way penalty term to satisfy \( \sum_{i=1}^{K} \pi_i \sum_{j=1}^{M} P^j_i - 1 = 0 \). Thus we have:

\[
J - J^* = \sum_{j=1}^{M} \sum_{l=j+1}^{M} |P_j - P_l|
\]

\[
= \sum_{j=1}^{M} \sum_{l=j+1}^{M} \left| \left( P_j - \frac{\sum_{i=1}^{M} P_i}{M} \right) - \left( P_l - \frac{\sum_{i=1}^{M} P_i}{M} \right) \right|.
\]

(24)

(25)

Let \( j^* = \arg\max_{j\in\{1,2,...,M\}} |P_j - \frac{\sum_{i=1}^{M} P_i}{M}| \). Without loss of generality assume \( P_{j^*} - \frac{\sum_{i=1}^{M} P_i}{M} \geq 0 \) and in that case there exists an \( l^* \) such that \( P_{l^*} - \frac{\sum_{i=1}^{M} P_i}{M} \leq 0 \). Therefore we have:

\[
J - J^* \geq \left| \left( P_{j^*} - \frac{\sum_{i=1}^{M} P_i}{M} \right) - \left( P_{l^*} - \frac{\sum_{i=1}^{M} P_i}{M} \right) \right|
\]

\[
\geq \left| P_{j^*} - \frac{\sum_{i=1}^{M} P_i}{M} \right| = \beta.
\]

(26)

(27)

**Proof of Lemma**

Consider a split with a fixed purity factor \( \alpha \). \( J_{\text{purity}}^\alpha \) denotes the sum of the class integrity and multi-way penalty terms of the objective function. When subtracting them from the total value of the objective at node \( n \) we obtain the balancing term. Thus we have:

\[
J - J_{\text{purity}}^\alpha = \sum_{j=1}^{M} \sum_{l=j+1}^{M} |P_j - P_l|
\]

\[
= \sum_{j=1}^{M} \sum_{l=j+1}^{M} \left| \left( P_j - \frac{\sum_{i=1}^{M} P_i}{M} \right) - \left( P_l - \frac{\sum_{i=1}^{M} P_i}{M} \right) \right|.
\]

(28)

(29)

13
Let \( j^* = \arg \max_{j \in \{1, \ldots, M\}} |P_j - \frac{\sum_{i=1}^{M} P_i}{M}|. \) Without loss of generality assume \( P_{j^*} - \frac{\sum_{i=1}^{M} P_i}{M} \geq 0 \) and in that case there exists an \( l^* \) such that \( P_{l^*} - \frac{\sum_{i=1}^{M} P_i}{M} \leq 0. \) Therefore we have:

\[
J - J_{\text{purity}}^\alpha \geq \left| \left( P_{j^*} - \frac{\sum_{i=1}^{M} P_i}{M} \right) - \left( P_{l^*} - \frac{\sum_{i=1}^{M} P_i}{M} \right) \right| \tag{30}
\]

\[
\geq \left| P_{j^*} - \frac{\sum_{i=1}^{M} P_i}{M} \right| = \beta. \tag{31}
\]

Next lemma shows that in isolation, when the balancedness of the split is perfect, decreasing the value of the objective leads to recovering more pure splits.

**Lemma 6.** If a node split is perfectly balanced and assuming that the following condition holds: \( \lambda_1(M - 1) \geq \lambda_2 \geq \lambda_1 \frac{M - 1}{2}, \) then

\[
\alpha \leq (J + \lambda_2) \frac{2}{M(2\lambda_2 - \lambda_1(M - 1))}. \tag{32}
\]

