Angle-based hierarchical classification using exact label embedding

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Abstract

Hierarchical classification problems are commonly seen in practice. However, most existing methods do not fully utilize the hierarchical information among class labels. In this paper, a novel label embedding approach is proposed, which keeps the hierarchy of labels exactly, and reduces the complexity of the hypothesis space significantly. Based on the newly proposed label embedding approach, a new angle-based classifier is developed for hierarchical classification. Moreover, to handle massive data, a new (weighted) linear loss is designed, which has a closed form solution and is computationally efficient. Theoretical properties of the new method are established and intensive numerical comparisons with other methods are conducted. Both simulations and applications in document categorization demonstrate the advantages of the proposed method.

Keywords: Angle-based large-margin; Computational efficiency; Hierarchical classification; Label embedding

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1 Introduction

Hierarchical classification problems are commonly encountered in many scientific fields (Silla and Freitas, 2011), including but not limited to image classification (Akata et al., 2015, 2016), text categorization (Koller and Sahami, 1997), protein function prediction (Vens et al., 2008), music genre classification (DeCoro et al., 2007; Silla Jr. and Freitas, 2009), and online commerce (Chen and Warren, 2013). In hierarchical classification, the hierarchy of the classes can be pre-defined by a graph, where each node stands for a class, and a directed edge from the node $\nu$ to the node $\nu'$ means that if an instance is assigned to $\nu'$, then it must be assigned to $\nu$ first. We call $\nu$ a parent of $\nu'$, and $\nu'$ a child of $\nu$. A node without any child is referred to a leaf, and it does not necessarily locate at the last layer. If each node has at most one parent, then the graph is of a tree structure; otherwise, we call it a Directed Acyclic Graph (DAG). An illustrative example of a tree structure is shown in Figure 1. In this article, we focus on tree structures. Moreover, we assume that each node either is a leaf or has at least two children, and that an instance to be classified belongs to at most one node at any layer in the hierarchy, namely single-labeled.

For hierarchical classification, the simplest approach is to apply a flat classifier, which predicts only the leaf nodes, completely ignoring the hierarchy (Hayete and Bienkowska, 2005; Barbedo and Lopes, 2006). Another popular approach is to sequentially train a multicategory classifier locally at each parent node (Davies et al., 2007), or train a binary classifier at each node (Cesa-Bianchi et al., 2006). The classifier may suffer from a small training sample and be suboptimal. Besides, to incorporate the hierarchical structure among nodes in learning classification rules, various other methods have been developed during the past several decades including imposing inequality constraints directly (Wang et al., 2009), designing regularized loss functions (Gopal and Yang, 2013), and considering cost-sensitive learning (Fan et al., 2015; Charuvaka and Rangwala, 2015). A detailed survey of hierarchical classification can be found in Silla and Freitas (2011).

Besides the methods mentioned above, several methods on label embedding have been
developed for both multicategory classification (Lange and Wu, 2008; Wu and Lange, 2010; Wu and Wu, 2012; Zhang and Liu, 2014) and hierarchical classification (Cai and Hofmann, 2004; Tsochantaridis et al., 2005; Bengio et al., 2010), though some of them did not use this particular term. Label embedding aims to map nodes into a set of points in the Euclidean space, such that the Euclidean distance between these points mimics the dissimilarity between the nodes as much as possible. Such a method has obvious advantages in computation, as the classification problem can be naturally transformed into a regression task. It has been proven useful in many application domains such as image classification (Akata et al., 2016; Chollet, 2016) and text categorization (Weinberger and Chapelle, 2009).

For hierarchical classification, there are two crucial factors for the success of label embedding, the hierarchy of the embedded points and the dimension of the embedded Euclidean space. A desired embedding approach is to embed nodes into points in a low-dimensional space while keeping the hierarchy. Suppose there are \( q \) nodes totally excluding the root. The classical approach maps each node into a \( q \)-dimensional vector (Cai and Hofmann, 2004; Tsochantaridis et al., 2005). As shown in Section 2, the Euclidean distance between these vectors cannot mimic the dissimilarity between the nodes properly, and thus they do not maintain the hierarchy well. In addition, the embedded space has the dimension \( q \), which leads to a complex hypothesis space. To reduce the dimension of the embedded space, some existing papers developed approximated embedding (Weinberger and Chapelle, 2009; Bengio et al., 2010). However, these approximated embedding approaches cannot keep the hierarchy exactly. It is desirable to propose an embedding method such that the embedded points keep the hierarchy exactly as well as locate in a low-dimensional Euclidean space.

Motivated by the existing work, we develop a label embedding method that keeps the hierarchy exactly, i.e. it satisfies two basic properties of dissimilarities between nodes on the hierarchical tree. Surprisingly, the dimension of the embedded space is only \( n_{\text{leaf}} - 1 \), where \( n_{\text{leaf}} \) denotes the number of leaf nodes, much smaller than \( q \), the number of nodes excluding the root, especially when the tree is complicated. In addition, note that this dimension
is exactly the same as the one required for the multiclassification classification on leaf nodes by the label embedding approach of [Lange and Wu (2008) and Zhang and Liu (2014)]. This observation sheds light on the long-standing phenomenon that flat classifiers which ignore the hierarchy, can still be competitive, compared with some hierarchical classifiers (Babbar et al., 2013; Hoyoux et al., 2016). Flat classifiers directly applying to leaf nodes involve a lower-dimensional hypothesis space, while some hierarchical classifiers utilizing the hierarchical information involve a much higher-dimensional hypothesis space. In this sense, our embedding method takes the advantages of both aspects, keeping the hierarchy exactly and reducing the complexity of the hypothesis space (or equivalently the number of unknown parameters) simultaneously. Based on our embedded points, we then extend the angle-based method [Zhang and Liu (2014)] to the hierarchical case.

There are several key contributions in this paper. Firstly, we address that an ideal dissimilarity measurement between nodes on the hierarchical tree should satisfy two basic properties, called hierarchical and symmetric (H.S.) properties. Then we define a novel dissimilarity measurement that satisfies the properties. Secondly, we develop an exact label embedding procedure to construct points in a low-dimensional Euclidean space. Thirdly, we propose an angle-based method for hierarchical classification and establish some statistical properties. The convergence rate of the proposed method has advantages over existing approaches. Fourthly, we design a (weighted) linear loss function, under which the estimator can be derived in a closed form without complicated optimization. It is particularly useful when the tree is complex or the sample size is large, which is the case in big data analyses.

The remaining of this article is organized as follows. In Section 2, we state H.S. properties and define a novel dissimilarity measurement. In Section 3, we develop an exact label embedding procedure. In Section 4, we propose the angle-based method and the linear loss functions. Some theoretical properties of the estimator including Fisher consistency and asymptotic results on generalization errors are established in Section 5. Simulations and real data analyses are presented in Section 6. Finally, we make discussions in Section 7.
Before proceeding, we introduce some notations used in the paper. For any positive integers \( m \) and \( i \) with \( i \leq m \), let \( \mathbf{e}_i = (0, \cdots, 0, 1, 0, \cdots, 0)^\top \in \mathbb{R}^m \) with the \( i \)-th coordinate being 1 and others being 0. For any vector \( \mathbf{u} = (u_1, \cdots, u_m)^\top \in \mathbb{R}^m \), \( \|\mathbf{u}\| \) denotes the \( l_2 \) norm, and \( \mathbf{u}^{(\tilde{m})} \) denotes the subvector consisting of the first \( \tilde{m} \) coordinates of \( \mathbf{u} \) with \( \tilde{m} \leq m \). For any set \( S \), \( |S| \) denotes the cardinality of \( S \).

2 Dissimilarity between classes

2.1 Hierarchical and symmetric (H.S.) properties

We first introduce some notations and definitions. The ancestor of a node is its parent or recursively the parent of an ancestor. The offspring of a node is referred to its child or the child of an offspring. Siblings are nodes sharing the same parent. For a node, denote its parent, children, ancestors, offsprings and siblings respectively as \( \text{Par}(\cdot) \), \( \text{Chi}(\cdot) \), \( \text{Anc}(\cdot) \), \( \text{Off}(\cdot) \), and \( \text{Sib}(\cdot) \). For a tree structure, assume it has \( k \) layers in total. Denote \( C_1 \) as the node at the first layer which is the root, and \( C_{1,j_2} \) as the child of \( C_1 \) with index \( j_2 = 1, 2, \cdots, N_1 \) at the second layer from left to right, where \( N_1 \) is the number of children for the node \( C_1 \). In general, for \( 3 \leq m \leq k \), \( C_{1,j_2,\cdots,j_{m-1},j_m} \) denotes the child of \( C_{1,j_2,\cdots,j_{m-1}} \) with index \( j_m = 1, 2, \cdots, N_{1,j_2,\cdots,j_{m-1}} \) at the \( m \)-th layer from left to right, where \( N_{1,j_2,\cdots,j_{m-1}} \) denotes the number of children for \( C_{1,j_2,\cdots,j_{m-1}} \). Denote the collection of all nodes as \( \mathcal{C} = \{C_1\} \cup \{C_{j_1,j_2,\cdots,j_s} : j_1 \equiv 1, j_s = 1, \cdots, N_{j_1,j_2,\cdots,j_{s-1}}, s = 2, \cdots, k \} \). For the example shown in Figure 1, there are \( k = 4 \) layers. Here, \( C_1 \) denotes the root node. It has two children \( C_{1,1} \) and \( C_{1,2} \) with \( N_1 = 2 \). In addition, \( C_{1,1} \) has two children \( C_{1,1,1} \) and \( C_{1,1,2} \) with \( N_{1,1} = 2 \). Similarly, \( C_{1,2} \) has three children \( C_{1,2,1} \), \( C_{1,2,2} \) and \( C_{1,2,3} \) with \( N_{1,2} = 3 \). Finally, \( C_{1,1,1} \) has two children \( C_{1,1,1,1} \) and \( C_{1,1,1,2} \) with \( N_{1,1,1} = 2 \).

Let \( \mathcal{C}_H = \mathcal{C} \setminus \{C_1\} \) with cardinality \( q = |\mathcal{C}| - 1 \). Sort the nodes in \( \mathcal{C}_H \) by layers from top to bottom, and the nodes at the same layer from left to right. For the example in Figure 1, nodes are ordered as \( C_{1,1}, C_{1,2}; C_{1,1,1}, C_{1,1,2}, C_{1,2,1}, C_{1,2,2}, C_{1,2,3}; C_{1,1,1,1}, C_{1,1,1,2} \). Rename
the ordered nodes as $C_{(1)}, \cdots, C_{(q)}$ and let $C_{(0)}$ denote the root node. The classical label embedding method [Cai and Hofmann, 2004; Tsochantaridis et al., 2005] maps node $C_{(i)}$ into a $q$-dimensional binary vector $u(C_{(i)}) = (u_1, \cdots, u_q)^\top$, where $u_j = 1$ if $C_{(j)}$ is an ancestor of $C_{(i)}$ or $j = i$, and 0 otherwise for $1 \leq j \leq q$. For the example in Figure 1, the embedded points of the classical method are

$$
\begin{pmatrix}
C_{1,1} & C_{1,2} & C_{1,1,1} & C_{1,1,2} & C_{1,2,1} & C_{1,2,2} & C_{1,1,1,1} & C_{1,1,1,2} \\
1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\
0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 
\end{pmatrix}.
\tag{2.1}
$$

Denote $d_E(\cdot, \cdot)$ as the Euclidean distance. For any two nodes $C, C'$ in $\mathcal{C}_H$, let $d_{\mathcal{C}_H}(C, C') = d_E(u(C), u(C'))$. It can be seen that the distance between vectors in (2.1) does not mimic the dissimilarity between the nodes well. For example, one can see that $d_{\mathcal{C}_H}(C_{1,1}, C_{1,2}) = d_{\mathcal{C}_H}(C_{1,1,1}, C_{1,1,2}) = \sqrt{2}$. Note that $C_{1,1,1} = \{\text{African elephant}\}$ and $C_{1,1,2} = \{\text{Asian elephant}\}$ have the latest common ancestor $C_{1,1} = \{\text{Elephant}\}$. On the other hand, $C_{1,1} = \{\text{Elephant}\}$ and $C_{1,2} = \{\text{Dog}\}$ have the latest common ancestor $C_1 = \{\text{Animal}\}$. Since $C_{1,1}$ is a child

Figure 1: An example of a hierarchical tree of 4 layers.
of \( C_1 \), it is more reasonable to require \( d_{C_{H}}(C_{1,1}, C_{1,2}) > d_{C_{H}}(C_{1,1}, C_{1,1}) \). To proceed, we define the concept of the layer of the latest common ancestor (LLCA) as follows.

**Definition 1. (LLCA)** For any two nodes \( C_{i_1,i_2,...,i_m} \) at the \( m \)-th layer and \( C_{j_1,j_2,...,j_l} \) at the \( l \)-th layer, where \( i_1 = j_1 \equiv 1 \) and \( 1 \leq m, l \leq k \), define \( I_{i_1,i_2,...,i_m; j_1,j_2,...,j_l} \) as the layer at which the latest common ancestor (LLCA) of nodes \( C_{i_1,i_2,...,i_m} \) and \( C_{j_1,j_2,...,j_l} \) locates, that is, \( I_{i_1,i_2,...,i_m; j_1,j_2,...,j_l} = \max \{ t : (i_1, i_2, \ldots, i_t) = (j_1, j_2, \ldots, j_t), 1 \leq t \leq \min \{m, l\} \} \).

