Partition Tree Ensembles for Improving Multi-Class Classification

Miran Özdogan[1][a], Alan Jeffares[2][b] and Sean Holden[3][c]
[1]*Department of Computer Science, Oxford University, U.K.*
[2]*Department of Applied Mathematics and Theoretical Physics, Cambridge University, U.K.*
[3]*Department of Computer Science, Cambridge University, U.K.*

Keywords: Multi-Class Classification, Non-Convex Optimization, AutoML.

Abstract: We propose the *Partition Tree Ensemble (PTE)*, a novel tree-based ensemble method for classification problems. This differs from previous approaches in that it combines ideas from reduction methods—that decompose multi-class classification problems into binary classification problems—with the creation of specialised base learners that are trained on a subset of the input space. By exploiting multi-class reduction, PTEs adapt concepts from the *Trees of Predictors (ToP)* method to successfully tackle multi-class classification problems. Each inner node of a PTE splits either the feature space or the label space into subproblems. For each node our method then selects the most appropriate base learner from the provided set of learning algorithms. One of its key advantages is the ability to optimise arbitrary loss functions. Through an extensive experimental evaluation, we demonstrate that our approach achieves significant performance gains over the baseline ToP and AdaBoost methods, across various datasets and loss functions, and outperforms the *Random Forest* method when the label space exhibits clusters where some classes are more similar to each other than to others.

1 INTRODUCTION

Ensemble methods have gained popularity in supervised machine learning as a strategy for maximising performance by aggregating the predictions of multiple base learners. It is often advantageous to organise these base learners using a tree structure. Examples of such tree-based ensembles include *Nested Dichotomies (NDs)* (Frank and Kramer, 2004), *Model Trees (MTs)* (Quinlan et al., 1992) and *Trees of Predictors (ToPs)* (Yoon et al., 2018b; Yoon et al., 2018a).

ToPs employ tree structures to decompose classification problems. They apply distinct base learners to various subsets of the feature space, and optimise for arbitrary loss functions. This can be an advantage, especially in the field of healthcare where it is often appropriate to evaluate classifier performance in terms of AUC (Cortes and Mohri, 2003) or other non-standard measures (Yoon et al., 2018a; Beneke et al., 2023). Yoon *et al.* (Yoon et al., 2018b) demonstrated that ToPs can yield substantial performance gains when compared to frequently utilised methods such as Random Forests and AdaBoost (Yoon et al., 2018b). However, their evaluation of the ToPs approach was limited to binary classification problems. Our preliminary experiments showed that their performance compared to baselines diminishes with an increasing number of classes.

This inspired us to devise an ensemble method that, similarly to the ToP approach, is able to optimise for arbitrary loss functions and overcome the shortcomings of ToPs for multi-class problems. We introduce the PTE, a novel tree-based ensemble approach that combines ideas from reduction techniques (Frank and Kramer, 2004), which decompose multi-class classification problems, with the creation of specialised base learners that are trained on a subset of the input space, as exemplified by the ToP approach.

We draw inspiration from the *Nested Dichotomies (NDs)* (Frank and Kramer, 2004) reduction technique, which achieves state-of-the-art performance compared to competitors such as *One-VS-One* or *One-VS-Rest* (Wever et al., 2023; Leathart, 2019). In PTEs, each inner node of a PTE splits either the feature space or the label space. For the latter, we divide the set of possible classes into two subsets that define three classification problems: "Which of the two

[a] https://orcid.org/0009-0008-7776-6107
[b] https://orcid.org/0009-0003-8744-0876
[c] https://orcid.org/0000-0001-7979-1148

Özdogan, M., Jeffares, A. and Holden, S.
Partition Tree Ensembles for Improving Multi-Class Classification.
DOI: 10.5220/0013163400003905
Paper published under CC license (CC BY-NC-ND 4.0)
In *Proceedings of the 14th International Conference on Pattern Recognition Applications and Methods (ICPRAM 2025)*, pages 55-69
ISBN: 978-989-758-730-6; ISSN: 2184-4313
Proceedings Copyright © 2025 by SCITEPRESS – Science and Technology Publications, Lda.

subsets does a sample belong to?" and "Given that a sample is part of one of the subsets, which of its classes does it belong to?".. By exploiting such *Class Dichotomies*, we can more effectively decompose the original learning problem, and extend the advantages of ToPs to multi-class problems.

We assess the value of this approach through an experimental evaluation, comparing its performance with ToPs, Random Forests and AdaBoost. Our evaluation employs nine datasets from the UCI repository (Dua and Graff, 2017). In addition, we conduct experiments on optimising for two different loss functions, specifically the AUC (Cortes and Mohri, 2003) and the F1-Measure (Chicco and Jurman, 2020).

In summary, our contributions are as follows:

- We introduce the PTE and provide a comprehensive formal description of the method.
- We present a detailed mathematical derivation of the computational complexity associated with training PTEs.
- In an extensive experimental evaluation, we compare PTEs against ToPs and additional baselines of Random Forests (Breiman, 2001) and AdaBoost (Freund et al., 1999). We are able to show that PTEs can lead to substantial performance gains over ToPs and AdaBoost.

2 RELATED WORK

An overview of the respective differences between PTEs, ToPs, NDs and Model Trees can be found in Table 1. We acknowledge that other tree-based ensemble methods exist, including *Filter trees* (Beygelzimer et al., 2007) and *Kernel Regression Tree* (Torgo, 1997b). However, we will focus on NDs, ToPs and Model Trees as these are the methods most similar to PTEs.

Table 1: Comparison of PTEs with Existing Tree-Based Ensemble Methods.

Method	PTE	MT	ND	ToP
Multiple Base Learners	✔	✘	✘	✔
Partition $\mathcal{X}$	✔	✔	✘	✔
Partition $\mathcal{Y}$	✔	✘	✔	✘
Non-Convex Loss	✔	✘	✘	✔
Classification	✔	✘	✔	✔
Regression	✘	✔	✘	✔

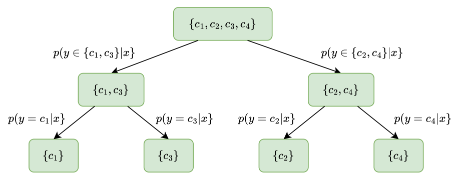


Figure 1: Illustrative example of a Nested Dichotomy with $\mathcal{Y} = \{c_1, c_2, c_3, c_4\}$. Figure adapted to our notation from (Wever et al., 2023).