**Proof of Lemma**

The perfectly balanced split is attained when \( P_1 = P_2 = \ldots = P_M. \) This zeros out the balancing term in the objective function. Hence:

\[
J = -\lambda_1 \sum_{i=1}^{K} \sum_{j=1}^{M} \sum_{l=j+1}^{M} \pi_{i} |P^i_j - P^i_l| + \lambda_2 \left( \sum_{j=1}^{M} P_j - 1 \right) \tag{33}
\]

\[
= -\lambda_1 \sum_{i=1}^{K} \sum_{j=1}^{M} \sum_{l=j+1}^{M} \pi_{i} |P^i_j - P^i_l| + \lambda_2 \left( \sum_{i=1}^{K} \sum_{j=1}^{M} P^i_j - 1 \right) \tag{34}
\]

\[
\geq -\lambda_1 \frac{M - 1}{2} \sum_{i=1}^{K} \sum_{j=1}^{M} \pi_{i} P^i_j + \lambda_2 \left( \sum_{i=1}^{K} \sum_{j=1}^{M} P^i_j - 1 \right) \tag{35}
\]

thus we have:

\[
J + \lambda_2 \geq \left( \lambda_2 - \lambda_1 \frac{M - 1}{2} \right) \sum_{i=1}^{K} \sum_{j=1}^{M} \pi_{i} P^i_j \tag{36}
\]

\[
\geq \left( \lambda_2 - \lambda_1 \frac{M - 1}{2} \right) \sum_{i=1}^{K} \sum_{j=1}^{M} \pi_{i} \min(P^i_j, \sum_{l=1}^{M} P^i_l - P^i_j) \tag{37}
\]

\[
\geq \left( \lambda_2 - \lambda_1 \frac{M - 1}{2} \right) M \alpha \tag{38}
\]

**Proof of Lemma**

Consider a split with a fixed balancedness factor \( \beta. \) \( J_{\text{balance}}^\beta \) denotes the balancing term of the objective function. When subtracting it from the total value of the objective at node \( n \) we will obtain the sum of the class integrity and multi-way penalty terms. Hence:

\[
J - J_{\text{balance}}^\beta = -\lambda_1 \sum_{i=1}^{K} \sum_{j=1}^{M} \sum_{l=j+1}^{M} \pi_{i} |P^i_j - P^i_l| + \lambda_2 \left( \sum_{j=1}^{M} P_j - 1 \right) \tag{39}
\]

\[
= -\lambda_1 \sum_{i=1}^{K} \sum_{j=1}^{M} \sum_{l=j+1}^{M} \pi_{i} |P^i_j - P^i_l| + \lambda_2 \left( \sum_{i=1}^{K} \sum_{j=1}^{M} P^i_j - 1 \right) \tag{40}
\]