Motivated from the phylogenetic tree, an ideal dissimilarity measurement denoted as \( s_C(\cdot, \cdot) \) between nodes should satisfy the following H.S. properties.

**Definition 2. (H.S. properties)**

**H.S.1** (Hierarchical property) For two pairs of classes \( \{C_{i_1,i_2,...,i_m}, C'_{i_1',i_2',...,i_m'}\} \) and \( \{C_{j_1,j_2,...,j_l}, C'_{j_1',j_2',...,j_l'}\} \), if \( I_{i_1,i_2,...,i_m; j_1,j_2,...,j_l} < I_{i_1',i_2',...,i_m'; j_1',j_2',...,j_l'} \), then \( s_C(C_{i_1,i_2,...,i_m}, C'_{i_1',i_2',...,i_m'}) > s_C(C_{j_1,j_2,...,j_l}, C'_{j_1',j_2',...,j_l'}) \).

**H.S.2** (Symmetric property) For two pairs of classes \( \{C_{i_1,i_2,...,i_m}, C'_{i_1',i_2',...,i_m'}\} \) and \( \{C_{i_1,i_2,...,i_m}, C'_{j_1,j_2,...,j_l}\} \), if \( I_{i_1,i_2,...,i_m; j_1,j_2,...,j_l} = I_{i_1',i_2',...,i_m'; j_1',j_2',...,j_l'} \), then \( s_C(C_{i_1,i_2,...,i_m}, C'_{i_1',i_2',...,i_m'}) = s_C(C_{i_1,i_2,...,i_m}, C'_{j_1,j_2,...,j_l}) \).

The property (H.S.1) means that if the LLCA for the pair \( C_{i_1,i_2,...,i_m} \) and \( C'_{i_1',i_2',...,i_m'} \) is smaller than that of the pair \( C_{j_1,j_2,...,j_l} \) and \( C'_{j_1',j_2',...,j_l'} \), then the dissimilarity between the first pair is larger than that of the second pair. This is similar to a phylogenetic tree. For our example in Figure 1, \( C_{1,1} = \{\text{Elephant}\} \) and \( C_{1,2} = \{\text{Dog}\} \) have the latest common ancestor \( C_1 = \{\text{Animal}\} \), while \( C_{1,1,1} = \{\text{African elephant}\} \) and \( C_{1,1,2} = \{\text{Asian elephant}\} \) have the latest common ancestor \( C_{1,1} = \{\text{Elephant}\} \). Thus, we require \( s_C(C_{1,1,1}, C_{1,1,2}) > s_C(C_{1,1,1}, C_{1,1,1}) \).

The property (H.S.2) means that for a node \( C_{i_1,i_2,...,i_m} \) at the \( m \)-th layer and other two nodes \( C'_{i_1',i_2',...,i_m'} \) and \( C'_{j_1',j_2',...,j_l'} \) which are both located at the \( m \)-th layer, if the LLCA of \( \{C_{i_1,i_2,...,i_m}, C'_{i_1',i_2',...,i_m'}\} \) is the same as that of \( \{C_{i_1,i_2,...,i_m}, C'_{j_1',j_2',...,j_l'}\} \), then the dissimilarity between the first pair is the same as that of the second pair. This property guar-
Step 1. (Between a parent and a child) Add an edge between any non-leaf node \(C_{j_1,j_2,\ldots,j_{m-1}}\) at the \((m-1)\)-th layer (\(2 \leq m \leq k\)) and any of its children \(C_{j_1,j_2,\ldots,j_m} = 1,\ldots,N_{j_1,j_2,\ldots,j_{m-1}}\). Define the dissimilarity \(s_C(C_{j_1,j_2,\ldots,j_{m-1}}, C_{j_1,j_2,\ldots,j_m}) = \omega_{m-1}\), where \(\omega_{m-1}\) is a constant that will be specified later. Note that \(\omega_{m-1}\) only depends on the layer that the node locates at, regardless of the node itself.

Step 2. (Between two siblings) For \(2 \leq m \leq k\), add an edge between any pair of siblings in \(\{C_{j_1,j_2,\ldots,j_m}, j_m = 1,\ldots,N_{j_1,j_2,\ldots,j_{m-1}}\}\) with the same parent \(C_{j_1,j_2,\ldots,j_{m-1}}\), and assign the dissimilarity between them as \(\psi_{j_1,j_2,\ldots,j_{m-1}}\), which is a constant depending on \((j_1, j_2, \ldots, j_{m-1})\) and will be specified later. That is, \(s_C(C_{j_1,j_2,\ldots,j_{m-1}}, C_{j_1,j_2,\ldots,j_{m-1},j'}_{m}) = \psi_{j_1,j_2,\ldots,j_{m-1}},\) for any \(1 \leq j'_m \neq j''_m \leq N_{j_1,j_2,\ldots,j_{m-1}}, 2 \leq m \leq k\).

Now we have a graph \(G\) with the nodes set \(\mathcal{C}\) and the edges set \(\mathcal{E} = \{\text{edges between a parent and any node of its children}\} \cup \{\text{edges between two siblings}\}\). An example is shown in Figure 1. Then we can define the dissimilarity between any two different nodes, \(C_{i_1,i_2,\ldots,i_m}\) at the \(m\)-th layer and \(C_{j_1,j_2,\ldots,j_l}\) at the \(l\)-th layer, where \(1 \leq m, l \leq k\) and \(i_1 = j_1 \equiv 1\). Without any loss of generality, assume \(m \leq l\). Denote \(\text{Path}_{\text{min}}(C_{i_1,i_2,\ldots,i_m}, C_{j_1,j_2,\ldots,j_l})\) as the
path with the minimum number of connected edges between these two nodes on the graph \(G\), and \(\tilde{t} = i_{\tilde{t}},i_{\tilde{t}+1},\ldots,i_m,j_{\tilde{t}},\ldots,j_l\). Specifically, there are two cases as follows:

(i) If \(\tilde{t} = m\), then \(m < l\) and \(C_{i_1,i_2,\ldots,i_m}\) is the ancestor of \(C_{j_1,j_2,\ldots,j_l}\). Then we have the following Path\(_{\text{min}}(C_{i_1,i_2,\ldots,i_m},C_{j_1,j_2,\ldots,j_l})\),

\[
C_{i_1,i_2,\ldots,i_m} \to C_{i_1,i_2,\ldots,i_m,j_{m+1}} \to \cdots \to C_{i_1,i_2,\ldots,i_m,j_{m+l}}.
\]  

(2.2)

(ii) Otherwise, by the definition of \(\tilde{t}\), it holds that \((i_1,i_2,\ldots,i_{\tilde{t}}) = (j_1,j_2,\ldots,j_{\tilde{t}})\). Then we have \(C_{i_1,i_2,\ldots,i_{\tilde{t}+1}}\) and \(C_{j_1,j_2,\ldots,j_{\tilde{t}+1}}\) being siblings. Thus, Path\(_{\text{min}}(C_{i_1,i_2,\ldots,i_m},C_{j_1,j_2,\ldots,j_l})\) is the combinations of Path\(_{\text{min}}(C_{i_1,i_2,\ldots,i_m},C_{i_1,i_2,\ldots,i_{\tilde{t}+1}})\), the edge between \(C_{i_1,i_2,\ldots,i_{\tilde{t}+1}}\) and \(C_{j_1,j_2,\ldots,j_{\tilde{t}+1}}\), and Path\(_{\text{min}}(C_{j_1,j_2,\ldots,j_{\tilde{t}+1}},C_{j_1,j_2,\ldots,j_l})\), that is,

\[
C_{i_1,i_2,\ldots,i_m} \to \cdots \to C_{i_1,i_2,\ldots,i_{\tilde{t}+1}} \to C_{j_1,j_2,\ldots,j_{\tilde{t}+1}} \to \cdots \to C_{j_1,j_2,\ldots,j_l}.
\]  

(2.3)

Based on Path\(_{\text{min}}(C_{i_1,i_2,\ldots,i_m},C_{j_1,j_2,\ldots,j_l})\), we can define the dissimilarity between two nodes as follows.

**Definition 3. (Dissimilarity between two nodes)** Rename the nodes along Path\(_{\text{min}}(C_{i_1,i_2,\ldots,i_m},C_{j_1,j_2,\ldots,j_l})\) as \(\nu_i, 1 \leq i \leq r\), where \(r\) is the total number of nodes in the path, then define the dissimilarity 

\[
s_C(C_{i_1,i_2,\ldots,i_m},C_{j_1,j_2,\ldots,j_l}) = \left(\sum_{i=1}^{r} s_C(\nu_i,\nu_{i+1})\right)^{1/2}.
\]

Combining with the definition in Steps 1 and 2, we get the explicit form of the dissimilarity between any two nodes as shown in Proposition \ref{prop1}.

**Proposition 1.** The dissimilarity between nodes \(C_{i_1,\ldots,i_m}\) and \(C_{j_1,\ldots,j_l}\) is defined as

\[
s_C(C_{i_1,\ldots,i_m},C_{j_1,\ldots,j_l}) = \begin{cases} 
\left(\frac{\max\{m,l\}-1}{\sum_{i=\tilde{t}}^{m,l} \omega_i^2}\right)^{1/2}, & \tilde{t} = \min\{m,l\}, \\
\left(\sum_{i=1}^{m-l} \omega_i^2 + \sum_{i=1}^{l-\tilde{t}} \omega_i^2 - 2 \sum_{i=1}^{\tilde{t}} \omega_i^2\right)^{1/2}, & \tilde{t} < \min\{m,l\}.
\end{cases}
\]

(2.4)
where \( \tilde{t} = I_{t_{1}, \ldots, t_{m}; j_{1}, \ldots, j_{l}} \) and \( j_{1} = i_{1} \equiv 1 \).

Take the example in Figure 1 for an illustration. The path with the minimum step between nodes \( C_{1,1,1,1} \) and \( C_{1,2,1} \) is \( C_{1,1,1,1} \rightarrow C_{1,1,1} \rightarrow C_{1,1} \rightarrow C_{1,2} \rightarrow C_{1,2,1} \). Thus, the dissimilarity between these two nodes is \( s_{C}(C_{1,1,1,1}, C_{1,2,1}) = (\psi_{1}^{2} + 2\omega_{2}^{2} + \omega_{3}^{2})^{1/2} \). To ensure that the dissimilarity defined in (2.4) satisfies H.S. properties, we need the following assumption.

**Assumption 1.** Given \( \omega_{1} > 0 \) and a constant \( \delta > 1 \), assume that \( \omega_{m} = \omega_{m-1}/\delta \) for \( 2 \leq m \leq k \) and that

\[
\omega_{m-1} < \psi_{j_{1}, j_{2}, \ldots, j_{m-1}} \leq 2\omega_{m-1}, \quad 2 \leq m \leq k. \tag{2.5}
\]

Assumption \( \omega_{m} = \omega_{m-1}/\delta \) means that the dissimilarity between a parent and any node of its children decreases when the layer increases along the tree, which is reasonable. The left part of (2.5) means that the dissimilarity between a node and its parent is not larger than that between it and its sibling. The right part of (2.5) is in a similar spirit as that of the triangle inequality. In Section 3.2, we give a specific form of \( \psi_{j_{1}, j_{2}, \ldots, j_{m-1}} \) satisfying Assumption 1. By Assumption 1, the following Theorem 1 shows that H.S. properties hold.

**Theorem 1.** Under Assumption 1 with \( \delta^{2} \geq 2\sqrt{2} + 2 \), the dissimilarity defined in (2.4) satisfies H.S. properties.

### 3 Exact label embedding

In this section, we consider the exact label embedding in hierarchical classification, by establishing an isometry (i.e. the Euclidean distance between embedded points is exactly equal to the dissimilarity between nodes on the tree). We first consider the case of \( q \)-class multicategory classification, where the label embedding approach has been considered in literature (Lange and Wu 2008; Zhang and Liu 2014). We give a different way to con-
Algorithm 1 : Label embedding in multicategory classification

1. **Initialization:** Given a constant $c > 0$, set $\xi^{(1)}_1 = c/2, \xi^{(1)}_2 = -c/2$.

2. **Iteration:** For $m = 2, \cdots, \tilde{q} - 1$, repeat the following steps (1) and (2).

   (1) Set $\xi^{(m)}_i = ((\xi^{(m-1)}_i)^\top, 0)^\top \in \mathbb{R}^m, i = 1, \cdots, m$;

   (2) $\xi^{(m)}_{m+1} = m^{-1} \sum_{i=1}^m \xi^{(m)}_i + a_m e^{(m)}_m$, where $a_m = \sqrt{c^2 - d_{m-1}^2}$ with $d_{m-1} = \|m^{-1} \sum_{i=1}^m \xi^{(m-1)}_i - \xi^{(m-1)}_m\|$, and $e_m \in \mathbb{R}^m$ with the $m$-th coordinate being 1 and others being 0.

3. **Centralization:** Let $\xi_i \leftarrow \xi_i - (\tilde{q} - 1) \sum_{j=1}^{\tilde{q}} \xi_j, i = 1, \cdots, \tilde{q}$.