2.1 Nested Dichotomies

Nested Dichotomies (NDs) (Frank and Kramer, 2004) are ensembles that employ a binary tree structure to recursively break down a multi-class classification problem into a set of binary classification problems. They facilitate the application of classifiers that are inherently binary to multi-class problems.

We can represent an ND as a binary tree, where each node corresponds to a subset of classes from the original multi-class classification problem. The subtrees of a node recursively divide its set of classes into distinct subsets, forming the *meta-classes* that correspond to its two children until a subset contains only a single element. At each internal node, the division constitutes a binary classification problem that is addressed by a *base learner* (Frank and Kramer, 2004). An illustration of this method can be found in Figure 1.

Since the initial work by Frank and Kramer (Frank and Kramer, 2004), extensive research has been conducted on the selection of good ND structures (Leathart, 2019). We now discuss two contemporary state-of-the-art methods. Leathart *et al.* (Leathart, 2019) sought to create trees with easier binary classification problems by employing dichotomies that group together classes that are "similar". This method is called Random Pair Nested Dichotomies (RPNDs). In this approach, an initial pair of classes is randomly selected. Then each of the other classes is grouped with one of those two. The assignment of other classes is determined by training a binary classifier on the initial classes. This classifier is applied to the remaining data and the remaining classes are assigned based on the classifier's predictions through hard voting. Note, that the binary classifier employed for class grouping is discarded, and a new binary classifier is trained to differentiate between the two meta-classes. Leathart *et al.* (Leathart, 2019) demonstrated that ensembles constructed using this technique exhibit state-of-the-art predictive performance while being less runtime-intensive than competing methods.

Wever *et al.* (Wever et al., 2023) propose a co-evolutionary algorithm *CONDA* aimed at discovering advantageous ensembles of NDs. In contrast with

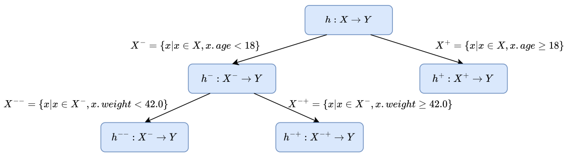

$h : X \to Y$
$X^- = \{x | x \in X, x.age < 18\}$
$X^+ = \{x | x \in X, x.age \geq 18\}$
$h^- : X^- \to Y$
$h^+ : X^+ \to Y$
$X^{--} = \{x | x \in X^-, x.weight < 42.0\}$
$X^{-+} = \{x | x \in X^-, x.weight \geq 42.0\}$
$h^{--} : X^- \to Y$
$h^{-+} : X^{-+} \to Y$

Figure 2: Illustrative example of a Tree of Predictors.

RPNDs, this requires a comprehensive optimisation of the entire tree structure, rather than the successive growth of the ND tree. It demonstrates superior predictive performance when compared to RPNDs, albeit at the expense of a significant increase in runtime (Wever et al., 2023).

Interestingly, Mohr *et al.* (Mohr et al., 2018) found that, for multi-class problems, implementing partial NDs of depth 1 (referred to simply as "Dichotomies" in the statistical literature) can sometimes enhance performance, when compared to using individual base learners.

2.2 Trees of Predictors

In this section, we describe the ToPs ensemble method as introduced in (Yoon et al., 2018a; Yoon et al., 2018b). We will assume that categorical features are one-hot encoded and continuous features are normalised such that $\mathcal{X}_j \in [0,1]$ for every feature j and $\mathcal{X} \subseteq [0,1]^d$. For subsets $\mathcal{Z}_1, \mathcal{Z}_2 \subseteq \mathcal{X}$ of the feature space, if predictors $h_1 : \mathcal{Z}_1 \mapsto \mathcal{Y}$ and $h_2 : \mathcal{Z}_2 \mapsto \mathcal{Y}$ are constructed such that $\mathcal{Z}_1 \cap \mathcal{Z}_2 = \emptyset$, we define $h_1 \vee h_2 : \mathcal{Z}_1 \cup \mathcal{Z}_2 \mapsto \mathcal{Y}$ as $h_1 \vee h_2(z) = h_i(z)$ for $z \in \mathcal{Z}_i$.

2.2.1 Formal Definition

A Tree of Predictors can be represented as a binary tree, denoted $\mathcal{T}$. Each node N within this tree corresponds to a subset $\mathcal{X}$ of the feature space and is associated with a classifier h_N. The corresponding subset is used interchangeably to refer to a node and vice versa. The root node of $\mathcal{T}$ must corresponds to the entire feature space $\mathcal{X}$. For any given node $N \in \mathcal{T}$ its children, denoted $\{N^+, N^-\}$, partition N. For a node $N \in \mathcal{T}$, its corresponding classifier h_N is generated by training an algorithm $A_N \in \mathcal{A}$ on a set N^*, where $N^* = N$ or N^* corresponds to one of the predecessors of N. Formally, this relationship is expressed as $h_N = A_N(N^*)$ with $N^* \in N^\uparrow$.

The set of leaves, denoted $\overline{\mathcal{T}}$, forms a partition of the feature space $\mathcal{X}$. We denote the leaf corresponding to some feature vector $x \in \mathcal{X}$ as $\overline{N}(x)$. An illustrative example of a Tree of Predictors is provided in Figure 2.

Note that this approach allows for a node's classifier to be trained on a set that corresponds to one of its predecessors. This design choice is driven by the understanding that partitioning the training set may result in performance enhancement for one subset, while degrading performance for another.

2.2.2 Growing a Tree of Predictors

Growing a ToP requires a finite set $\mathcal{A} = A_1, \ldots, A_m$ of base learner algorithms as input, as well as a training set D and two validation sets V^1 and V^2. The predictor that is obtained by training an algorithm $A \in \mathcal{A}$ on some subset $E \subseteq D$ of the training data is denoted $A(E)$. Let $\mathcal{E}$ be a collection of subsets of the training data D. We then define $\mathcal{A}(\mathcal{E}) = \{A(E) : A \in \mathcal{A}, E \in \mathcal{E}\}$ as the set of predictors obtained from training each algorithm in $\mathcal{A}$ on every set in $\mathcal{E}$. Given a subset $N \subset \mathcal{X}$ of the feature space and a subset $E \subset D$ of the dataset, we let $E(N) = \{(x_i, y_i) \in E : x_i \in N\}$. When provided with disjoint sets $E_1, \ldots, E_t$ and corresponding predictors h_l on E_l, we denote the overall loss as $L(\bigvee h_i, \bigcup E_i)$.