\[
\geq -\lambda_1 \frac{M - 1}{2} \sum_{i=1}^{K} \sum_{j=1}^{M} \pi_{i} P^i_j + \lambda_2 \left( \sum_{i=1}^{K} \sum_{j=1}^{M} P^i_j - 1 \right) \tag{41}
\]
We next expand the \( R \) where \( w \)
\[
\sum \rho \]
\[
\text{Note that the tree, denoted as}
\]
\[
\text{Next we will find the Shannon entropy bound with respect to the error and show that the entropy of the tree.}
\]
\[
\text{Proof of Theorem 1. Since we assume the objective is minimized in every node of the tree, therefore each node is sending examples to only one of its children and consequently each example descends to only one leaf. Thus in any leaf \( l \), we store label histograms and assign first \( R \) labels from the histogram to any example reaching that leaf, i.e. \( y(x) = \{ j_1, j_2, \ldots, j_R \} \), where \( j_1 = \arg\max_{k \in \{1,2,\ldots,K\}} \rho_k \), \( j_2 = \arg\max_{k \in \{1,2,\ldots,K\} \setminus j_1} (\rho^i_k) \), \( j_R = \arg\max_{k \in \{1,2,\ldots,K\} \setminus \{j_1,\ldots,j_{R-1}\}} (\rho^i_k) \) and \( \rho^i_k \) is the probability that the data point \( x \) has label \( i \) given that \( x \) has reached leaf \( l \), i.e. \( \rho^i_k = P(i \in t(x)|x \text{ reached } l) \).
\]
\[
\text{We next expand the } R\text{-level multi-label error as follows:}
\]
\[
\epsilon_R(T) = \frac{1}{R} \sum_{i=1}^{K} P(i \in t(x), i \notin y_R(x))
\]
\[
= \frac{1}{R} \sum_{l \in L} w(l) \sum_{i=1}^{K} P(i \in t(x), i \notin y_R(x)|x \text{ reached } l)
\]
\[
= \frac{1}{R} \sum_{l \in L} w(l) \sum_{i \notin j_1, \ldots, j_R} P(i \in t(x)|x \text{ reached } l)
\]
\[
= \frac{1}{R} \sum_{l \in L} w(l) \left( \sum_{i=1}^{K} \rho^i_k - \max_{k \in \{1,2,\ldots,K\} \setminus j_1} (\rho^i_k) - \max_{k \in \{1,2,\ldots,K\} \setminus \{j_1,j_2\}} (\rho^i_k) - \cdots - \max_{k \in \{1,2,\ldots,K\} \setminus \{j_1,j_2,\ldots,j_{R-1}\}} (\rho^i_k) \right)
\]
\[
\text{where } w(l) \text{ denote the probability that example } x \text{ reaches leaf } l \text{ and } L \text{ denote the set of all leaves of the tree.}
\]
\[
\text{Next we will find the Shannon entropy bound with respect to the error and show that the entropy of the tree, denoted as } G(T), \text{ upper-bounds the error. Note that:}
\]
\[
G(T) := \sum_{l \in L} w(l) \sum_{i=1}^{K} \rho^i_k \ln \left( \frac{1}{\rho^i_k} \right)
\]
\[
\geq \sum_{l \in L} w(l) \sum_{i \notin j_1, \ldots, j_R} \rho^i_k \ln \left( \frac{1}{\rho^i_k} \right)
\]
\[
\text{Note that } \sum_{i=1}^{K} \rho^i_k = R. \text{ Thus for any } i = 1, 2, \ldots, K \text{ such that } i \neq j_1, \ldots, j_R \text{ it must hold that } \rho^i_k \leq \frac{1}{2}. \text{ We continue as follows}
\]
\[
G(T) \geq \sum_{l \in \mathcal{L}} w(l) \sum_{i=1}^{K} \rho_i^l \ln(2)
\]  
\[
\geq \ln(2) \sum_{l \in \mathcal{L}} w(l) \left( \sum_{i=1}^{K} \rho_i^l \right) - \max_{k \in \{1,2,\ldots,K\}} \rho_k^l - \max_{k \in \{1,2,\ldots,K\} \setminus j_1 \cup \{j_1, j_2\}} \rho_k^l
\]  
\[
= \ln(2) R \epsilon_R(T)
\]  
\[
(51)
\]  
\[
(52)
\]

From Lemma 4 (for binary tree) and Lemma 1 (for M-ary tree) it follows that for any node in the tree, the corresponding split is balanced and the following holds: \(|P_j^i - P_j^j| = 1\) for all labels \(i = 1, 2, \ldots, K\) and all pairs of children nodes \((j, j')\) of the considered node such that \(j, j' \in \{1,2,\ldots,M\}\) and \(j \neq j'\). Thus when splitting any node, its label histogram is divided in such a way that its children have non-overlapping label histograms, i.e.

\[
\forall i = 1, 2, \ldots, K \forall j, j' \in \{1,2,\ldots,M\}, j \neq j' \quad \rho_i^{j} (j') = 0,
\]

where \(\rho_i^j\) and \(\rho_i^{j'}\) denote the \(i\)-th entry in the normalized label histograms of children nodes \(j\) and \(j'\) respectively. After \(\log_M(K/R)\) splits we obtain leaves with non-overlapping histograms, i.e. for any two leaves \(l_1, l_2 \in \mathcal{L}\) and \(l_1 \neq l_2, \forall i = 1, 2, \ldots, K \rho_i^{(l_1)}(j) = \rho_i^{(l_2)}(j) = 0\). In each leaf the label histogram contains \(R\) non-zero entries. Based on the above it follows that \(G^c(T) = 0\). Consequently, using Equation 52 we obtain that the multi-label error \(\epsilon_R(T)\) is equal to zero as well. This directly implies that \(\epsilon_R(T) = 0\) for any \(r = 1, 2, \ldots, R\). \(\square\)