4. **Scaling:** $\tilde{\xi}_i \leftarrow T_{\tilde{q}}^{-1} \xi_i$ for $1 \leq i \leq \tilde{q}$, where $T_{\tilde{q}}$ is given in Proposition 2.

struct points for multicategory classification in Section 3.1, and then extend to hierarchical classification in Section 3.2.

### 3.1 Label embedding in multicategory classification

In this subsection, we give the procedure to construct $\tilde{q}$ ($\tilde{q} \geq 2$) points with equal pairwise distances in the $\mathbb{R}^{\tilde{q}-1}$ Euclidean space, which is similar in spirit to the methods in Lange and Wu (2008), Wu and Lange (2010), Wu and Wu (2012) and Zhang and Liu (2014) for $\tilde{q}$-class multicategory classification problems. The $\tilde{q}$ points $\{\xi_i\}_{i=1}^{\tilde{q}}$ in $\mathbb{R}^{\tilde{q}-1}$ with an equal pairwise distance can be constructed by Algorithm 1, which indeed formulate a simplex. Recall that $u^{(m)}$ denotes the subvector consisting of the first $m$ coordinates of $u$.

**Proposition 2.** The following conclusions hold.

1. For $\{\xi_i\}_{i=1}^{\tilde{q}}$ constructed in Steps 1-3 of Algorithm 1,

   (i) $\|\xi_i - \xi_j\| = c$ for $1 \leq i \neq j \leq \tilde{q}$;

   (ii) $\|\xi_i\| = T_{\tilde{q}}$ for $1 \leq i \leq \tilde{q}$, where $T_{\tilde{q}} = c[(\tilde{q} - 1)/2\tilde{q}]^{1/2}$;

   (iii) the angles $\angle(\xi_i, \xi_j)$ are all equal for $1 \leq i \neq j \leq \tilde{q}$ with $\cos \angle(\xi_i, \xi_j) = -1/(\tilde{q} - 1)$.

2. For $\{\tilde{\xi}_i\}_{i=1}^{\tilde{q}}$ constructed in Steps 1-4 of Algorithm 1,
(i) \( \| \xi_i \| = T \) for \( 1 \leq i \leq \tilde{q} \);

(ii) \( \| \xi_i - \xi_j \| = c_{\tilde{q}} \) for \( 1 \leq i \neq j \leq \tilde{q} \), where \( c_{\tilde{q}} = T[2\tilde{q}/(\tilde{q} - 1)]^{1/2} \).

Proposition 2 shows that \( \{ \xi_i \}_{i=1}^{\tilde{q}} \) constructed in Steps 1–3 have an equal pairwise distance \( c \). Thus, if constructing points of an equal pairwise distance \( c \) is the goal, implementing Steps 1–3 is sufficient. In some cases, it is desirable to require further the constructed points having the same norm \( T \). To this end, in Step 4, we scale the points \( \{ \xi_i \}_{i=1}^{\tilde{q}} \). After Step 4, the points \( \{ \tilde{\xi}_i \}_{i=1}^{\tilde{q}} \) have the equal pairwise distance \( c_{\tilde{q}} \) and the same \( l_2 \) norm \( T \).

Remark 1. Points constructed in Algorithm 1 are in the space spanned by \( \{ e_j \in \mathbb{R}^{\tilde{q}-1}, 1 \leq j \leq \tilde{q} \} \), where \( e_j \)'s are the coordinate bases of \( \mathbb{R}^{\tilde{q}-1} \). For integers \( a \) and \( b \) with \( b \geq a + \tilde{q} - 1 \) and \( a \geq 0 \), Algorithm 1 can be directly extended to construct points in the subspace spanned by the coordinate bases \( \{ e_j \in \mathbb{R}^b, a + 1 \leq j \leq a + \tilde{q} - 1 \} \), by extending the vector \( \tilde{\xi}_i \) to \( (0_a^\top, \tilde{\xi}_i^\top, 0_{b-a-\tilde{q}+1}^\top) \), \( 1 \leq i \leq \tilde{q} \).

For the example in Figure 1, if we ignore the tree structure and consider multicategory classification on leaf nodes, the points constructed by Algorithm 1 given \( T = 1 \) are

\[
\begin{pmatrix}
C_{1,1,1,1} & C_{1,1,1,2} & C_{1,1,2} & C_{1,2,1} & C_{1,2,2} & C_{1,2,3} \\
-\sqrt{15}/5 & \sqrt{15}/5 & 0 & 0 & 0 & 0 \\
-\sqrt{5}/5 & -\sqrt{5}/5 & 2\sqrt{5}/5 & 0 & 0 & 0 \\
-\sqrt{10}/10 & -\sqrt{10}/10 & -\sqrt{10}/10 & 3\sqrt{10}/10 & 0 & 0 \\
-\sqrt{6}/10 & -\sqrt{6}/10 & -\sqrt{6}/10 & -\sqrt{6}/10 & 2\sqrt{6}/5 & 0 \\
-1/5 & -1/5 & -1/5 & -1/5 & -1/5 & 1
\end{pmatrix}.
\]

The points in (3.1) incorporate no hierarchy, and the distance is \( 2\sqrt{15}/5 \) for all pairs of leaf nodes. As stated in (H.S.1), it is more reasonable to require \( d_{C_H}(C_{1,1,1}, C_{1,1,2}) < d_{C_H}(C_{1,1,2}, C_{1,2,1}) \). In the following subsection, we propose an approach, which incorporates the hierarchical information while requiring the same dimension as (3.1).

3.2 Label embedding in hierarchical classification

We now extend the idea in Section 3.1 to hierarchical classification. Note that the root is meaningless, and we ignore it. Recall \( n_{\text{leaf}} \) is the number of leaf nodes on the tree and \( j_1 \equiv 1 \).
For $2 \leq m \leq k$, denote the nodes at the $m$-th layer and their corresponding embedding points respectively as $C_{H,m} = \{C_{j_1,j_2,\ldots,j_m}, j_s = 1, \ldots, N_{j_1,j_2,\ldots,j_{s-1}}, s = 2, \ldots, m\}, E_{H,m} = \{\xi_{j_1,j_2,\ldots,j_m} \in \mathbb{R}^K : j_s = 1, \ldots, N_{j_1,j_2,\ldots,j_{s-1}}, s = 2, \ldots, m\}$, where the dimension $K \geq n_{\text{leaf}} - 1$. In fact, Proposition 3 below shows that it is sufficient to set $K = n_{\text{leaf}} - 1$.

For $m = 2$, there are $N_{j_1}$ nodes in $C_{H,2}$. Let $D_2 = N_{j_1} - 1$. Then we construct points $\{\xi_{j_1,j_2} \in \mathbb{R}^K, j_2 = 1, \ldots, N_{j_1}\}$, where the subvectors $\{\xi_{j_1,j_2}^{(D_2)} : j_2 = 1, \ldots, N_{j_1}\}$ of dimension $D_2$ are constructed by Algorithm 1 with a given norm $T(1)$, and the coordinates of $\xi_{j_1,j_2}$ with indices larger than $D_2$ are set zero. For $m = 3, \ldots, k$, $E_{H,m}$ is constructed by Algorithm 2. We see that the $i$-th ($i > D_k$) coordinate of any point $\xi_{j_1,j_2,\ldots,j_m}$ is zero. Furthermore, Proposition 3 shows that $D_k = n_{\text{leaf}} - 1$. Thus, it is sufficient to set $K = n_{\text{leaf}} - 1$.

Algorithm 2: Label embedding in hierarchical classification

For $m = 3, \ldots, k$, repeat the following Steps 1-3:

1. Sort all non-leaf nodes in $C_{H,m-1}$ from left to right and rename them as $C_{i}^{(m-1)} \cdot \cdot \cdot , C_{n_{m-1}}^{(m-1)}$, where $n_{m-1}$ is the number of non-leaf nodes at the $(m-1)$-th layer. Then for any $1 \leq i \leq n_{m-1}$, there exists some index $(j'_2, \ldots, j'_{m-1})$ such that $C_i^{(m-1)} = C_{j'_1,j'_2,\ldots,j'_{m-1}}$ with $j'_1 = 1$. For each non-leaf node $C_i^{(m-1)} = C_{j'_1,j'_2,\ldots,j'_{m-1}}$, it has children $\text{Chi}(C_i^{(m-1)}) = \{C_{j_1,j'_2,\ldots,j'_{m-1}}, j_m = 1, \ldots, N_{j'_1,j'_2,\ldots,j'_{m-1}}\}$ at the $m$-th layer with $N_{j_1,j'_2,\ldots,j'_{m-1}} \geq 2$ according to our assumption that each parent node has at least two children. Let $d_{m,i} = N_{j'_1,j'_2,\ldots,j'_{m-1}} - 1, i = 1, \ldots, n_{m-1}$ and $T^{(m-1)} = T^{(m-2)}/\delta$ with $\delta$ being the constant defined in Assumption 1.

2. For any $C_i^{(m-1)}$ ($1 \leq i \leq n_{m-1}$) and its children $\text{Chi}(C_i^{(m-1)})$, we construct $N_{j'_1,j'_2,\ldots,j'_{m-1}}$ points denoted as $\{n_{j'_1,j'_2,\ldots,j'_{m-1}} : j_m = 1, \ldots, N_{j'_1,j'_2,\ldots,j'_{m-1}}\}$ based on Algorithm 1 and Remark 1 in Section 3.1 with the given norm $T^{(m-1)}$ in the subspace

$$\text{span} \left\{ e_j \in \mathbb{R}^K : D_{m-1} + 1 + \sum_{s=0}^{i-1} d_{m,s} \leq j \leq D_{m-1} + \sum_{s=0}^{i} d_{m,s} \right\} \quad (3.2)$$

where $d_{m,0} = 0$ and $e_j$’s are the coordinate bases in $\mathbb{R}^K$. Then let

$$\xi_{j'_1,j'_2,\ldots,j'_{m-1}} = \xi_{j'_1,j'_2,\ldots,j'_{m-1}} + n_{j'_1,j'_2,\ldots,j'_{m-1}}, \quad j_m = 1, \ldots, N_{j'_1,j'_2,\ldots,j'_{m-1}}. \quad (3.3)$$

3. Repeat Step 2 for all $n_{m-1}$ non-leaf nodes in $C_{H,m-1}$ and set $D_m = D_{m-1} + \sum_{i=1}^{n_{m-1}} d_{m,i}$.

Proposition 3. It holds that $D_k = n_{\text{leaf}} - 1$ and for any $i > D_k$, the $i$-th coordinate of any
point $\xi_{j_1,j_2,\ldots,j_m} \in \bigcup_{l=2}^k E_{H,l}$ is zero. Thus, the dimension of the embedded space can be set as $K = D_k = n_{\text{leaf}} - 1$.

Note that for a different $i$, the subspaces $(3.2)$ are orthogonal. The coordinates of $\xi_{j_1',j_2',\ldots,j_{m-1}'}$ with an index larger than $D_{m-1}$ are all zero by the proof of Proposition 3, while the first $D_{m-1}$ coordinates of $\eta_{j_1',j_2',\ldots,j_{m-1}'}$ are all zero. Thus, $(3.3)$ in Step 3 indicates that the constructed points inherit the coordinates from its parent node, and then incorporate the hierarchical information. Recall $C_H = C / \{C_1\} = \bigcup_{m=2}^k C_{H,m}$. Let $E_H = \bigcup_{m=2}^k E_{H,m}$. Define the map $F_H : C_H \rightarrow E_H$ satisfying $F_H(C_{j_1,j_2,\ldots,j_m}) = \xi_{j_1,j_2,\ldots,j_m}$. Then the following theorem shows that $F_H$ is an isometry.

**Theorem 2.** Assume that $\delta^2 \geq 2\sqrt{2} + 2$. Let $\psi_{j_1,j_2,\ldots,j_{m-1}} = \omega_m \left[ 2N_{j_1,\ldots,j_{m-1}} / (N_{j_1,\ldots,j_{m-1}} - 1) \right]^{1/2}$, $2 \leq m \leq k$, where $j_1 \equiv 1$. Then $\psi_{j_1,j_2,\ldots,j_{m-1}}$ satisfies Assumption 1. In addition, for any two nodes $C_{i_1,i_2,\ldots,i_m}$ and $C_{j_1,j_2,\ldots,j_l}$, it holds that

$$s_C(C_{i_1,i_2,\ldots,i_m}, C_{j_1,j_2,\ldots,j_l}) = \frac{\omega_1}{T(1)} d_E(F_H(C_{i_1,i_2,\ldots,i_m}), F_H(C_{j_1,j_2,\ldots,j_l})).$$

Specifically, setting $T(1) = \omega_1$, we have that $F_H$ is an isometry from $(C_H, s_C)$ to $(E_H, d_E)$.

**Remark 2.** Without loss of generality, we set $\omega_1 = 1$ and consequently $T(1) = 1$ to keep the isometry property. In fact, classification results are invariant for any $T(1) > 0$ according to the results in Sections 4 and 5. Moreover, as long as $\delta^2 \geq 2\sqrt{2} + 2$, preliminary experiments show that the effect of $\delta$ is limited. In this paper, we set $\delta = \sqrt{2}$. In addition, $\delta$ is a constant independent of $m$, and it can be extended to allow $\delta$ depending on $m$, i.e. $\omega_m = \omega_{m-1}/\delta_m$.