The process is initialised with the root node $\mathcal{X}$ and the corresponding classifier $h_{\mathcal{X}}$. The classifier is chosen such that $h_{\mathcal{X}} = A(D(\mathcal{X}))$, where A is selected from the set of algorithms $\mathcal{A}$ such that it minimises the validation loss on V^1.

Then the children of each leaf $N \in \overline{\mathcal{T}}$ are recursively created. For this, the corresponding feature space is split along the feature i and threshold $\tau_i \in [0,1]$ that result in the best validation loss measured on V_1. We write

$$N^-_{\tau_i} = \{x \in N : x_i < \tau_i\}, N^+_{\tau_i} = \{x \in N : x_i \geq \tau_i\} \quad (1)$$

In practice, for each continuous feature up to 9 candidate thresholds are selected at the 10th, 20th, ..., 90th percentiles. For every candidate threshold τ_i, the predictors $h^- \in \mathcal{A}(N^{-\uparrow}_{\tau_i})$, $h^+ \in \mathcal{A}(N^{+\uparrow}_{\tau_i})$ are chosen such that they minimise the validation loss where $N^\uparrow$ to denotes the set consisting of node N and all its predecessors that correspond to the same label space. From these predictors we then determine $h_{N^-_{\tau^*i}}$, $h_{N^+_{\tau^*_i}}$ that minimise the total validation loss.

A node N is only split if its loss is strictly higher than the total loss of its children $N^-_{\tau_i}$ and $N^+_{\tau_i}$. The pseudo-code for this can be found in Algorithm 1.

2.2.3 Weighting Predictors for Optimal Predictions

Once the locally optimal tree is established, the next step is to determine how to weight the various predictors. The prediction for a sample x is determined by the sequence of nodes $\prod$, which spans the path from the root node to the leaf node $\overline{N}(x)$ that corre-

Algorithm 1: Growing the Optimal Tree of Predictors. Adapted from (Yoon et al., 2018b).

```
Require: Feature space $\mathcal{X}$, set of algorithms $\mathcal{A}$,
    training set $D$, first validation set $V^1$

    $h_X \leftarrow \arg\min_{h \in \mathcal{A}(D)} L(h, V^1)$
    $\mathcal{T} \leftarrow (\mathcal{X}, h_X)$,
    Recursive step:
    Input: Current Tree of Predictors $\mathcal{T}$
    for each leaf $N \in \overline{\mathcal{T}}$ do
        for each feature i and threshold $\tau_i$ do
            $N^-_{\tau_i} \leftarrow \{x \in N : x_i < \tau_i\}$
            $N^+_{\tau_i} \leftarrow \{x \in N : x_i \geq \tau_i\}$
        end
        let $h^-_{\tau_i} \in \mathcal{A}(N^-_{\tau_i})$, $h^+_{\tau_i} \in \mathcal{A}(N^+_{\tau_i})$
        $(i^\star, \tau^\star_i, h_{N^-_{\tau_i}}, h_{N^+_{\tau_i}}) \leftarrow$
        $\arg\min L\left(h^-_{\tau_i} \vee h^+_{\tau_i}; V^1(N)\right)$
    end
    Stopping criterion:
    $L(h_N; V^1(N)) \leq$
    $\min_L \left(h^-_{\tau_i} \vee h^+_{\tau_i}; V^1(N^-_{\tau_i}) \cup V^1(N^+_{\tau_i})\right)$
```

sponds to x. Each leaf node is assigned an individual weight vector $\vec{w} = (w_N)_{N \in \prod}$, which defines the weights of predictors corresponding to nodes on the root-leaf path. These weights are used to generate predictions for samples associated with $\overline{N}(x)$. The entire weight vector of a leaf is individual; that is, the common ancestor of two leaves might have different weights assigned by them.

Weights are required to be non-negative and sum to one. For each leaf, weight vectors are chosen by utilising linear regression to minimise the empirical loss on the corresponding subset of the second validation set $V^2(\overline{N}(x))$.

2.3 Model Trees

Model Trees (Quinlan et al., 1992), are a tree-based ensemble method for solving regression tasks. They combine a conventional Decision Tree structure with the possibility of linear regression functions at the leaf nodes (Wang and Witten, 1997).

In the first phase of Model Tree construction, a Decision Tree induction algorithm (Breiman et al., 1984) is employed. As a splitting criterion it minimises the variation in class values within each subset across the branches. During the second phase, it prunes the tree, starting from each leaf and working upwards. This aims to reduce overfitting by removing or replacing less informative nodes (Breiman et al., 1984; Quinlan, 1986). A key distinction from conventional pruning methods is that, when pruning back to an internal node, the method involves replacing that node with a regression plane rather than a constant value (Wang and Witten, 1997).

Several works have expanded on the original Model Tree method. Torgo (Torgo, 1997a) introduced an approach that allows for different models within the leafs of the tree. However, Torgo's method remains constrained to growing the tree based on a single base learner. Malerba *et al.* (Malerba et al., 2001) proposed a Model Tree induction algorithm that has some similarities with our PTE method. It employs a splitting criterion based on how well linear models fit the data at a node during tree growth.

2.3.1 Differences to Partition Tree Ensembles

Primarily, Model Trees are designed to address regression tasks, whereas PTEs are designed for classification problems. Additionally, PTEs do not utilise pruning or smoothing techniques. Instead, they employ Stacked Generalisation (Wolpert, 1992) to determine the weights assigned to models along the path from the root to the leaf node. Furthermore, Model Trees solely partition the feature space, whereas PTEs have the versatility to partition both the feature space and the label space.

Importantly, Model Trees are induced using a single base learner algorithm while PTEs provide the flexibility to select the most suitable base learner at each tree node.