**Proof of Theorem 2** In our algorithm we store label histograms for each node, and at testing we assign to an example top \(r\) labels obtained from averaging the histograms of the leaves to which this example has descended to. At training, we recursively find the node with the highest priority and partition it to two children. Here we are examining the change of error with one node split. We consider examples reaching that node and without loss of generality we assume they have reached only this node. For each such example \(x\) we assign the top \(r\) labels from the histogram of the analyzed node, i.e. \(y(x) = \{k_1, k_2, \ldots, k_r\}\), where \(k_1 = \arg\max_{k \in \{1,2,\ldots,K\}} \rho_k, k_2 = \arg\max_{k \in \{1,2,\ldots,K\} \setminus j_1} \rho_k, \ldots, k_r = \arg\max_{k \in \{1,2,\ldots,K\} \setminus \{j_1, j_2, \ldots, j_{r-1}\}} \rho_k\) and \(\rho_i\) is the probability that the data point \(x\) has label \(i\) given that \(x\) has reached node \(n\), i.e. \(\rho_i = P(i \in t(x)|x \text{ reached } n)\). For simplicity, we assume that each example has \(r\) labels. After \(t\) splits the recall can be expanded as follows:

\[
(R@r)^t = \frac{1}{r} \sum_{i=1}^{K} P(i \in t(x), i \in y_r(x))
\]  
\[
= \frac{1}{r} \left( \max_{k \in \{1,2,\ldots,K\}} \rho_k + \max_{k \in \{1,2,\ldots,K\} \setminus j_1} \rho_k + \cdots + \max_{k \in \{1,2,\ldots,K\} \setminus \{j_1, j_2, \ldots, j_{r-1}\}} \rho_k \right)
\]  
\[
= \max_{k \in \{1,2,\ldots,K\}} \pi_k + \max_{k \in \{1,2,\ldots,K\} \setminus j_1} \pi_k + \cdots + \max_{k \in \{1,2,\ldots,K\} \setminus \{j_1, j_2, \ldots, j_{r-1}\}} \pi_k
\]  
\[
= \pi_{k_1} + \cdots + \pi_{k_r},
\]

where the last line comes from the fact that \(\pi_i\) is a normalized fraction of examples containing label \(i\) in their labels. After the node split, the recall is defined as the combination of the recalls of its children. For simplicity we consider equal contribution of each of the edges to \(P_{\text{multi}} = \left| \sum_{j=1}^{M} P_j \right| - 1\).
Therefore we can write the recalls of the children as:

\[(R@r)^{t+1} = (P_1 - \frac{1}{M} P_{\text{multi}})(R@r)^1 + \cdots + (P_M - \frac{1}{M} P_{\text{multi}})(R@r)^M\]  \hspace{1cm} (57)

\[= (P_1 - \frac{1}{M} P_{\text{multi}}) \left( \max_{i \in \{1, 2, \ldots, K\}} \pi_i \left( \frac{P_i^1 - \frac{1}{M} P_{\text{multi}}}{P_i - \frac{1}{M} P_{\text{multi}}} \right) + \cdots \right) + \cdots \]  \hspace{1cm} (58)

\[+ (P_M - \frac{1}{M} P_{\text{multi}}) \left( \max_{j \in \{1, 2, \ldots, K\}} \pi_j \left( \frac{P_j^M - \frac{1}{M} P_{\text{multi}}}{P_M - \frac{1}{M} P_{\text{multi}}} \right) + \cdots \right)\]  \hspace{1cm} (59)

Therefore we can write the recalls of the children as:

\[\max_{i \in \{1, 2, \ldots, K\}} \pi_i (P_i^1 - \frac{1}{M} P_{\text{multi}}) + \cdots\]  \hspace{1cm} (60)

\[+ \max_{j \in \{1, 2, \ldots, K\}} \pi_j (P_j^M - \frac{1}{M} P_{\text{multi}}) + \cdots\]  \hspace{1cm} (61)

Note that the subtraction of \((1/M)P_{\text{multi}}^i\) and \((1/M)P_{\text{multi}}\) in the coefficients is done to compensate the recall calculation for examples being sent to multiple directions. Let the top \(r\) labels assigned to the first child be denoted as \(y_1(x) = \{i_1, i_2, \ldots, i_r\}\), where

\[i_1 = \arg\max_{i \in \{1, 2, \ldots, K\}} \pi_i ((P_i^1 - P_2^1) + (P_i^2 - P_3^1) + \cdots (P_i^1 - P_M^1))\]

\[i_2 = \arg\max_{k \in \{1, 2, \ldots, K\} \setminus \{i_1\}} \pi_i ((P_i^1 - P_2^1) + (P_i^1 - P_3^2) + \cdots (P_i^1 - P_M^1))\]

\[\ldots\]

\[i_r = \arg\max_{k \in \{1, 2, \ldots, K\} \setminus \{i_1, \ldots, i_{r-1}\}} \pi_i ((P_i^1 - P_2^1) + (P_i^1 - P_3^2) + \cdots (P_i^1 - P_M^r))\]