Combining Theorems 1 and 2, we can show that the embedded points also satisfy H.S. properties as stated in the following proposition.

**Proposition 4.** For $\delta^2 \geq 2\sqrt{2} + 2$, it holds that

1. For any two pairs of points $\{\xi_{i_1,\ldots,i_m}, \xi'_{i_1',\ldots,i_m'}\}$ and $\{\xi_{j_1,\ldots,j_l}, \xi'_{j_1',\ldots,j_l'}\}$, if $I_{i_1,\ldots,i_m,i_1',\ldots,i_m'} < I_{j_1,\ldots,j_l,j_1',\ldots,j_l'}$, then $d_E(\xi_{i_1,\ldots,i_m}, \xi'_{i_1',\ldots,i_m'}) > d_E(\xi_{j_1,\ldots,j_l}, \xi'_{j_1',\ldots,j_l'}).$
For any two pairs of points \( \{\xi_{i_1, \ldots, i_m}, \xi_{i'_1, \ldots, i'_m}\} \) and \( \{\xi_{i_1, \ldots, i_m}, \xi_{j'_1, \ldots, j'_m}\} \), if \( I_{i_1, \ldots, i_m} = I_{i'_1, \ldots, i'_m; j'_1 \ldots, j'_m} \), then \( d_E(\xi_{i_1, \ldots, i_m}, \xi_{i'_1, \ldots, i'_m}) = d_E(\xi_{i_1, \ldots, i_m}, \xi_{j'_1, \ldots, j'_m}) \).

For the example in Figure 1, the whole label embedding matrix is constructed as

\[
\begin{pmatrix}
C_{1,1} & C_{1,2} & C_{1,1,1} & C_{1,1,2} & C_{1,2,1} & C_{1,2,2} & C_{1,1,2,1} & C_{1,1,2,2} \\
-1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\
0 & 0 & -\sqrt{5}/5 & \sqrt{5}/5 & 0 & 0 & -\sqrt{5}/5 & -\sqrt{5}/5 \\
0 & 0 & 0 & 0 & -\sqrt{15}/10 & \sqrt{15}/10 & 0 & 0 \\
0 & 0 & 0 & 0 & -\sqrt{5}/10 & -\sqrt{5}/10 & \sqrt{5}/5 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1/5 & 1/5
\end{pmatrix}
\] (3.4)

The dimension of the embedding space is 5, much smaller than 9 required by the classical label embedding method [2.1], and is the same as that of the multicategory case in (3.1), where the hierarchical information is ignored. The distance matrix associated with (3.4) is

\[
\begin{pmatrix}
C_{1,1} & C_{1,2} & C_{1,1,1} & C_{1,1,2} & C_{1,2,1} & C_{1,2,2} & C_{1,1,2,1} & C_{1,1,2,2} \\
2 & \sqrt{5}/5 & \sqrt{5}/5 & \sqrt{105}/5 & \sqrt{105}/5 & \sqrt{105}/5 & \sqrt{6}/5 & \sqrt{6}/5 \\
\sqrt{105}/5 & \sqrt{105}/5 & \sqrt{5}/5 & \sqrt{5}/5 & \sqrt{5}/5 & \sqrt{106}/5 & \sqrt{106}/5 \\
2\sqrt{5}/5 & \sqrt{110}/5 & \sqrt{110}/5 & \sqrt{110}/5 & 1/5 & 1/5 & 1/5 \\
\sqrt{110}/5 & \sqrt{110}/5 & \sqrt{110}/5 & \sqrt{110}/5 & \sqrt{21}/5 & \sqrt{21}/5 & \sqrt{21}/5 \\
\sqrt{15}/5 & \sqrt{15}/5 & \sqrt{15}/5 & \sqrt{11}/5 & \sqrt{11}/5 & 2/5 & 2/5 \\
\sqrt{15}/5 & \sqrt{15}/5 & \sqrt{15}/5 & \sqrt{15}/5 & \sqrt{11}/5 & \sqrt{11}/5 & \sqrt{11}/5 & \sqrt{11}/5 \\
\sqrt{11}/5 & \sqrt{11}/5 & \sqrt{11}/5 & \sqrt{11}/5 & \sqrt{11}/5 & \sqrt{11}/5 & \sqrt{11}/5 & \sqrt{11}/5 \\
2/5 & 2/5 & 2/5 & 2/5 & 2/5 & 2/5 & 2/5 & 2/5
\end{pmatrix}
\]

It can be seen that our embedding points incorporate the hierarchy. Recall that \( C_{1,1} = \{\text{Elephant}\}, C_{1,2} = \{\text{Dog}\}, C_{1,1,1} = \{\text{African elephant}\}, C_{1,1,2} = \{\text{Asian elephant}\}, C_{1,2,1} = \{\text{Herding dog}\} \). Then we have \( d_{C_H}(C_{1,1}, C_{1,2}) = 2 \), which is larger than \( d_{C_H}(C_{1,1,1}, C_{1,1,2}) = 2\sqrt{5}/5 \), and the latter is smaller than \( d_{C_H}(C_{1,1,2}, C_{1,2,1}) = \sqrt{110}/5 \).

4 Angle-based hierarchical classification via exact label embedding

In hierarchical classification, denote \( Z = (X, Y) \in \mathcal{X} \times \mathcal{Y} \), where \( \mathcal{X} \subset \mathbb{R}^p \) and \( \mathcal{Y} \) is the set of paths from the root to a leaf on the tree. Specifically, \( X \in \mathbb{R}^p \) is a \( p \)-dimensional input.
vector, and \( Y = \{ Y^{(1)}, \ldots, Y^{(L(Y))} \} \) is the corresponding output with \( Y^{(m)} \) indicating the label at the \( m \)-th layer and \( L(Y) \) being the layer where the leaf locates, i.e. \( Y^{(1)} = C_1 \), and \( Y^{(m)} \in \text{Chi}(Y^{(m-1)}) \) for \( m = 2, \ldots, L(Y) \). For example, two possible paths in Figure 1 are \( y = \{ C_1, C_{1,1}, C_{1,1,1}, C_{1,1,1,1} \} \) with \( L(y) = 4 \) and \( y = \{ C_1, C_{1,2}, C_{1,2,1} \} \) with \( L(y) = 3 \).

### 4.1 Hierarchical classification with the top-down strategy

Different from multicategory classification, the strategies for hierarchical classification are more complicated. The most commonly used strategy is the top-down (TD) (Wang et al., 2011), which is adopted in this paper. It means given an instance classified to a node at the \((m-1)\)-th layer, we only consider to classify it into one of its children at the \( m \)-th layer.

For \( m = 2, \ldots, L(y) \), define \( \xi_m(y) = F_H(y^{(m)}) \) being the corresponding constructed point, i.e. \( \xi_m(y) = \xi_{j_1, \ldots, j_m} \) if \( y^{(m)} = C_{j_1, \ldots, j_m} \). Denote the learning function as \( f(x) = (f_1(x), \ldots, f_K(x))^\top \in \mathbb{R}^K \), where \( K = n_{\text{leaf}} - 1 \). Similar to Zhang and Liu (2014), we define a linear discriminant function \( g : (f(x), \xi_m(y)) \rightarrow \langle f(x), \xi_m(y) \rangle \), where \( \langle \cdot, \cdot \rangle \) denotes the inner product in the Euclidean space. We denote by \( \hat{y} = \mathcal{H}(f(x)) \in \mathcal{Y} \) the predicted path for \( x \) according to the following hierarchical classification rule with given \( f(x) \). Note that \( \hat{y}^{(1)} \equiv C_1 \).

**Definition 4. (TD)** For \( m \geq 2 \), assume \( x \) has been assigned to the label \( \hat{y}^{(m-1)} \) at the \((m-1)\)-th layer. When \( \hat{y}^{(m-1)} \) is not a leaf node, we assign \( x \) to one of its children \( \hat{y}^{(m)} \in \text{Chi}(\hat{y}^{(m-1)}) \) at the \( m \)-th layer, if the corresponding embedded point \( \xi_m(\hat{y}) \) has the largest inner product at the \( m \)-th layer, that is, for any \( \tilde{y} \in \mathcal{E}_m(\hat{y}) = \{ \tilde{y} : \tilde{y}^{(m)} \neq \hat{y}^{(m)}, \tilde{y}^{(m)} \in \text{Chi}(\tilde{y}^{(m-1)}) \} \),

\[
g(f(x), \xi_m(\hat{y})) \geq g(f(x), \xi_m(\tilde{y})). \tag{4.1}
\]

Note that \( \xi_m(\tilde{y}) \) depends only on \( \tilde{y}^{(m)} \). It is possible that there are many \( \tilde{y} \in \mathcal{E}_m(\hat{y}) \) with the same label \( \tilde{y}^{(m)} \) at the \( m \)-th layer. If this is the case, taking only one of them as the rep-
representative and denoting the set of representatives as \([E_m(\hat{y})]\), we only need to require that (4.1) holds for any \(\hat{y} \in [E_m(\hat{y})]\). Take the example in Figure 1 for an illustration. Let \(\hat{y}^{(1)} = C_1\). We consider the children \(C_{1,1}\) and \(C_{1,2}\). Then \(x\) is assigned with \(\hat{y}^{(2)} = C_{1,1}\), if (4.1) holds for any \(\tilde{y} \in E_2(\hat{y})\) with \(E_2(\hat{y}) = \{\{C_1, C_{1,2}, C_{1,2,1}\}, \{C_1, C_{1,2}, C_{1,2,2}\}, \{C_1, C_{1,2}, C_{1,2,3}\}\}\). The three paths in \(E_2(\hat{y})\) have the same label \(C_{1,2}\) at the second layer, then it is sufficient to take any of them as the representative, and require (4.1) holds, i.e. \(\langle f(x), \xi_{1,1} \rangle > \langle f(x), \xi_{1,2} \rangle\); otherwise, we set \(\hat{y}^{(2)} = C_{1,2}\). Supposing \(\hat{y}^{(2)} = C_{1,2}\), we then consider the children of \(C_{1,2}\), that is, \(C_{1,2,1}, C_{1,2,2}, C_{1,2,3}\). Computing \(\langle f(x), \xi_{1,2,1} \rangle, \langle f(x), \xi_{1,2,2} \rangle\) and \(\langle f(x), \xi_{1,2,3} \rangle\), \(\hat{y}^{(3)}\) is taken as the class that the corresponding embedded point has the largest inner product.

It is shown in Lemma 2 of the Supplementary Material that all points \(\xi_m(\tilde{y})\) with \(\tilde{y} \in [E_m(\hat{y})]\) have the same norm. Therefore, (4.1) holds as long as \(d_E(f(x), \xi_m(\tilde{y})) \leq d_E(f(x), \xi_m(\tilde{y}))\), which shows that our classification strategy is essentially based on the Euclidean distance. Given the linear discriminant function \(g\), define \(G_m(f(x), y, \tilde{y}) = g(f(x), \xi_m(y)) - g(f(x), \xi_m(\tilde{y}))\), \(\tilde{y} \in [E_m(y)], m = 2, \cdots , L(y)\). For an instance \(z = (x, y)\), we define the following hierarchy margin \(M(f(x), y)\) associated with the strategy TD,

\[
M(f(x), y) = \min_{m=2, \cdots, L(y)} \left[ g(f(x), \xi_m(y)) - \max_{\tilde{y} \in [E_m(y)]} g(f(x), \xi_m(\tilde{y})) \right] = \min_{m=2, \cdots, L(y)} \min_{\tilde{y} \in [E_m(y)]} G_m(f(x), y, \tilde{y}).
\]

A positive margin is required for the classifier to assign the correct label along the whole path, which is equivalent to a set of linear constraints

\[
G_m(f(x), y, \tilde{y}) \geq 0, \quad \tilde{y} \in [E_m(y)], m = 2, \cdots , L(y).
\]  

(4.2)

A special case of the hierarchy margin is \(k = 2\) without any hierarchical structure. If \(M(f(x), y) \geq 0\), that is, \(\langle f(x), \xi_2(y) \rangle \geq \langle f(x), \xi_2(\tilde{y}) \rangle\) for any \(\tilde{y} \in [E_2(y)] = \{\tilde{y} : \tilde{y}^{(2)} \neq \hat{y}^{(2)}\}\), then \(x\) is correctly classified by \(f(x)\). This is exactly the same as the method of Zhang and Liu (2014) for multiclassification. Therefore, the hierarchy margin is
a natural extension of the margin in multicategory classification (Zhang and Liu 2014).

Recall $\mathcal{H}(f(x)) \in \mathcal{Y}$ is the classification rule by $f(x)$ with the top-down strategy. There are several definitions of the generalization error in hierarchical classification, and details can be referred to Wang et al. (2009, 2011); Babbar et al. (2016). In this paper, we use the 0-1 hierarchical loss and define $R(f) = E[I(Y \neq \mathcal{H}(f(X)))]$ (Wang et al. 2011; Babbar et al. 2016). One can verify that $I(Y \neq \mathcal{H}(f(X))) = I(M(f(X), Y) < 0)$. A classification error occurs if (4.2) fails, that is, $G_m(f(x), y, \tilde{y}) < 0$ for some $m$ and $\tilde{y} \in [E_m(y)]$.