Lastly, Model Trees are restricted to using convex loss functions (Yoon et al., 2018b). This can be disadvantageous when optimising for F-score or AUC, as is frequently done in medical applications. In contrast, PTEs offer the flexibility to optimise non-convex loss functions.

3 PARTITION TREE ENSEMBLES

In this section, we introduce PTEs. First, in Section 3.1 we explain the motivation for this method. Then in Section 3.2 we formally introduce Class Dichotomies, which constitute the inner nodes of Nested Dichotomies. (Note that in the statistical literature these are referred to simply as “Dichotomies”.) Inspired by (Leathart et al., 2016) we use the Random Pair method to select Class Dichotomies for PTEs. We describe this in Section 3.3. In Section 3.4 we provide a formal definition of PTEs. Then, in Section 3.5 we describe our method for inducing them. Finally, in Section 3.6 we describe how we aggregate base learner predictions into an overall prediction.

3.1 Motivation

In this section, we succinctly present the motivation underpinning our PTE algorithm. Previous work by Yoon *et al.* (Yoon et al., 2018b) highlighted how a Tree of Predictors can produce significant improvements over baseline methods such as AdaBoost, and Random Forest. However, their experimental analysis was confined to binary classification datasets. Our preliminary experiments applying ToPs to multi-class classification problems revealed that their performance advantage over the baselines diminishes with a higher number of classes.

Achieving high performance in terms of loss functions other than the cross-entropy loss can be pivotal, especially in healthcare applications. Conventional performance measures such as cross-entropy loss or accuracy are often not the most suitable metrics in medical settings (Yoon et al., 2018a). In many cases, employing other loss functions such as AUC-Loss (Cortes and Mohri, 2003) or the F-Measure (Gu et al., 2009) may be more appropriate. Hence, our goal was to identify an ensemble method comparable to Tree of Predictors, which can successfully optimise arbitrary loss functions for multi-class problems as well.

In response to this challenge, we present PTEs. Like ToPs, PTEs recursively split the classification problem into subproblems associated with the nodes of a binary tree. However, in addition to splitting the feature space, nodes within the tree can partition the label space using Class Dichotomies, thereby giving rise to sub-problems derived from the initial multi-class classification problem. Since these sub-problems have a lower number of classes compared to the original problem, we are able to obtain performance gains similar to those we observed for ToPs in binary classification problems.

3.2 Class Dichotomies

In this section, we provide a formal definition of Class Dichotomies, which serve as a means to partition a multi-class classification problem into three distinct sub-problems. Class Dichotomies are utilised at every inner node of a ND tree. In early machine learning literature, the individual nodes of a Nested Dichotomy were themselves referred to as Nested Dichotomies (Frank and Kramer, 2004). However, in contemporary usage, the term "Nested Dichotomies" has evolved to encompass the entire tree structure (Leathart, 2019).

Given a classification problem with $\mathcal{Y} = \{c_1, \ldots, c_k\}$, a Class Dichotomy partitions the set of classes into two subsets. Without loss of generality, let these subsets be $\mathcal{Y}^- = \{c_1, \ldots, c_j\}$ and $\mathcal{Y}^+ = \{c_{j+1}, \ldots, c_k\}$. It is important to note that Class Dichotomies may define arbitrary non-empty partitions, and the ordering of classes is not relevant to this. To construct a predictor that addresses the original multi-class problem, the Class Dichotomy combines predictions for three sub-problems, which are defined by the two subsets. First, the Class Dichotomy includes a predictor $h_{\mathcal{Y}^-,\mathcal{Y}^+}$ that differentiates between the two meta-classes determined by $\mathcal{Y}^-$ and $\mathcal{Y}^+$. This means that, for a given sample (x,y), $h_{\mathcal{Y}^-,\mathcal{Y}^+}(x)$ estimates the probability $p(y \in \mathcal{Y}^-|x)$. Also, the Class Dichotomy has two predictors, $h_{\mathcal{Y}^-}$ and $h_{\mathcal{Y}^+}$, which estimate the class probabilities of a sample, assuming it belongs to the respective subset; that is, $h_{\mathcal{Y}^r}$ estimates $p(y = c_i|x, y \in \mathcal{Y}^r)$ for all classes $c_i \in \mathcal{Y}^r$ where $\mathcal{Y}^r \in \{\mathcal{Y}^-, \mathcal{Y}^+\}$. We can simply multiply the conditional probability with the probability of its condition to obtain an overall class probability estimate:

$$p(y = c_i|x) = p(y = c_i|x, c_i \in Y^r) \cdot p(c_i \in Y^r|x) \quad (2)$$

Thus, for each class $c_i \in \mathcal{Y}^r$, if $\mathcal{Y}^r = \mathcal{Y}^-$, we can estimate $p(y = c_i|x)$ using $h_{\mathcal{Y}^-,\mathcal{Y}^+}(x) \cdot h_{\mathcal{Y}^-}(x)$, and if $\mathcal{Y}^r = \mathcal{Y}^+$, using $\left(1 - h_{\mathcal{Y}^-,\mathcal{Y}^+}(x)\right) \cdot h_{\mathcal{Y}^+}(x)$. We refer to this overall classifier as h_{CD}.

3.3 Random Pair Method

Inspired by (Leathart et al., 2016), we propose the use of the Random Pair method to generate Class Dichotomies within our PTEs. Our rationale is as follows: among methods that rely on iterative splitting, RPNDs have demonstrated the best performance in selecting NDs (Leathart, 2019). Although this may not directly translate to optimal performance for choosing individual Class Dichotomies, we believe it serves as a good proxy. In this section, we present a detailed explanation of the method along with the corresponding pseudocode.