Analogy holds for all other children. Thus for example the \(M\)th child’s labels are: \(y_M(x) = \{j_1, j_2, \ldots, j_r\}\). Therefore the difference between the recall of the parent node and its children can be written as:

\[(R@r)^{t+1} - (R@r)^t = \frac{1}{M} (\pi_{i_1} ((P_i^1 - P_2^1) + \cdots (P_i^1 - P_M^1) + 1) + \cdots)

+ \pi_{i_r} ((P_i^r - P_2^r) + \cdots (P_i^r - P_M^r) + 1) + \cdots\]  \hspace{1cm} (62)

For the ease of notation we show the case for the binary below:

\[\frac{1}{2} (\pi_{i_1} (P_{R1}^1 - P_{L1}^1 + 1) + \cdots + \pi_{i_r} (P_{R1}^r - P_{L1}^r + 1))

+ \frac{1}{2} (\pi_{j_1} (P_{R1}^1 - P_{L1}^1 + 1) + \cdots + \pi_{j_r} (P_{R1}^r - P_{L1}^r + 1))

- (\pi_{k_1} + \cdots + \pi_{k_r})\]  \hspace{1cm} (63)

Considering the Assumption 3.1 we have at least one label such that \(P_{R1}^1 - P_{L1}^1 = \gamma_1 > 0\), \(\gamma_1 \in (0, 1]\). Without loss of generality let \(P_{R1}^1 - P_{L1}^1 = \gamma_1 > 0\) for the top label in the parent node. Thus:

\[\pi_{i_1} (P_{R1}^1 - P_{L1}^1 + 1) \geq \pi_{k_1} (1 + \gamma_1)\] and

\[\pi_{j_1} (P_{R1}^1 - P_{L1}^1 + 1) \geq \pi_{k_1} (1 - \gamma_1)\]

Therefore we have \((R@r)^{t+1} - (R@r)^t \geq 0\). Due to the weak hypothesis assumption the histograms in the children nodes are different than in the parent on at least one position corresponding to one label. If that label is in the top \(r\) labels that we assign to the child node, the error will be reduced. If not, the
error is going to be the same, but that cannot happen forever, i.e. for some split the label(s) for which the weak hypothesis assumption holds will eventually be in the top \( r \) labels that are assigned to the children node. To put this intuition into more formal language, if any of the top \( r \) labels in any of the children are different from the top \( r \) parent labels, i.e. \( y_1 \neq y, y_2 \neq y, \ldots, \) or \( y_M \neq y \) we will have \( (R@r)^{t+1} - (R@r)^t \geq 0 \). Because of the weak hypothesis assumption, the latter condition is inevitable and will eventually hold after some node split. This shows that the recall error is monotonically decreasing.

9 Experimental setup

LdSM was implemented in C++. The regressors in the tree nodes were trained with either SGD [42] (Mediamill) or NAG [43] (remaining data sets) with step size chosen from \([0.001, 1]\). The trees were trained with up to 20 passes through the data and we explored trees with up to \( 64K \) nodes for Mediamill and Bibtext, up to \( 32K \) for Delicious, and up to \( 2K \) for the rest of the data sets. \( \lambda_1 \) and \( \lambda_2 \) were chosen from the set \([0.5, 1, 1.5, 2, 4]\) and \( M \) was set to either 2 or 4. FastXML, PFastreXML, CRAFTML and LdSM algorithms use tree ensembles of size \( \sim 50 \). PLT and LPSR use a single tree, and GBDT-S uses up to 100 trees. Since the two largest data sets (WikiLSHTC-325k and Amazon-670k) suffer from the tail label problem, we use re-ranking approach for them similar to [8]. This is applied at testing, after our tree is built and trained. Re-ranking increases the test time by \( \sim 9\% \) for WikiLSHTC-325k and \( \sim 15\% \) for Amazon-670k.