Let $\{z_i : z_i = (x_i, y_i)\}_{i=1}^n$ be a set of $n$ labeled training samples. The empirical generalization error is defined as $n^{-1} \sum_{i=1}^n I(M(f(x_i), y_i) < 0)$, which is computationally infeasible because of the discontinuity. Given a convex surrogate loss $\ell$, the optimization problem can be formulated as $\min_{f \in \mathcal{F}} n^{-1} \sum_{i=1}^n \ell(M(f(x_i), y_i)) + \lambda J(f)$, or equivalently $\min_{f \in \mathcal{F}} n^{-1} \sum_{i=1}^n \ell(M(f(x_i), y_i))$, subject to $J(f) \leq s_{\lambda}$, where $\mathcal{F}$ is the set of candidate functions, $J(f)$ is a penalty function of $f$, and $\lambda$ and $s_{\lambda} > 0$ are tuning parameters. However, solving the above problem is computationally heavy because of the discontinuity of the derivative of $M(f(x_i), y_i)$. For example, for the linear classifier $f(x) = Ax$ where $A \in \mathbb{R}^{K \times p}$ and the first coordinate of $x$ is set to 1, one can see that $\partial M(Ax_i, y_i)/\partial A$ is discontinuous. To improve the computational efficiency, we then replace $\ell(M(f(x_i), y_i))$ by $V_\ell(f, z_i) = \sum_{m=2}^{c(y_i)} \sum_{\tilde{y} \in [E_m(y)]} \ell(G_m(f(x_i), y_i, \tilde{y}))$, and estimate $\hat{f}_{\lambda}$ by solving

$$\hat{f}_{\lambda} = \arg \min_{f \in \mathcal{F}} n^{-1} \sum_{i=1}^n V_\ell(f, z_i) + \lambda J(f).$$

For general loss functions, $\mathcal{F}$ is regularly chosen as the set of linear functions or the set of all measurable functions. To reduce computation, we introduce in Section 4.2 a special linear loss $\ell(u) = -u$. As shown in the Supplementary Material, a restriction $E(\|f\|^2) \leq 1$ is required in the theoretical analysis for the linear loss. Thus, for the linear loss, $\mathcal{F}$ should be restricted on the set $\{f : E(\|f\|^2) \leq 1\}$ in (4.3), e.g. $\{\text{all linear functions}\} \cap \{f : E(\|f\|^2) \leq 1\}$ or $\{\text{all measurable functions}\} \cap \{f : E(\|f\|^2) \leq 1\}$. As $\lambda \to 0$, (4.3) is argmin$_{f \in \mathcal{F}} n^{-1} \sum_{i=1}^n V_\ell(f, z_i)$. The theoretical properties of $\hat{f}_{\lambda}$ is established in Section 5.
Remark 3. For the linear loss, solving (4.3) might be involved due to the restriction $E(\|f\|^2) \leq 1$. For easy of computation, we approximate $\hat{f}_\lambda$ by first solving (4.3) without the restriction $E(\|f\|^2) \leq 1$, getting an unscaled estimator, and then scaling it to guarantee $E(\|\hat{f}_\lambda\|^2) \leq 1$. For a large $\lambda$, the unscaled estimator can satisfy the restriction $E(\|f\|^2) \leq 1$, that is, $\hat{f}_\lambda$ can be calculated directly by removing the restriction $E(\|f\|^2) \leq 1$. When $\lambda$ is small, there may be a small gap between the actual method and the theoretical analysis. In particular, when a linear classifier is applied, one can verify that the estimator calculated in this way is tuning-parameter free and leads to the same classification result as that obtained in the next Section 4.2.

For the linear classifier $f(x) = Ax \in \mathcal{F}$ and $J(f)$ being the square of the Frobenius norm of $A$, we have

$$\hat{A}_\lambda = \arg\min_A n^{-1} \sum_{i=1}^n V_i(Ax_i, z_i) + \lambda \|A\|_F^2.$$  \hspace{1cm} (4.4)

The estimated classifier is $\hat{f}_\lambda(x) = \hat{A}_\lambda x$.

The estimators derived from (4.3) and (4.4) have two advantages. First, it is computationally efficient. Second, as shown in Section 5.1, the population version of the estimator is Fisher consistent under mild conditions, which ensures the validity of the estimator. Simulation and application results in Section 6 show that our approach has obvious advantages in classification accuracy and computation, compared with other existing methods. In order to reduce computation further, in Section 4.2, we propose two specific loss functions, the linear loss and the weighted linear loss, under which a closed form of $\hat{A}_\lambda$ can be obtained.

4.2 Linear loss functions

To improve the computational efficiency of our method for massive data, we propose a linear loss function similar to that in the SVM binary classification problem (Shao et al.).
It leads to a closed form solution, avoiding iterations in optimization.

Define the linear loss function \( \ell_{\text{lin}}(u) = -u \), which is equivalent to the loss \( \tilde{\ell}_{\text{lin}}(u) = 1 - u \) in the sense that both lead to the same estimator. Note that \( \ell_{\text{hinge}}(u) = \max\{\tilde{\ell}_{\text{lin}}(u), 0\} \) can be viewed as the truncated version of \( \tilde{\ell}_{\text{lin}}(u) \). Under the linear loss, we denote the unscaled minimizer of (4.4) as \( \hat{A}_{\text{lin}, \lambda} \). As shown in the Supplementary Material, we have

\[
\hat{A}_{\text{lin}, \lambda} = -B/(2\lambda),
\]

where \( B = n^{-1} \sum_{i=1}^{n} \sum_{m=2}^{\mathcal{E}(y_i)} \sum_{\hat{y} \in [\mathcal{E}_m(y_i)]} (\xi_m(\hat{y}) - \xi_m(y_i)) x_i^\top \). Note that for any two siblings \( \xi_{j_1,j_2,\ldots,j_m} \) and \( \xi_{j_1,j_2,\ldots,j_m}' \), it holds that \( \langle \xi_{j_1,j_2,\ldots,j_m}, \hat{A}_{\text{lin}, \lambda} x \rangle \leq \langle \xi_{j_1,j_2,\ldots,j_m}', \hat{A}_{\text{lin}, \lambda} x \rangle \) for any \( \kappa > 0 \). Thus, there is no need to scale (4.5) as discussed in Remark 3. Since the estimator \( \hat{A}_{\text{lin}, \lambda} \) is a linear function of \( \lambda^{-1} \), it is clear that the value of \( \lambda \) does not affect the classification results. Therefore, the estimator under the linear loss is tuning-parameter free, which can reduce computation significantly. We simply set \( \lambda = 1 \) in (4.5) and denote the estimator as \( \hat{A}_{\text{lin}} \).

Although the linear loss function is simple in computation, it may not be robust to outliers. To alleviate the impact of possible outliers, we apply the idea of Wu and Liu (2013) and propose an adaptive weighted linear loss. We consider

\[
\hat{A}_{\text{ada}, \lambda} = \arg\min_{A} n^{-1} \sum_{i=1}^{n} w_i V_{\text{lin}}(A x_i, z_i) + \lambda \| A \|^2_F,
\]

where \( w_i \) is the adaptive weight for the \( i \)-th training sample. According to Wu and Liu (2013), we set \( w_i = 1/(1 + \| \hat{A}_{\text{lin}} x_i \|_F^\gamma) \), where \( \gamma > 0 \) is a tuning parameter. One advantage of the weighted linear loss is that the solution still has a closed form. Specifically, \( \hat{A}_{\text{ada}, \lambda} = -B_{\text{ada}}/(2\lambda) \), where \( B_{\text{ada}} = n^{-1} \sum_{i=1}^{n} \sum_{m=2}^{\mathcal{E}(y_i)} \sum_{\hat{y} \in [\mathcal{E}_m(y_i)]} w_i (\xi_m(\hat{y}) - \xi_m(y_i)) x_i^\top \). The proof is similar to that of (4.5), and we omit it. Clearly, the value of \( \lambda \) does not affect the classification results. We simply set \( \lambda = 1 \) and denote the estimator as \( \hat{A}_{\text{ada}} \). In Section 6, we see that this loss is competitive in classification accuracy and computational efficiency.
In our simulation, we also consider the hinge loss function $\ell_{\text{hinge}}(\cdot)$ in optimization problem (4.4), which can be solved by the dual quadratic program regularly, that is,

$$\min_{A \in \mathbb{R}^{K \times p}} n^{-1} \sum_{i=1}^{n} V_{\ell_{\text{hinge}}}(Ax_i, z_i) + \lambda \|A\|_F^2.$$ 

5 Statistical properties

5.1 Fisher consistency

As stated in Section 4, the generalization error is defined based on the 0-1 hierarchical loss, that is, $R(f) = E [I(Y \neq \mathcal{H}(f(X)))]$ (Wang et al. 2011; Babbar et al. 2016). The minimizer $\bar{f}$ of $R(f)$ is known as the Bayes rule. Wang et al. (2011) proved the Bayes rule $\bar{f}$ satisfying $\mathcal{H}(\bar{f}) = \arg\max_{y \in Y} P(y|X = x)$. However, solving the optimization problem associated with the 0-1 loss is difficult. A surrogate loss $\ell(u)$ is used instead. For a surrogate loss $\ell(u)$, denote $R_{V\ell}(f) = E[V\ell(f, Z)]$ where $V\ell(f, Z) = \sum_{m=2}^{C(y)} \sum_{Y \in [\mathcal{E}_m(Y)]} \ell(G_m(f(X), Y, \tilde{Y}))$.

Define $f^* = \arg\inf_{f \in \mathcal{F}_0} R_{V\ell}(f)$, where $\mathcal{F}_0$ is the set of all measurable functions. A loss $\ell(u)$ is called Fisher consistent, if $f^*$ leads to the same classification rule as the Bayes rule under TD. We establish the Fisher consistency of $\ell(u)$ under the following mild conditions.

Denote $P(Y^{(m)}|X = x)$ as the conditional distribution of the label at the $m$-th layer, where $P(Y^{(m)} = C|X = x) = \sum_{y \in Y: y^{(m)} = C} P(y|X = x)$.

Assumption 2. Given $x \in \mathcal{X}$, denote by $\tilde{y} = \{C_{j_1}, C_{j_1,j_2}, \ldots, C_{j_1,j_2,\ldots,j_{m_0}}\}$ the Bayes rule with $j_1 \equiv 1$, that is, $\tilde{y} = \arg\max_{y \in Y} P(y|X = x)$. Assume that, for any $m = 2, \ldots, m_0$,

$$C_{j_1,j_2,\ldots,j_m} = \arg\max_{C \in \text{Chi}(C_{j_1,j_2,\ldots,j_{m-1}})} P(Y^{(m)} = C|X = x).$$

Assumption 2 requires the conditional probability that an instance belongs to the node $C_{j_1,j_2,\ldots,j_m}$ on the path $\tilde{y}$ is the largest one among siblings $\{C_{j_1,j_2,\ldots,j_m'}: j_m' = 1, \ldots, N_{j_1,\ldots,j_{m-1}}\}$ for $m = 2, \ldots, m_0$, which is natural in hierarchical classification. Taking the example in
Figure 1 as an illustration, if the Bayes classifier assigns an instance to the path \( \{ C_1 = \{ \text{Animal} \}, C_{1,1} = \{ \text{Elephant} \}, C_{1,1,1} = \{ \text{African elephant} \}, C_{1,1,1,1} = \{ \text{Loxodonta africana} \} \} \), Assumption 2 requires that the conditional probability it belongs to \( C_{1,1} \) is larger than that it belongs to \( C_{1,2} = \{ \text{Dog} \} \), the conditional probability it belongs to \( C_{1,1,1} \) is larger than that it belongs to \( C_{1,1,2} = \{ \text{Asian elephant} \} \), and the conditional probability it belongs to \( C_{1,1,1,1} \) is larger than that it belongs to \( C_{1,1,1,2} = \{ \text{Loxodonta cyclotis} \} \).

**Theorem 3.** Under Assumption 2, the loss \( \ell \) is Fisher consistent by TD respect to \( R_V(\ell) \), if (i) \( \ell(u) \) is differentiable with \( \ell'(u) < 0 \) for any \( u \); (ii) \( \ell'(u) \) is nondecreasing in \( u \).

According to Theorem 3, the exponential loss \( \ell(u) = e^{-u} \), the deviance loss \( \ell(u) = \log(1 + \exp(-u)) \), and the linear loss \( \ell(u) = -u \) satisfy the conditions in Theorem 3 and thus are Fisher consistent. Though the hinge loss is not differentiable and the conditions above fail, Liu et al. (2011) showed that the hinge loss is a limit of a set of large-margin unified machine loss functions, which satisfy the conditions, and then are Fisher consistent.

**Remark 4.** For a surrogate loss function \( \ell(u) \), the minimizer of \( E[\ell(M(f(X), Y))] \) can be Fisher consistent without Assumption 2. Details are referred to Theorem S1 in the Supplementary Material. However, as argued in Section 4, solving optimization problem associated with \( R_V(\ell) \) is more computational efficient than that with \( E[\ell(M(f(X), Y))] \).