The process begins by randomly selecting two classes, c^- and c^+, from the label space $\mathcal{Y}$ without replacement. Following this, we utilise the available training data for these classes to train a binary classifier h_{c^-,c^+} to distinguish between the two classes. This classifier is applied to the remaining training data and the remaining classes are assigned to one of two sets $\mathcal{Y}^-, \mathcal{Y}^+$ based on the classifier's predictions through hard voting. Specifically, if the classifier predicts that the majority of data points belonging to class c_i are in class c^-, class c_i will be allocated to the subset $\mathcal{Y}^-$ surrounding c^-. Otherwise, it will be assigned to the subset $\mathcal{Y}^+$. Once the two *meta-classes* $\mathcal{Y}^-$ and $\mathcal{Y}^+$ are formed, we discard h_{c^-,c^+}

and train a new classifier $h_{\mathcal{Y}^-,\mathcal{Y}^+}$ using the training set $\{(x,0)|(x,y) \in D, y \in \mathcal{Y}^-\} \cup \{(x,1)|(x,y) \in D, y \in \mathcal{Y}^+\}$ to distinguish between the two meta-classes. To form a complete Class Dichotomy, we also train and select $h_{\mathcal{Y}^-} = \arg\min_{A \in \mathcal{A}} L\left(A(D^-), V_1^-\right)$ and $h_{\mathcal{Y}^+} = \arg\min_{A \in \mathcal{A}} L\left(A(D^+), V_1^+\right)$ which constitute the optimal models for the two respective sub-problems.

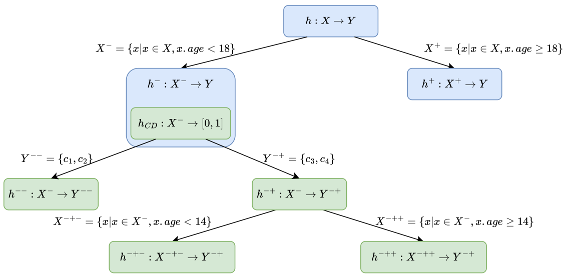
We choose this method to create Class Dichotomies because it has been used to develop state-of-the-art NDs (Leathart et al., 2016). Although evolutionary algorithms NDEA (Wever et al., 2018) and CONDA (Wever et al., 2023) have recently outperformed RPNDs, these methods optimise the entire ND tree instead of individual dichotomies. Consequently, they are not suitable for our purposes.

3.4 Formal Definition

In this section, we provide a formal introduction to the PTE method. We employ the same notation as in Section 2.2, and we continue to assume that categorical features are represented in binary form and continuous features are normalised. For our PTE method, we require a finite set of m candidate algorithms, denoted as $\mathcal{A} = \{A_1, \dots, A_m\}$, as well as a set of m_{CD} candidate algorithms $\mathcal{A}_{CD}$ that we use to create predictors which distinguish between the meta-classes in Class Dichotomies.

Each node N within this tree corresponds to a subset of the feature space $\mathcal{X}_N \subseteq \mathcal{X}$ and a subset of the label space $\mathcal{Y}_N \subseteq \mathcal{Y}$. A classifier h_N is associated with each node, mapping the feature space to the respective subset of the label space. It is generated by training an algorithm $A_N \in \mathcal{A}$ on a subset of the feature space corresponding to node N^*, where N^* is either N or one of its predecessors that corresponds to the same subset of the label space $\mathcal{Y}_N$. Formally, this relationship is expressed as $h_N = A_N(N^*)$ where $(N^* \in N^*\uparrow) \wedge (\mathcal{Y}_{N^*} = \mathcal{Y}_N)$. For any given node $N \in \mathcal{T}$, its children, denoted as $\{N^-, N^+\}$, partition the local feature space $\mathcal{X}_N$ and correspond to the local label space $\mathcal{Y}_N$ or vice versa. If and only if a node's successors split the label space, it contains an additional predictor $h_{\mathcal{Y}_N^-,\mathcal{Y}_N^+}$ that is generated by training an algorithm $A_{CD} \in \mathcal{A}_{CD}$ to distinguish between the two meta-classes defined by the subsets $\mathcal{Y}_N^-$ and $\mathcal{Y}_N^+$.

To grow a Partition Tree, we randomly partition the available dataset into the training set D and two validation sets V_1 and V_2. Given a subset of the feature space $N \subset \mathcal{X}$ and a subset of the dataset $Z \subset D$, we let $Z(N) = \{(x_i, y_i) \in Z : x_i \in N\}$. Our general model accommodates the optimisation of arbitrary loss functions. An illustrative example of a PTE is provided in Figure 3.



$h : X \to Y$
$X^- = \{x|x \in X, x.age < 18\}$
$X^+ = \{x|x \in X, x.age \geq 18\}$
$h^- : X^- \to Y$
$h^+ : X^+ \to Y$
$h_{CD} : X^- \to [0,1]$
$Y^{--} = \{c_1, c_2\}$
$Y^{-+} = \{c_3, c_4\}$
$h^{--} : X^- \to Y^{--}$
$h^{-+} : X^- \to Y^{-+}$
$X^{-+-} = \{x|x \in X^-, x.age < 14\}$
$X^{-++} = \{x|x \in X^-, x.age \geq 14\}$
$h^{-+-} : X^{-+-} \to Y^{-+}$
$h^{-++} : X^{-++} \to Y^{-+}$

Figure 3: Illustrative example of a Partition Tree Ensemble with $\mathcal{Y} = \{c_1, c_2, c_3, c_4\}$.

3.5 Growing a Partition Tree

In this subsection, we introduce our algorithm for growing Partition Trees, building upon the algorithm for growing ToPs from Section 2.2. This extension enables splits of the label space, utilising the concept of Class Dichotomies introduced earlier.

Similarly to the procedure for growing ToPs, we begin with the trivial Partition Tree containing only the root node corresponding to $(\mathcal{X}, \mathcal{Y})$. When creating children for each node, we first estimate the optimal split of the feature space, as for ToPs. Instead of immediately generating the children based on this optimal split, we further create a candidate Class Dichotomy for each $A_{CD} \in \mathcal{A}_{CD}$. For this purpose, we utilise the Random Pair method, as outlined in Section 3.3, to create two meta-classes. Then, the algorithm A_{CD} is trained on these meta-classes, yielding $h_{\mathcal{Y}^-,\mathcal{Y}^+}$. Using the validation set V^1, we select the optimal algorithms $A^-, A^+ \in \mathcal{A}$ to create $h_{\mathcal{Y}^-}$ and $h_{\mathcal{Y}^+}$. These three predictors collectively form $h_{\mathcal{Y},CD}$. The optimal $h^*_{\mathcal{Y},CD}$ is chosen from the m_{CD} Class Dichotomies created in this manner, based on the validation set V^1. If $h^*_{\mathcal{Y},CD}$ demonstrates a lower loss compared to the optimal split of the feature space, then we create the node's children based on this Class Dichotomy instead of splitting the feature space. In this case, the children will correspond to partitions of the local label space $\mathcal{Y}^-$ and $\mathcal{Y}^+$, while sharing the same local feature space. Additionally, the current node will be assigned the meta-classifier $h_{\mathcal{Y}^-,\mathcal{Y}^+}$, which is used to combine the predictions of its children. This recursive process of creating the children's offspring continues until neither the best Class Dichotomy nor the optimal feature space split can further improve the local loss. The pseudocode for PTEs is in Algorithm 2.