| Data Sets    | #Features | #Labels | #Training samples | #Testing samples | Avg. Labels per Point | Avg. Points per Label |
|--------------|-----------|---------|-------------------|------------------|-----------------------|-----------------------|
| Mediamill    | 120       | 101     | 30993             | 12914            | 4.38                  | 1902.15               |
| Bibtext      | 1836      | 159     | 4880              | 2515             | 2.40                  | 111.71                |
| Delicious    | 500       | 983     | 12920             | 3185             | 19.03                 | 311.61                |
| Eurlex       | 5000      | 3993    | 15539             | 3809             | 5.31                  | 25.73                 |
| AmazonCat-13k| 203882    | 13330   | 1186239           | 306782           | 5.04                  | 448.57                |
| Wiki10-31k   | 101938    | 30938   | 14146             | 6616             | 18.64                 | 8.52                  |
| Delicious-200k| 782585   | 205443  | 196606            | 100095           | 75.54                 | 72.29                 |
| WikiLSHTC-325k| 1617899 | 325056  | 1778351           | 587084           | 3.19                  | 17.46                 |
| Amazon-670k  | 135909    | 670091  | 490449            | 153025           | 5.45                  | 3.99                  |

Table 3: Data set statistics.

| Data Sets     | Depth | Arity |
|---------------|-------|-------|
| Mediamill     | 9     | 4     |
| Bibtext       | 9     | 4     |
| Delicious     | 10    | 4     |
| AmazonCat-13k | 18    | 2     |
| Wiki10-31k    | 10    | 4     |
| Delicious-200k| 46    | 2     |
| WikiLSHTC-325k| 22    | 2     |
| Amazon-670k   | 25    | 2     |

Table 4: Experimental setup that was used to obtain results for various data sets with LdSM method: the depth of the deepest tree in the ensemble and tree arity.
10 Additional experimental results

Table 5: Prediction time [ms] per example for tree-based approaches: GBDT-S, CRAFTML, FastXML, PFastreXML, LdSM (LPSR and PLT are NA) and other (not purely tree-based) methods: Parabel, DisMEC [19], PD-Sparse [20], PPD-Sparse [21], OVA-Primal++ [22] and SLEEC [44] on various data sets. The best result among tree-based methods is in bold, and among all methods is underlined.

| Tree-based | GBDT-S | CRAFTML | FastXML | PFastreXML | LdSM |
|------------|--------|---------|---------|------------|------|
| Mediamill  | 0.05   | NA      | 0.27    | 0.37       | **0.05** |
| Bibtex     | NA     | NA      | 0.64    | 0.73       | **0.013** |
| Delicious  | 0.04   | NA      | NA      | NA         | **0.017** |
| AmazonCat-13k | NA     | 5.12    | 1.21    | 1.34       | **0.09** |
| Wiki10-31k | **0.20** | NA      | 1.38    | NA         | **0.2** |
| Delicious-200k | **0.14** | 8.6     | 1.28    | 7.40       | 5.65 |
| WikiLSHTC-325k | NA     | 7.67    | **1.02** | 1.47       | 2.77 |
| Amazon-670k | NA     | 5.02    | **1.48** | 1.98       | 3.04 |

| Other | Parabel | DISMEC | PD-Sparse | PPD-Sparse | OVA-Primal++ | SLEEC |
|-------|---------|--------|-----------|------------|--------------|-------|
| Mediamill | NA     | 0.142  | 0.004     | 0.078      | NA           | 4.95  |
| Bibtex     | NA     | 0.28   | 0.007     | 0.094      | NA           | 0.70  |
| AmazonCat-13k | NA    | 0.20   | 0.87      | 1.82       | NA           | 13.36 |
| Wiki10-31k | NA     | 116.66 | NA        | NA         | NA           | NA    |
| Delicious-200k | NA    | 311.4  | 0.43      | 275        | NA           | 2.69  |
| WikiLSHTC-325k | 1.17   | 65     | 3.89      | 290        | NA           | 4.85  |
| Amazon-670k | 1.13   | 148    | NA        | 20         | NA           | 6.94  |