**Remark 5.** Given \( y \), define \( \eta_m(y) = \eta_{j_1, \ldots, j_m} \) if \( y^{(m)} = C_{j_1, \ldots, j_m} \) for \( m = 2, \ldots, \mathcal{L}(y) \). As shown in the Supplementary Material, for the linear loss, we have \( f^* = \lim_{c \to +\infty} cV_0 \), where \( V_0 = \sum_{y \in \mathcal{Y}} \sum_{m=2}^{\mathcal{L}(y)} P(y|x)(|\text{Sib}(\eta_m(y))| + 1)\eta_m(y) \). In fact, all learners in the set \( \{ cV_0 : c > 0 \} \) lead to the same classification result. Taking this into account, we define \( f^* = \arg\min_{f \in \mathcal{F}_0 : E[\|f\|^2] \leq 1} R_V(f) = V_0/[E(\|V_0\|^2)]^{1/2} \) with \( c = [E(\|V_0\|^2)]^{-1/2} \). We prove in the Supplementary Material that the linear loss is also Fisher consistent under this definition.
5.2 Asymptotic results on the generalization error

In this subsection, we study the convergence rate of the excess $\ell$-risk and the excess risk (Bartlett et al., 2006). Recall that $f^*$ is the underlying function that minimizes the expected loss $R_{V_{\ell}}(f)$, that is, $f^* = \arg\inf R_{V_{\ell}}(f)$. (For the linear loss, $f^*$ is defined in Remark 5.) Consequently, $R_{V_{\ell}}(f^*)$ represents the ideal performance under the surrogate loss $\ell$, whereas $R(f^*)$ is the ideal generalization performance of $f^*$. Based on the Fisher consistency by Theorem 3, we have $H(f^*) = H(\bar{f})$, and consequently $R(\bar{f})$. The excess $\ell$-risk is then defined as $e_{V_{\ell}}(f, f^*) = R_{V_{\ell}}(f) - R_{V_{\ell}}(f^*)$, and the excess risk is $e(f, f^*) = R(f) - R(f^*)$. Clearly, the excess $\ell$-risk measures the difference between any learning function $f$ and $f^*$ in terms of the expectation $\ell$-risk, while the excess risk quantifies the difference between the hierarchical misclassification errors between $f$ and the Bayes rule.

For any $\dot{f}$ and $\ddot{f}$ in $F$, let $d(\dot{f}, \ddot{f}) = [E(\|\dot{f}(X) - \ddot{f}(X)\|^2)]^{1/2}$. Remind that $\dot{f}_\lambda$ is the minimizer of (4.3), where $F$ has been specified accordingly. To give asymptotic results on the generalization error, we introduce the following assumptions.

**Assumption 3.** Assume the loss function $\ell(u)$ is Lipschitz with a constant $0 < \alpha < \infty$, that is, $|\ell(u_1) - \ell(u_2)| \leq \alpha |u_1 - u_2|$ for any bounded $u_1$ and $u_2$.

**Assumption 4.** There exists constants $1 \leq \gamma_1 < +\infty, 0 < \gamma_2 \leq +\infty$ and $\beta_i > 0, i = 1, 2$ such that, for all small $\epsilon > 0$,

$$
\inf \{f \in F : d(f, f^*) \geq \epsilon\} e_{V_{\ell}}(f, f^*) \geq \beta_1 \epsilon^{\gamma_1},
$$

$$
\sup \{f \in F : d(f, f^*) \leq \epsilon\} |e(f, f^*)| \leq \beta_2 \epsilon^{\gamma_2}.
$$

Assumption 4 from Zhang and Liu (2014) enables us to control $e(\dot{f}_\lambda, f^*)$ through $e_{V_{\ell}}(\dot{f}_\lambda, f^*)$ in a small neighborhood of $f^*$. In the Supplementary Material, we verify that under mild conditions, $\gamma_1 = 2$. Note that $\gamma_2$ depends on $f^*$ and the distribution of $Z = (X, Y)$. We give an illustrative example in the Supplementary Material, showing that $\gamma_2 = 1$ when $F$ is the set of linear learners.
Before giving Assumption\ref{ass:5} we define a complexity measure of a function space $\mathcal{F}$. Given any $\epsilon > 0$, denote $\{(f^i, f_i^*)\}$ as an $\epsilon$-bracketing function set of $\mathcal{F}$ if for any $f \in \mathcal{F}$, there exists an $i$ such that $f^i \leq f \leq f_i^*$ and $[\epsilon(\|f^i - f_i^*\|) + \epsilon]^{1/2} \leq \epsilon, i = 1, 2, \ldots$. Then the metric entropy with bracketing $\mathcal{H}_B(\epsilon, \mathcal{F})$ is the logarithm of the cardinality of the smallest $\epsilon$-bracketing set for $\mathcal{F}$. Denote $V_{\ell}^T(f, z) = \tilde{T} \wedge V_{\ell}(f, z)$, where $\tilde{T}$ is a truncation constant.

Let $f_0 = f^*$ when $f^* \in \mathcal{F}$; otherwise, $f_0 \in \mathcal{F}$ is chosen as an approximation in $\mathcal{F}$ to $f^*$. Let $\mathcal{F}^V_{\ell}(t) = \{V_{\ell}^T(f, z) - V_{\ell}(f_0, z) : f \in \mathcal{F}, J(f) \leq J_0 t\}$ with $J_0 = \max\{J(f_0), 1\}$.

**Assumption 5.** For some constants $c_i > 0, i = 1, \ldots, 3$, there exists some $\epsilon_n > 0$ such that

$$\sup_{t \geq 1} \phi(\epsilon_n, t) \leq c_1 n^{1/2}, \quad \phi(\epsilon_n, t) = \int_{c_2 L}^{c_3 L} \mathcal{H}_B^{1/2}(u, \mathcal{F}_{\ell}(t)) du / L$$

with $\beta_3 = 2/\gamma_1$ and $L = L(\epsilon_n, \lambda, t) = \min\{\epsilon_n^2 + \lambda J_0(t/2 - 1), 1\}$.

Assumption\ref{ass:5} measures the complexity of $\mathcal{F}^V_{\ell}(t)$ via the metric entropy. It was previously used in\cite{shen2007, wang2009, wang2011}. We establish the convergence rate in the following theorem by the approach of\cite{wang2011}.

**Theorem 4.** Under Assumptions\ref{ass:3,4,5} there exists constants $c_4$ and $c_5$ such that

$$P(\epsilon(f_\lambda, f^*) \geq c_4 \delta_n^{2\beta_1}) \leq 3.5 \exp(-c_5 n(\lambda J_0)^{2-\min(\beta_3, 1)})$$

provided that $\lambda^{-1} \geq 2\delta_n^{-2} J_0$, where $\delta_n = \min\{\epsilon_n^2 + 2\epsilon V_{\ell}(f_0, f^*), 1\}, J_0 = \max\{J(f_0), 1\}, \beta_4 = \gamma_2 / \gamma_1$, and $\beta_3$ and $\epsilon_n$ are defined in Assumption\ref{ass:5}.

**Corollary 1.** Under the assumptions in Theorem\ref{thm:4}, $|\epsilon(f_\lambda, f^*)| = O_p(\delta_n^{2\beta_1})$ provided that $n(\lambda J_0)^{2-\min(\beta_3, 1)}$ is bounded away from 0 as $n \to \infty$.

When $\mathcal{F}$ is the set of linear functions, we have the following explicit expression on $\mathcal{H}_B(\epsilon, \mathcal{F}^V_{\ell}(t))$.

**Lemma 1.** Assume $J_0$ is bounded. Considering $\mathcal{F}$ as the set of linear functions, it holds that $\mathcal{H}_B(\epsilon, \mathcal{F}^V_{\ell}(t)) \leq O(c_7 p \log(c_0^{1/2}/\epsilon))$, where $c_0 = \max_{y \in Y} \sum_{m=2}^{L(y)} |\text{Sib}(y^{(m)})| T^{(m)}$ and $c_7 = \max_{y \in Y} \sum_{m=2}^{L(y)} |\text{Sib}(y^{(m)})|$.
For the illustrative example in the Supplementary Material, we show that $\gamma_1 = 2$ and $\gamma_2 = 1$ under mild conditions. Consequently, it holds that $\beta_3 = 1$ and $\beta_4 = 1/2$ there. Assuming that $p$ is bounded, we have $\mathcal{H}_B(\epsilon, \mathcal{F}^{V_t}(t)) \leq O(c_7 \log(c_6 t^{1/2}/\epsilon))$ by Lemma 1 when $\mathcal{F}$ is the set of linear learners. Then by the definitions of $\phi(\epsilon_n, t)$ and $L$, it follows that $\sup_{t \geq 1} \phi(\epsilon_n, t) \leq O((c_7 \log(c_6/\epsilon_n))^{1/2}/\epsilon_n)$, and consequently $\epsilon_n = (c_7 n^{-1} \log n)^{1/2}$ by Assumption 5. Since $f^* \in \mathcal{F}$ as shown in the Supplementary Material, the convergence rate is of the order $\sqrt{(\log n)}/n$ for this example.

For a better illustration, we compare the proposed method, named the angle-based hierarchical classification via label embedding (HierLE), with other methods by the following example of a binary tree [Wang et al. 2011]. Specifically, we consider two methods, where the convergence rates have been given in literature: (1) multicategory SVM considering only leaf nodes (MSVM); (2) hierarchical SVM of [Wang et al. 2011] (HSVM).

Example. For a binary tree with depth $k$, it has $n_{\text{leaf}} = 2^{k-1}$ leaf nodes and $2^k - 2$ non-root nodes. Recall $\mathcal{C}_H = \{C(1), \ldots, C(q)\}$ is the set of non-root nodes, and $Y$ is a path from the root to a leaf node. Denote the set of leaf nodes as $\mathcal{C}_{\text{leaf}} = \{\tilde{C}(i), i = 1, \ldots, 2^{k-1}\} \subset \mathcal{C}_H$. The conditional probability of $Y = y$ can be expressed as $P(Y = y|X = x) = P(y \cap \mathcal{C}_{\text{leaf}}|X = x)$. Let $X \in \mathbb{R}^2$ sampled from the uniform distribution over $[0, 1]^2$. Given $x = (x_1, x_2)^\top$, when $x_1 \in [(i-1)/2^{k-1}, i/2^{k-1}), i = 1, \ldots, 2^{k-1}$, define the probability $P(\tilde{C}(i) \in Y|X = x) = 1 - 2^{-(k-1)}$, and for any $\tilde{C}(j) \in \mathcal{C}_{\text{leaf}}$ with $j \neq i$, let $P(\tilde{C}(j) \in Y|X = x) \equiv 2^{-(k-1)}/(2^{k-1} - 1)$. Moreover, for any non-leaf node $C(i) \in \mathcal{C}_H \setminus \mathcal{C}_{\text{leaf}}$, let $P(C(i) \in Y|X = x) = \sum_{t \in \text{Off}(C(i))} P(t \in Y|X = x)$. We consider the linear classifiers for this example. One can verify the optimal minimizer is $f^*(x) = (f_1(x), f_2(x), \ldots, f_K(x))^\top \in \mathcal{F}$ with $f_1(x) = x_1 - 2^{k-2}/2^{k-1}$, $f_j(x) = f_{[j/2]} + [2I(j \mod 2 = 0) - 1](x_1 - f_{[j/2]})/2$ for $j = 2, \ldots, K$.

Let us consider our HierLE estimator first. By [Wang et al. 2011], we have $\beta_3 = 1$ and $\beta_4 = 1/2$. Recall that $\mathcal{H}_B(\epsilon, \mathcal{F}^{V_t}(t)) \leq O(c_7 \log(c_6 t^{1/2}/\epsilon))$ in Lemma 1. Then by the definitions of $\phi(\epsilon_n, t)$ and $L$, it follows that $\sup_{t \geq 1} \phi(\epsilon_n, t) \leq O((c_7 \log(c_6/\epsilon_n))^{1/2}/\epsilon_n)$, and
consequently that $\varepsilon_n = (c_7n^{-1}\log n)^{1/2}$ by Assumption 5. Moreover, for this example, one can compute that $c_7 = k - 1$. By Theorem 4 and Corollary 1, we have $|e(\hat{f}, f^*)| = O_p(\varepsilon_n) = O_p((kn^{-1}\log n)^{1/2})$.

For comparisons, we consider the rates of MSVM and HSVM for this example. The convergence rate of MSVM is $O_p(\left(n_{\text{leaf}}(n_{\text{leaf}} - 1)n^{-1}\log n/2\right)^{1/2})$ (Wang et al., 2011). For any given tree, define $c_8 = \sum_{j=0}^{q} |\text{Chi}(C(j))| |\text{(Chi}(C(j))| - 1)/2$, where $\{C(j), q = 0, \cdots, q\}$ is the set of all nodes one the tree. For the binary tree above, we have $c_8 = 2^{k-1} - 1 = n_{\text{leaf}} - 1$. By Wang et al. (2011), the HSVM has the convergence rate $O_p((n_{\text{leaf}}n^{-1}\log n)^{1/2})$. Clearly, $c_7$ is much smaller than $n_{\text{leaf}}$ and $n_{\text{leaf}}(n_{\text{leaf}} - 1)/2$ for this example. Therefore, the proposed estimator has advantages compared with these two existing methods.