If a node's children partition the label space, it is necessary to assign them a new second validation set V^2. To achieve this, we split off a new validation set from the training set at the current node and pass it to the children as the V^2 set. This step is crucial because, Algorithm 2: Growing the Optimal Partition Tree Ensemble.

```
**Require:** Training set $D$, the first validation set $V_1$, a set of base estimators $\mathcal{A}$, a set of binary base estimators for Class Dichotomies $\mathcal{A}_{CD}$
    $h_X \leftarrow \arg\min_{A \in \mathcal{A}} L(A(D); V_1)$
    $root \leftarrow (X, h_X)$,
    **Recursive step:**
    **Require:** node $(N, h_N)$ **for** *a feature i and a threshold* $\tau_i$ **do**
        $N^-_{\tau_i} \leftarrow \{x \in N : x_i < \tau_i\}$
        $N^+_{\tau_i} \leftarrow \{x \in N : x_i \geq \tau_i\}$
    **end**
    **let** $h^-_{\tau_i} \in \mathcal{A}(D(N^-_{\tau_i})), h^+_{\tau_i} \in \mathcal{A}(D(N^+_{\tau_i}))$ :
    $(i^\star, \tau^\star_i, h_{N^-_{\tau_i}}, h_{N^+_{\tau_i}}) \leftarrow \arg\min L\left(h^-_{\tau_i} \cup h^+_{\tau_i}; V_1(N)\right)$
    $h_{CD} \leftarrow randomPair(D(N), V_1(N), \mathcal{A}, \mathcal{A}_{CD})$
    $L_{\tau_i} \leftarrow L(h^-_{\tau^\star_i} \cup h^+_{\tau^\star_i}, V_1(N))$
    $L_{CD} \leftarrow L(h_{CD}, V_1(N)))$
    $L_N \leftarrow L(h_N, V_1(N))$
    **if** $(L_{\tau_i} < L_N) \wedge (L_{\tau_i} \leq L_{CD})$ **then**
        $node.left \leftarrow (N^-_{\tau^\star_i}; h^+_{\tau^\star_i})$
        $node.right \leftarrow (N^+_{\tau^\star_i}; h^+_{\tau^\star_i})$
        $recurse(node.left)$
        $recurse(node.right)$
    **end**
    **if** $(L_{CD} < \min(L_N, L_{\tau_i})$ **then**
        $node.CD \leftarrow h_{CD}$
        $recurse(node.CD.left)$
        $recurse(node.CD.right)$
    **end**
    **Stopping criterion:**
    $(L_N \leq \min(L_{CD}, L_{\tau_i})$
```

without it, stacking would be biased towards assigning higher weights to predictions resulting from Class Dichotomies. The reason for this will become more clear in the next section.

3.6 Weighting and Assembling Predictions

In PTEs, we cannot assemble predictions in the same manner as in ToPs. This is because base learners below a Class Dichotomy are trained on a sub-problem with fewer classes. Therefore, integrating their predictions into the original multi-class problem requires the use of predictor $h_{\mathcal{Y}^-,\mathcal{Y}^+}$, which has been trained on the meta-classes at the Class Dichotomy node.

To tackle this, we conceptually regard nodes containing a Class Dichotomy as leaf nodes, and their subtrees as independent PTEs. This strategy enables us to integrate the two subtrees and the meta-classifier at a Class Dichotomy into a single predictor h_{CD}. Consequently, our tree now resembles a tree of predictors, with the exception that we have an added predictor h_{CD} at each leaf node containing a Class Dichotomy. We can then employ linear regression to define a weight vector $\vec{w}$, allocating non-negative weights to each of the predictors on the path from the root to the leaf node, including the additional h_{CD}.

However, to make this feasible, the subtrees of the Class Dichotomy must be functional PTEs, implying that weight vectors must have already been assigned to them. Therefore, we initiate this process at the lowest Class Dichotomies and work our way up the tree. Now, the need for creating new V^2 sets for the children at nodes with Class Dichotomies becomes apparent. If we use the same validation set V^2 to assign the weight vectors to the children, the estimated performance of h_{CD} on V^2 will be biased, and the weight assigned to it will likely be higher than optimal.

4 IMPLEMENTATION

We implement PTEs in Python 3.11.1 and adhere to the guidelines for developing scikit-learn estimators (Pedregosa et al., 2011).

In our implementation we introduce an additional hyperparameter, *minLeafSize*, which serves as an additional stopping criterion. If either the training or one of the two validation sets at a node contains fewer samples than *minLeafSize*, we will not split the node further. The rationale behind this is that a small validation set may lead to a higher probability of overfitting.

4.1 Computational Complexity

The computational complexity of PTE can be expressed as:

$$O\left(n\left(nd\sum_{i=1}^{m}\left(T_i(n,d)\right)+\sum_{j=1}^{m_{CD}}\left(T_j^{CD}(n,d)+\sum_{i=1}^{m}\left(T_i(n,d)\right)\right)\right)\right). \quad (3)$$

Here $T_i(n,d)$ denotes the computational complexity of the i^{th} base learner algorithm, m represents the number of such algorithms, $T_j^{CD}(n,d)$ signifies the computational complexity of the jth base learner algorithm used to create Class Dichotomies, and m_{CD} is the number of those algorithms. As previously defined, n refers to the number of samples, and d to the feature count. We provide a proof for this complexity bound in Appendix 6.

When using Logistic Regression as the only base learner our method has a training time complexity

Table 2: Properties of the UCI datasets we use in our experiments.