Table 6: Training time [s] for tree-based approaches: GBDT-S, CRAFTML, FastXML, PFastreXML, LdSM (LPSR and PLT are NA) and other (not purely tree-based) methods: Parabel, DisMEC, PD-Sparse, PPD-Sparse, SLEEC, on various data sets. The best result among tree-based methods is in bold, and among all methods is underlined.

| Tree-based | GBDT-S | CRAFTML | FastXML | PFastreXML | LdSM |
|------------|--------|---------|---------|------------|------|
| Mediamill  | NA     | NA      | 276.4   | 293.2      | **52.7** |
| Bibtex     | NA     | NA      | 21.68   | 21.47      | **20.69** |
| Delicious  | NA     | NA      | NA      | NA         | **65** |
| AmazonCat-13k | NA     | **2876** | 115.35 | 13985      | **2865** |
| Wiki10-31k | **1044** | NA      | 1275.9  | NA         | **1033** |
| Delicious-200k | NA    | **1174** | 8832.46 | 8807.51    | 29067 |
| WikiLSHTC-325k | NA     | **5092** | 19160   | 20070      | 124131 |
| Amazon-670k | NA     | **1487** | 5624    | 6559       | 72121 |

| Other | Parabel | DISMEC | PD-Sparse | PPD-Sparse | OVA-Primal++ | SLEEC |
|-------|---------|--------|-----------|------------|--------------|-------|
| Mediamill | NA     | 12.15  | 34.1      | 23.8       | NA           | 9504  |
| Bibtex     | 0.203  | 7.71   | 0.232     | NA         | 296.86       |
| AmazonCat-13k | 11828  | 2789   | 122.8     | 7330       | 119840       |
| Wiki10-31k | NA     | NA     | NA        | NA         | 1364         | NA    |
| Delicious-200k | 38814  | 5137.4 | 2869      | NA         | 4838.7       |
| WikiLSHTC-325k | 13032  | 271407 | 94343.5   | 353        | 39000        |
| Amazon-670k | 1512   | 174135 | NA        | **921.9**  | **20904** |

**Remark 1** (Training time). The training time of LdSM can be reduced order of magnitudes by using lower number of epochs at the expense of ~ 1% loss in the accuracy. However, we report the training times that correspond to the best accuracy results obtained with LdSM.
Table 7: Precisions: $P@1$, $P@3$, and $P@5$ (%) and nDCG: $N@1$, $N@3$, and $N@5$ (%) obtained for tree-based approaches: GBDT-S, CRAFTML, FastXML, PFastXML, LPSR, PLT, and LdSM and other (not purely tree-based) methods: Parabel, DisMEC, PD-Sparse, PPD-Sparse, OVA-Primal++, LEML, and SLEEC, on various data sets. LdSM ($d,M$) denotes the LdSM approach with the depth of the deepest tree in the ensemble $d$ and arity $M$ for various multi-label data sets. The best result among tree-based methods is in bold, and among all methods is underlined.
Figure 4: The behavior of precision/nDCG score as a function of the number of trees in the ensemble. Plots were obtained for Delicious, Bibtex, Mediamill, and Wiki10 data sets.
Figure 5: The behavior of precision/nDCG score as a function of the number of nodes $T_{max}$ (including leaves) and tree depth of the deepest tree in the ensemble. Plots were obtained for Delicious, Bibtex, Mediamill, AmazonCat, and Wiki10 data sets.
In Figure 6 we show how the objective function is optimized as we move from the root deeper into the tree. We present results on two exemplary LdSM trees. Intuitively root faces the most difficult optimization task as it sees the entire data set and consequently the objective function there is optimized more weakly, i.e. to a higher level, than in case of nodes lying deeper in the tree. As we move closer to the leaves, the convergence is faster due to the “cleaner” nature of the data received by the nodes there (less label variety).

In Figure 7 we show how the objective function is optimized as we move from the root deeper into the tree. We present results on two exemplary LdSM trees. Intuitively root faces the most difficult optimization task as it sees the entire data set and consequently the objective function there is optimized more weakly, i.e. to a higher level, than in case of nodes lying deeper in the tree. As we move closer to the leaves, the convergence is faster due to the “cleaner” nature of the data received by the nodes there (less label variety).