For better illustration, we check the candidate set $\mathcal{F}$ when the linear classifier is applied. For our method, the candidate set of linear classifiers is $\mathcal{F} = \{f : f = Ax \in \mathbb{R}^K, A \in \mathbb{R}^{K \times p}, x \in \mathbb{R}^p\}$, where the intercept is included in $x$. For HSVM, the candidate set is $\mathcal{F} = \{f : f = Wx \in \mathbb{R}^q, W \in \mathbb{R}^{q \times p}, x \in \mathbb{R}^p\}$ (Wang et al., 2011). It is seen that the candidate set $\mathcal{F}$ for our method is related to the dimension $K$ of embedding space, while $\mathcal{F}$ for HSVM is associated with $q$, the total number of nodes except the root. As shown in Section 3, $K$ is smaller than $q$. On the other hand, Assumption 2 is required for our method to obtain Fisher consistency. For HSVM, Fisher consistency can be established in more general situations without Assumption 2.

### 6 Simulation and real data analysis

In this section, we evaluate the proposed method under three loss functions denoted as $\text{HierLE}_{\text{lin}}$ (linear loss), $\text{HierLE}_{\text{wl}}$ (weighted linear loss) and $\text{HierLE}_{\text{hinge}}$ (hinge loss), and compare them with some competitors. Specifically, we consider (1) MSVM (Chang and Lin, 2011); (2) sequential hierarchical SVM training SVMs separately for each parent node and using the top-down strategy to assign labels (Davies et al., 2007) (SHSVM); (3) sequential hierarchical binary SVM training binary SVMs separately for each node and using the top-
down strategy to assign labels (Cesa-Bianchi et al. 2006) (SBSVM); (4) traditional label embedding method for hierarchical classification (Cai and Hofmann 2004) (HofSVM); (5) HSVM (Wang et al. 2011); (6) cost-sensitive learning method for hierarchical classification that can be used for massive data (Charuvaka and Rangwala 2015) (HierCost).

6.1 Evaluation measures

Given the test set \( \{(x_i, y_i)\}_{i=1}^{n_{te}} \) of size \( n_{te} \), denote \( \hat{y}_i = \{\hat{y}_i^{(1)}, \cdots, \hat{y}_i^{(L(\hat{y}_i))}\} \) as the estimated path of \( x_i \), \( i = 1, \cdots, n_{te} \). We introduce first four losses and then the hierarchical f-measure suggested by Silla and Freitas (2011). Note that smaller values are preferred for the four losses, and larger values are preferred for hF.

The first evaluation metric is the 0-1 loss (Cai and Hofmann 2004), which gives loss of 0 if \( x_i \) is labeled correctly in the whole path, and 1 otherwise, that is, \( \ell_{0-1} = \sum_{i=1}^{n_{te}} I(\hat{y}_i \neq y_i) / n_{te} \). The symmetric loss \( \ell_\Delta \) is calculated as follows (Kosmopoulos et al., 2015), \( \ell_\Delta = \sum_{i=1}^{n_{te}} |(\hat{y}_i \setminus y_i) \cup (y_i \setminus \hat{y}_i)| / n_{te} \). The symmetric loss treats each node on the tree equally. Cesa-Bianchi et al. (2004) defined a hierarchical loss function which views the mistakes made at higher layers being more important than those at lower layers. Note that \( y_i \) and \( \hat{y}_i \) may have different lengths. We transform \( y_i \) into a binary vector \( Q(y_i) \in \mathbb{R}^q \), where the \( j \)-th coordinate \( Q(y_i)_j \) indicates whether the node \( C(j) \) defined in Section 2.1 is on the path \( y_i \). Define \( Q(\hat{y}_i) \) in the same way. The hierarchical loss is calculated as \( \ell_H = \sum_{i=1}^{n_{te}} \sum_{j=1}^{q} v_{C(i)} I(\{Q(\hat{y}_i)_j \neq Q(y_i)_j\} \land \{Q(\hat{y}_i)_s = Q(y_i)_s, \forall s < j\}) / n_{te} \). The coefficients \( 0 \leq v_{C(i)} \leq 1 \) are used for down-scaling the loss. There are two popular choices for \( v_{C(i)} \). Specifically, denote \( \ell_H \) as \( \ell_{H(sib)} \) when \( v_{C(i)} \) takes the form \( v_{C(i)} = 1, v_{C(j)} = v_{\text{Par}(C(j))}/|\text{Sib}(C(j))|, j = 1, \cdots, q \), where \(|\text{Sib}(C(j))|\) represents the number of siblings of the node \( C(j) \). Denote \( \ell_H \) as \( \ell_{H(sub)} \) when \( v_{C(i)} \) is of the form \( v_{C(j)} = q^{-1}|\text{subtree}(C(j))|, j = 1, \cdots, q \), where \(|\text{subtree}(C(j))|\) is the size of the subtree rooted by the node \( C(j) \).

Besides the four losses above, Silla and Freitas (2011) suggested using the hierarchical f-measure (Kiritchenko et al. 2005), as it can be effectively applied to any hierarchical
classification scenario, i.e. tree, DAG, single-labeled and multiple-labeled. It is defined as $hF = 2 \cdot hP \cdot hR / (hP + hR)$, where $hP$ and $hR$ are hierarchical precision and hierarchical recall, respectively defined as,

$$hP = \sum_{i=1}^{n_{te}} \frac{|\{\bigcup_{C(j) \in \hat{y}_i} \text{Anc}(C(j)) \cup \hat{y}_i\} \cap \{\bigcup_{C(j) \in y_i} \text{Anc}(C(j)) \cup y_i\}|}{\sum_{i=1}^{n_{te}} |\bigcup_{C(j) \in \hat{y}_i} \text{Anc}(C(j)) \cup \hat{y}_i|},$$

$$hR = \sum_{i=1}^{n_{te}} \frac{|\{\bigcup_{C(j) \in \hat{y}_i} \text{Anc}(C(j)) \cup \hat{y}_i\} \cap \{\bigcup_{C(j) \in y_i} \text{Anc}(C(j)) \cup y_i\}|}{\sum_{i=1}^{n_{te}} |\bigcup_{C(j) \in y_i} \text{Anc}(C(j)) \cup y_i|}.$$  

6.2 Simulation

In our simulations, samples are split into the training, the validation and the test sets, with sizes denoted as $n, n_{vl}$ and $n_{te}$, respectively. We set $n : n_{vl} : n_{te} = 1 : 1 : 2$. Let $T^{(1)} = 1$ and $\delta = \sqrt{5}$ in Algorithm 2 as discussed in Remark 2 in Section 3. We first learn classifiers on the training set and choose the best tuning parameter based on the validation set over 41 grid points $\{10^{i/10}, i = -20, -19, \cdots, 20\}$. Note that HierLE$_{\text{lin}}$ is tuning free. Then we apply the estimated learner on the test set to compute the evaluation metrics.

**Example 1.** We first consider a tree of $k$ layers. There are 4 nodes at the second layer and each node has two children at the lower layers. The tree structure is shown in Figure 2 (left), where the digits stand for labels. Note that all leaf nodes locate at the $k$-th layer. Simulate data $\{(x_i, y_i)\}_{i=1}^{4n}$ as follows, where $x_i = (x_{i1}, \cdots, x_{ip})^T$, $y_i = \{y_i^{(1)}, \cdots, y_i^{(k)}\}^T$. For $i = 1, 2, \cdots, 4n$, $y_i$ follows a discrete uniform distribution in the set of paths on the tree. Let $\mu_i$ be a zero vector of length $p$ except for the $y_i^{(m)}$-th element being $1/(m-1)$ for $m = 2, \cdots, k$. Taking $k = 3, y_i = \{0, 1, 5\}$ as an example, we have $\mu_i = (1, 0, 0, 0, 1/2, 0, \cdots, 0)^T$. Let $x_i|y_i \sim N(\mu_i, 0.1I_{p \times p})$. Then we randomly select 20% of the data and assign their labels randomly to generate non-separable cases. Set $n = 50$, $k = 3, 4$ and $p = 15, 30$.

The average results over 100 replications on $\ell_{0-1}, \ell_\Delta, \ell_{H(\text{sub})}, \ell_{H(\text{sub})}$, $hF$ and time cost (i.e. time on training, validating and testing) are shown in Table[1]. From Table 1, we see that in terms of the four loss measures and the $hF$ measure, SBSVM performs worst. Our proposed
three classifiers HierLE_{lin}, HierLE_{wl} and HierLE_{hinge} perform better than other methods with HierLE_{wl} being the best in all evaluation metrics. Compared to MSVM, all hierarchical classifiers get better as $k$ increases. Regarding the computational time, HofSVM takes the longest to run, followed by HSVM, HierCost, HierLE_{hinge}, SBSVM, MSVM, SHSVM, HierLE_{wl} and HierLE_{lin}. Our proposed method runs fast under the (weighted) linear loss since it has a closed form solution.

**Example 2.** In this example, we simulate a more complex tree and samples of a larger size. The hierarchy is of 5 layers. There are 12 nodes at the second layer and each node has two children at the lower layers. Thus, there are 24, 48, 96 nodes at the third, fourth and fifth layers, respectively, and 180 nodes except for the root in total. Note that all leaf nodes locate at the last layer. We simulate $\{(x_i, y_i)\}_{i=1}^{4n}$ as follows, where $x_i = (x_{i1}, \cdots, x_{ip})^\top$, $y_i = \{y_{i1}, y_{i2}, y_{i3}, y_{i4}, y_{i5}\}^\top$. For $i = 1, 2, \cdots, 4n$, $y_i$ follows a discrete uniform distribution in the set of paths on the tree. For each $x_i$, $x_i | y_i \sim N(\xi_5(y_i), 0.1I_{p \times p})$, where $\xi_5(y_i)$ is the constructed point corresponding to the leaf node $y_i^{(5)}$ and $p = n_{\text{leaf}} - 1$. Set $n = 2000$.

Since the size of this problem is large, HofSVM, HSVM and HierLE_{hinge}, involving quadratic programming with large amounts of constraints, are not considered because of computational inefficiency. The average results for MSVM, SHSVM, SBSVM, HierCost, HierLE_{lin} and HierLE_{wl} over 100 replications are shown in Table 1. It is seen that the proposed classifiers HierLE_{lin} and HierLE_{wl} have significant advantages over other methods in terms of both classification accuracy and computing costs for this large dataset.
Table 1: Average results as well as standard deviations for Example 1 and Example 2 over 100 replications. The best value in each column is boldfaced and the percentages in brackets are the amounts of improvement over MSVM.

|         | $\ell_{0-1}$ | $\ell_\Delta$ | $\ell_{\text{H(sib)}}$ | $\ell_{\text{H(sub)}}$ | hF         | Time |
|---------|--------------|----------------|--------------------------|--------------------------|------------|------|
| MSVM    | 0.541_{0.006} (0.0%) | 1.716_{0.023} (0.0%) | 0.107_{0.001} (0.8%) | 0.098_{0.001} (0.0%) | 0.571_{0.006} (0.0%) | 0.510 |
| SHSVM   | 0.521_{0.007} (3.7%) | 1.595_{0.023} (7.0%) | 0.100_{0.001} (7.0%) | 0.090_{0.001} (9.1%) | 0.601_{0.006} (5.3%) | 0.290 |
| SBSVM   | 0.589_{0.006} (-8.9%) | 1.910_{0.023} (-11.3%) | 0.119_{0.001} (-11.3%) | 0.110_{0.001} (-11.8%) | 0.522_{0.006} (-8.5%) | 0.777 |
| HofSVM  | 0.541_{0.006} (0.0%) | 1.744_{0.022} (-1.7%) | 0.109_{0.001} (-1.7%) | 0.101_{0.001} (-2.6%) | 0.564_{0.006} (-1.2%) | 31.421 |
| HSVM    | 0.517_{0.006} (4.5%) | 1.627_{0.022} (5.2%) | 0.102_{0.001} (5.2%) | 0.093_{0.001} (5.7%) | 0.593_{0.005} (3.9%) | 6.580 |
| HierCost| 0.517_{0.006} (4.4%) | 1.635_{0.023} (4.7%) | 0.102_{0.001} (4.7%) | 0.092_{0.001} (6.3%) | 0.591_{0.006} (3.5%) | 6.589 |
| HierLE_{lin} | 0.501_{0.006} (7.4%) | 1.518_{0.019} (11.5%) | 0.095_{0.001} (11.5%) | 0.085_{0.001} (13.9%) | 0.620_{0.005} (8.6%) | 0.014 |
| HierLE_{wle} | 0.498_{0.006} (8.0%) | 1.495_{0.018} (12.9%) | 0.093_{0.001} (12.9%) | 0.083_{0.001} (15.7%) | 0.626_{0.004} (9.7%) | 0.553 |
| HierLE_{hinge} | 0.507_{0.006} (6.2%) | 1.515_{0.021} (11.7%) | 0.095_{0.001} (11.7%) | 0.083_{0.001} (15.5%) | 0.621_{0.005} (8.8%) | 6.017 |