Dataset	Task ID	Size	Classes	Features
mfeat-fourier	14	2000	10	76
mfeat-karhunen	16	2000	10	64
mfeat-morph	18	2000	10	6
mfeat-pixel	20	2000	10	240
mfeat-zernike	22	2000	10	47
robot-navigation	9942	5456	4	4
plants-shape	9955	1600	100	64
semeion	9964	1593	10	256
cardiocotography	9979	2126	10	35

of $O(n^3d^2)$. This follows from inserting $O(nd)$—the computational complexity of Logistic Regression (Singh, 2023)—into the above formula:

$$O(n(nd(nd)+(nd+nd))) = O\left(n^3d^2\right). \quad (4)$$

5 EVALUATION

In this section, we conduct a thorough experimental evaluation of our proposed PTEs. In conducting these experiments, our main objectives are twofold. First, we aim to evaluate whether PTEs can exploit Class Dichotomies to more effectively decompose multi-class problems, compared to ToPs. Second, we investigate whether the capability of our approach to optimise arbitrary loss functions provides a competitive edge over widely-used ensemble methods for classification, such as AdaBoost and Random Forest. A performance comparison to NDs is not included in our analysis. This is because the primary goal of NDs is not to enhance the predictive performance for a specified base learner, but to reduce a multi-class problem into a set of binary problems.

We assess the performance of PTEs across different objectives. In Section 5.1, we examine the performance on the AUC-Loss function. This is followed by an evaluation with the F1-Score in Section 5.2.

For our experiments, we use nine distinct datasets from the UCI repository (Dua and Graff, 2017) (refer to Table 2

for more detail). We deliberately chose datasets featuring a sample size above 1500, and with a maximum of 5500. This range was selected to allow for the potential growth of a tree to a depth where the impact of our ensemble method could be adequately demonstrated. Larger datasets, while potentially informative, were not considered due to our computational constraints and the substantial processing time required. It is important to highlight that the quantity of features in a dataset also significantly influences the runtime of our method. The majority of the datasets chosen for our study comprise 10 classes. The underlying rationale for selecting datasets with a variety of classes is to provide sufficient opportunities for partitioning the label space to enable the PTEs method to show its effects in comparison to the ToPs method.

To ensure both comparability and reproducibility of our results, we adhere to a standardised testing methodology. We apply the same hyperparameter tuning procedure across all methods. Detailed information on this hyperparameter tuning process can be found in Appendix 6. To ensure the reliability of our findings, we utilise the Wilcoxon Signed Rank Test (Rey and Neuhäuser, 2011) for all performance results with a significance level, α, of 0.05.

For benchmarking purposes, we compare our PTEs against ToPs, using the same two sets of base learners as employed in (Yoon et al., 2018b), but with a slight modification: we replace Linear Regression with Logistic Regression. Logistic Regression is typically more appropriate for classification tasks, and the reason for the original choice of Linear Regression in (Yoon et al., 2018b) remains unclear. The two sets of base learners are LR = {Logistic Regression} and ALL = {Logistic Regression, Random Forest, AdaBoost}. Motivated by the successful application of Logistic Regression in NDs (Wever et al., 2018), we choose it as the singular base learner for creating Class Dichotomies in PTEs. From this point forward, we will denote ToPs and PTEs with the abbreviations ToP-LR, ToP-ALL, PTE-LR, and PTE-ALL to indicate the specific set of base learners being referred to. In addition to ToPs, we also evaluate the performance of our model against the two conventional ensemble methods Random Forest and AdaBoost, to provide additional baseline comparisons. We also include the performance of simple Logistic Regression to provide additional context for the evaluation. All our experiments were conducted in a high performance computing cluster using a dual Xeon Gold 6142 16C 2.6GHz CPU and 384GiB of RAM on nodes that run the Scientific Linux 7 operating system, which is based on CentOS 7.

5.1 Experiments Using AUC-Loss

In this section, we discuss our experimental results when using a loss function based on the Area Under the Receiver Operator Characteristic curve (AUC) (Cortes and Mohri, 2003). We employ a multi-class extension of the regular AUC-Measure, as detailed in Section 5.1.2.

Table 3: Loss of PTE-LR and baselines optimised for ROC-AUC.

Task ID	PTE-LR	ToP-LR	LR
14	0.0191±0.0041	0.0203±0.0048 ●	0.0189±0.0041
16	0.003±0.0016	0.0033±0.0021	0.0034±0.0019 ●
18	0.0614±0.0262	0.0887±0.014 ●	0.0873±0.0138 ●
20	0.002±0.0011	0.0022±0.0015	0.0019±0.001
22	0.0209±0.003	0.0207±0.0042	0.0207±0.0029
9942	0.0013±0.0028	0.0005±0.0008 ○	0.0011±0.0006
9955	0.0271±0.0055	0.0281±0.0055	0.0283±0.0052
9964	0.0045±0.0028	0.0052±0.0028 ●	0.0045±0.0026
9979	0.0434±0.0134	0.1517±0.0247 ●	0.1464±0.0242 ●

5.1.1 Motivation

In (Cortes and Mohri, 2003) Cortes and Mohri provide a statistical analysis of the AUC and theoretically determine its expected value and variance given a fixed error rate. They point out that algorithms minimising the error rate do not necessarily lead to optimal AUC values. It is an important measure in cases where we are interested in the quality of a classifier's ranking, thus directly optimising it can yield substantial benefits in such cases. Hand and Till argue in (Hand and Till, 2001) that such a ranking-based loss can often be useful in multi-class cases as well, primarily because it is challenging to assign realistic costs to different types of misclassification in practice. Moreover, we want to ensure comparebility with Yoon *et al.* (Yoon et al., 2018b) who adopted AUC as a loss function in their introduction of ToPs.

5.1.2 Multi-Class AUC

The multi-class generalisation of AUC we use is computed by assessing the average "separability" between each pair of classes. In this context, the separability between two classes c_i and c_j is quantified as the average of two probabilities: 1) the probability that a randomly drawn instance of class c_j has a lower estimated probability of belonging to class c_i than a randomly drawn instance of class c_i, and 2) the equivalent probability with c_i and c_j reversed (Hand and Till, 2001).