Example 1 \( k = 3, p = 15 \)

|         | $\ell_{0-1}$ | $\ell_\Delta$ | $\ell_{\text{H(sib)}}$ | $\ell_{\text{H(sub)}}$ | hF         | Time |
|---------|--------------|----------------|--------------------------|--------------------------|------------|------|
| MSVM    | 0.791_{0.005} (0.0%) | 3.684_{0.034} (0.0%) | 0.142_{0.001} (0.0%) | 0.134_{0.001} (0.0%) | 0.386_{0.006} (0.0%) | 0.807 |
| SHSVM   | 0.770_{0.005} (2.7%) | 3.398_{0.031} (7.8%) | 0.128_{0.001} (9.8%) | 0.119_{0.001} (11.5%) | 0.434_{0.005} (12.4%) | 1.023 |
| SBSVM   | 0.810_{0.005} (-3.2%) | 3.849_{0.034} (-4.5%) | 0.149_{0.001} (-4.6%) | 0.141_{0.002} (-4.7%) | 0.358_{0.006} (-7.1%) | 2.287 |
| HofSVM  | 0.779_{0.005} (1.6%) | 3.677_{0.033} (0.2%) | 0.143_{0.001} (-0.5%) | 0.136_{0.002} (-0.9%) | 0.387_{0.006} (0.3%) | 337.014 |
| HSVM    | 0.753_{0.005} (4.9%) | 3.401_{0.034} (7.7%) | 0.130_{0.001} (8.8%) | 0.121_{0.001} (9.8%) | 0.433_{0.006} (12.2%) | 29.643 |
| HierCost| 0.784_{0.005} (0.9%) | 3.563_{0.032} (3.3%) | 0.137_{0.001} (3.7%) | 0.129_{0.001} (4.2%) | 0.406_{0.005} (5.2%) | 18.799 |
| HierLE_{lin} | 0.735_{0.005} (7.2%) | 3.134_{0.028} (14.9%) | 0.117_{0.001} (17.5%) | 0.108_{0.001} (19.9%) | 0.478_{0.005} (23.8%) | 0.022 |
| HierLE_{wle} | 0.735_{0.005} (7.2%) | 3.130_{0.028} (15.0%) | 0.117_{0.001} (17.7%) | 0.107_{0.001} (20.1%) | 0.478_{0.005} (23.9%) | 0.842 |
| HierLE_{hinge} | 0.751_{0.005} (5.2%) | 3.148_{0.028} (14.5%) | 0.118_{0.001} (17.2%) | 0.108_{0.001} (19.6%) | 0.475_{0.005} (23.1%) | 9.890 |

Example 2

|         | $\ell_{0-1}$ | $\ell_\Delta$ | $\ell_{\text{H(sib)}}$ | $\ell_{\text{H(sub)}}$ | hF         | Time |
|---------|--------------|----------------|--------------------------|--------------------------|------------|------|
| MSVM    | 0.814_{0.001} (0.0%) | 4.288_{0.005} (0.0%) | 0.036_{0.000} (0.0%) | 0.033_{0.000} (0.0%) | 0.464_{0.001} (0.0%) | 258.470 |
| SHSVM   | 0.799_{0.001} (1.9%) | 4.001_{0.005} (6.7%) | 0.032_{0.000} (10.3%) | 0.030_{0.000} (11.4%) | 0.500_{0.001} (7.8%) | 105.416 |
| SBSVM   | 0.833_{0.001} (-2.5%) | 4.690_{0.006} (-9.4%) | 0.041_{0.000} (-14.2%) | 0.039_{0.000} (-15.8%) | 0.414_{0.001} (-10.8%) | 1452.514 |
| HierCost| 0.802_{0.001} (1.5%) | 4.098_{0.010} (4.4%) | 0.033_{0.000} (6.3%) | 0.031_{0.000} (7.0%) | 0.488_{0.001} (5.1%) | 575.524 |
| HierLE_{lin} | 0.790_{0.001} (3.1%) | 3.781_{0.005} (11.8%) | 0.029_{0.000} (17.9%) | 0.027_{0.000} (19.9%) | 0.527_{0.001} (13.7%) | 1.871 |
| HierLE_{wle} | 0.788_{0.001} (3.2%) | 3.742_{0.005} (12.7%) | 0.029_{0.000} (19.2%) | 0.026_{0.000} (21.4%) | 0.532_{0.001} (14.7%) | 58.129 |
6.3 Real data analysis: document categorization

Hierarchical classification has a wide range of applications in text categorization, particularly on the Web. As the complexity of the hierarchy and the number of documents increase, it is desirable to consider methods that incorporate the hierarchical information and that can be computed efficiently.

The first dataset is a part of Reuters [Lewis et al., 2004], which is an archive of manually categorized newswire stories. It is a multi-labeled (one sample may belong to several paths) hierarchical classification problem. There are 3000 samples in the original data set with 47236 features. From the whole tree, we select a subtree as shown in Figure 2 (right). It has four layers with 15 nodes in total and 10 leaf nodes. Then we select observations that only belong to one of the paths in our selected subtree as our samples. The sample size is 455 and the number of features is 7206 for this new small dataset.

The second dataset Chinese Hierarchical Text Classification (CHTC) is collected by the authors. We download 5241 advertisements from an online shopping website in China. The categories are organized in a hierarchical tree of 4 layers. There are 5 nodes at the second layer, indicating whether the advertisement belongs to food, amusements, life services, online shopping, or travel. There are 16 and 35 nodes at the third and fourth layers, respectively. Totally, there are 57 nodes with 40 leaf nodes. Detailed information is shown in the Supplementary Material. We perform documents parsing and tokenization to get 13103 terms. The covariates represent the frequency of these terms. For this dataset, we consider two cases, the first 3 layers of the whole tree and the whole tree itself.

For each dataset, we assign the sample into the training, validation and test sets with ratio 1:1:2. We perform feature screening via distance correlation [Li et al., 2012] to select 110 important features for Reuters and 1000 important features for the two cases of CHTC.

The average results over 100 replications are shown in Table 2. For the small subtree of Reuters, we compare all nine methods. Our methods HierLE\textsubscript{lin}, HierLE\textsubscript{wl} and HierLE\textsubscript{hinge}
are better than other methods in all evaluation measures and HierLEwl performs best. Regarding the computational time, the proposed methods HierLElin and HierLEwl are quite efficient, with HierLElin being the best one. For the large tree with $k = 3, 4$ of CHTC, we compare only MSVM, SHSVM, SBSVM, HierCost, HierLElin and HierLEwl because the other three methods are very time consuming. We can see that HierCost, HierLElin and HierLEwl perform better than MSVM in all metrics, while SHSVM and SBSVM are worse. Moreover, our proposed methods HierLElin and HierLEwl show great advantages in terms of classification accuracy and computational efficiency.

7 Discussion

In this paper, we propose an angle-based hierarchical classifier via exact label embedding. In contrast to existing label embedding approaches, our embedding approach is an isometry map into a lower-dimensional space, keeping the hierarchy exactly and reducing the complexity of the hypothesis space simultaneously. Under the (weighted) linear loss function, the solution is of a closed form, which makes it computationally efficient for massive data. Theoretical analyses show the advantages of the proposed method in the convergence rate over existing methods. Numerical experiments imply that our method performs excellently in both classification accuracy and computing, especially when the tree structure is complex and the sample size is large.

The idea of this paper can be extended in several aspects. First, we consider only the linear learner and the approach can be extended further into kernel learning. Second, we consider the exact label embedding for tree structure and single-labeled samples. Extending the idea to DAG structure or the multi-labeled case is an interesting future research topic. Third, when the number of features is large, some sparse penalty functions such as the $l_1$ penalty can be used to select features.
Table 2: Average results as well as standard deviations for Reuters and CHTC over 100 replications. The best value in each column is boldfaced and the percentages in brackets are the amounts of improvement over MSVM.

|         | ℓ_0−1     | ℓ_Δ       | ℓ_H(sib)  | ℓ_H(sub)  | hF       | Time     |
|---------|-----------|-----------|-----------|-----------|----------|----------|
| Reuters |           |           |           |           |          |          |
| MSVM    | 0.435,0.004 (0.0%) | 1.298,0.014 (0.0%) | 0.079,0.001 (0.0%) | 0.066,0.001 (0.0%) | 0.724,0.003 (0.0%) | 1.893    |
| SHSVM   | 0.430,0.003 (1.1%) | 1.225,0.012 (5.6%) | 0.073,0.001 (7.7%) | 0.060,0.001 (9.4%) | 0.738,0.003 (2.0%) | 1.236    |
| SBSVM   | 0.479,0.004 (-10.0%) | 1.361,0.012 (-4.8%) | 0.083,0.001 (-4.1%) | 0.068,0.001 (-3.1%) | 0.708,0.003 (-2.2%) | 3.196    |
| HofSVM  | 0.435,0.004 (0.2%) | 1.277,0.012 (1.6%) | 0.079,0.001 (0.2%) | 0.065,0.001 (0.9%) | 0.724,0.003 (0.1%) | 644.632  |
| HSVN    | 0.431,0.004 (1.1%) | 1.196,0.011 (7.8%) | 0.072,0.001 (9.0%) | 0.058,0.001 (12.4%) | 0.741,0.002 (2.4%) | 55.016   |
| Hier Cost | 0.475,0.004 (-9.2%) | 1.423,0.014 (-9.6%) | 0.089,0.001 (-11.9%) | 0.075,0.001 (-14.1%) | 0.691,0.003 (-4.6%) | 12.272   |
| Hier LElin | 0.428,0.004 (1.6%) | 1.161,0.013 (10.6%) | 0.068,0.001 (13.7%) | 0.055,0.001 (16.8%) | 0.750,0.003 (3.6%) | 0.050    |
| Hier LE_wl | 0.409,0.001 (6.0%) | 1.089,0.010 (16.1%) | 0.064,0.001 (19.5%) | 0.051,0.001 (23.0%) | 0.766,0.002 (5.8%) | 1.772    |
| Hier LE_hinge | 0.424,0.004 (2.5%) | 1.142,0.012 (12.0%) | 0.067,0.001 (15.8%) | 0.053,0.001 (19.4%) | 0.755,0.003 (4.3%) | 37.322   |

|         |           |           |           |           |          |          |
|---------|-----------|-----------|-----------|-----------|----------|----------|
| CHTC k = 3 |        |           |           |           |          |          |
| MSVM    | 0.425,0.001 (0.0%) | 1.464,0.004 (0.0%) | 0.068,0.000 (0.0%) | 0.061,0.000 (0.0%) | 0.634,0.001 (0.0%) | 551.649  |
| SHSVM   | 0.444,0.001 (-4.3%) | 1.506,0.004 (-2.9%) | 0.069,0.000 (-1.9%) | 0.063,0.000 (-3.6%) | 0.624,0.001 (-1.7%) | 432.623  |
| SBSVM   | 0.486,0.001 (-14.2%) | 1.668,0.004 (-14.0%) | 0.078,0.000 (-14.0%) | 0.071,0.000 (-16.6%) | 0.583,0.001 (-8.1%) | 900.615  |
| Hier Cost | 0.335,0.001 (21.1%) | 1.127,0.003 (23.0%) | 0.052,0.000 (24.2%) | 0.046,0.000 (23.4%) | 0.718,0.001 (13.3%) | 544.134  |
| Hier LElin | 0.335,0.001 (21.4%) | 1.100,0.003 (24.8%) | 0.050,0.000 (27.0%) | 0.045,0.000 (25.8%) | 0.725,0.001 (14.3%) | 0.548    |
| Hier LE_wl | 0.324,0.001 (23.8%) | 1.059,0.003 (27.6%) | 0.048,0.000 (30.0%) | 0.043,0.000 (29.0%) | 0.735,0.001 (15.9%) | 20.461   |

|         |           |           |           |           |          |          |
|---------|-----------|-----------|-----------|-----------|----------|----------|
| CHTC k = 4 |        |           |           |           |          |          |
| MSVM    | 0.499,0.001 (0.0%) | 2.298,0.006 (0.0%) | 0.068,0.000 (0.0%) | 0.076,0.000 (0.0%) | 0.603,0.001 (0.0%) | 582.101  |
| SHSVM   | 0.521,0.001 (-4.4%) | 2.359,0.006 (-2.6%) | 0.068,0.000 (0.5%) | 0.077,0.000 (-1.7%) | 0.594,0.001 (-1.5%) | 467.904  |
| SBSVM   | 0.565,0.001 (-13.2%) | 2.560,0.006 (-11.4%) | 0.076,0.000 (-11.9%) | 0.086,0.000 (-12.7%) | 0.556,0.001 (-7.8%) | 1027.250 |
| Hier Cost | 0.412,0.001 (17.5%) | 1.817,0.005 (20.9%) | 0.052,0.000 (23.2%) | 0.059,0.000 (21.9%) | 0.686,0.001 (13.8%) | 1202.397 |
| Hier LElin | 0.417,0.001 (16.4%) | 1.781,0.005 (22.5%) | 0.049,0.000 (27.8%) | 0.057,0.000 (25.6%) | 0.693,0.001 (14.9%) | 0.853    |
| Hier LE_wl | 0.403,0.001 (19.3%) | 1.707,0.004 (25.8%) | 0.047,0.000 (31.4%) | 0.054,0.000 (29.3%) | 0.705,0.001 (17.0%) | 32.877   |
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