5.1.3 Experimental Results

In Table 3 we present the results obtained from PTE-LR, ToP-LR, and individual Logistic Regression, each optimised using the multi-class AUC-Loss function as detailed above. The datasets are identified by their OpenML Task ID. The table provides the average loss and the corresponding standard deviation as obtained from cross-validation. Moreover, it highlights instances of statistical significance where applicable. A significant improvement of PTE-LR over a baseline is highlighted with symbol •. Conversely, a significant degradation in performance is indicated by the symbol ◦. To further elucidate our findings, Figure 4 provides a visual representation of the results obtained. We find that when employing Logistic Regression as the sole base learner, PTEs outperform ToPs in seven out of nine instances. Interestingly, in four of these seven cases, the improvement is statistically significant, while only one instance of significant degradation is observed.

This divergence in performance, where we observe slight performance degradation for some datasets and significant improvement for others, could potentially be attributed to the inherent nature of the classes within these datasets. In the field of statistics, the recommendation to employ NDs is contingent upon having a substantial rationale for selecting specific dichotomies. For instance, if there is some particular ordering of classes, it might be advantageous to cluster together classes that fall within the same order spectrum, either lower or higher (Fox, 2016). Hence, we hypothesise that datasets demonstrating significant improvements may possess such intrinsic characteristics, making them more apt for the application of Class Dichotomies.

We substantiate this hypothesis by examining the dataset where PTEs exhibit the most significant performance enhancement over ToPs. In the case of the cardiotocography dataset, we note a reduction in loss of over two-thirds, which is more than twice the rate of improvement observed in any other case. This dataset categorises each instance based on the class (1-10) of the fetal heart rate pattern, with classes 1-8 corresponding to normal baselines, class 9 to moderate bradycardia, and class 10 to severe bradycardia (Maso et al., 2012). Our conjecture is that, for this dataset, the similarity among certain classes (1-8, 9-10) makes the application of a Class Dichotomy especially advantageous.

Conversely, for datasets where such properties are absent, PTEs might experience minor degradations due to factors such as noise, or increased overfitting owing to their higher flexibility. Moreover, it is important to highlight that, in certain instances, the random-pair method might more readily discover a beneficial partitioning of classes compared to other scenarios.

We hypothesise that the substantial performance degradation observed on the wall-robot-navigation dataset is likely attributable to overfitting. Interestingly, this dataset has only four classes, while all others contain at least ten classes. This observation suggests that Class Dichotomies might be more advantageous for datasets with a greater number of classes.

While PTE-LR statistically outperforms simple

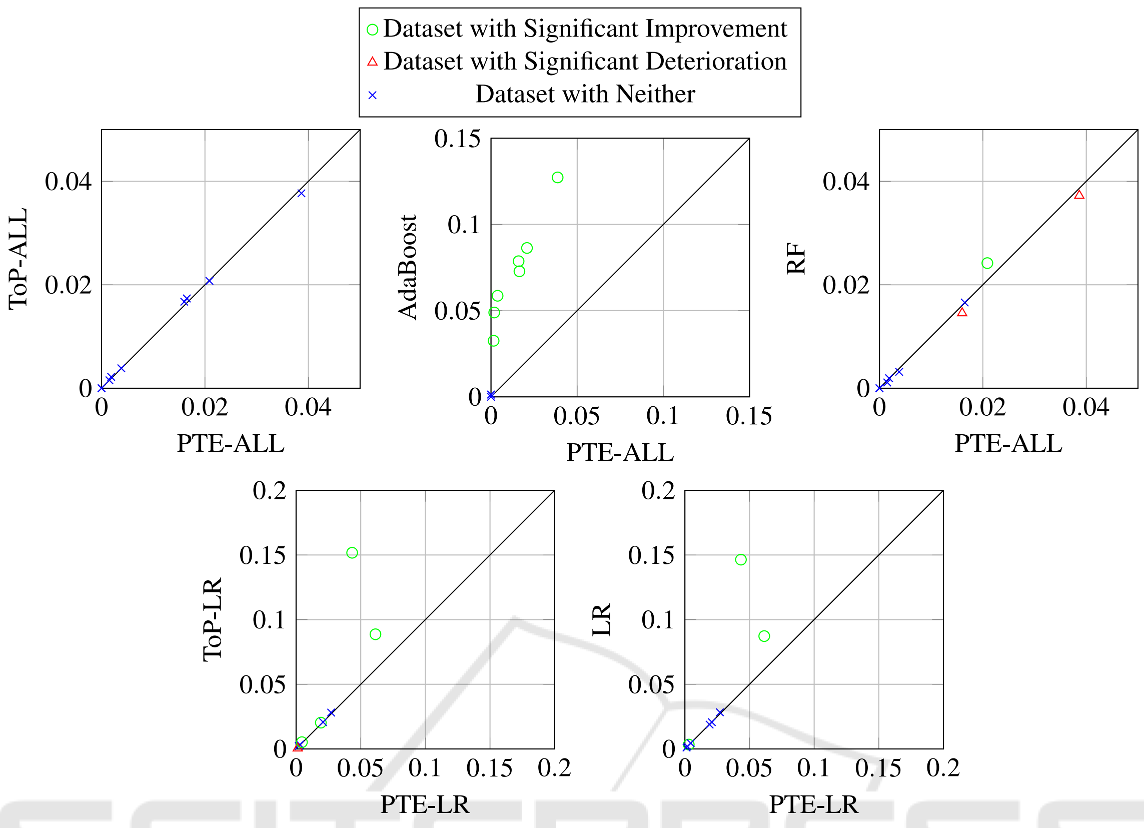


Figure 4: Scatter plots contrasting the AUC-Loss of PTE-ALL with baselines ToP-ALL, Random Forest, and AdaBoost, as well as the AUC-Loss of PTE-LR compared to ToP-LR and Logistic Regression. Each data point in these plots represents the mean loss obtained over the ten cross-validation folds for a specific OpenML task. Data points are color-coded to highlight the statistical significance of the performance difference between PTE and the respective baselines.

Table 4: Loss of PTE-ALL and baselines optimised for ROC-AUC.

Task ID	PTE-ALL	ToP-ALL	RF	AdaBoost
14	0.0165±0.003	0.0174±0.0039	0.0166±0.0032	0.0728±0.0184 •
16	0.0019±0.0009	0.0022±0.0012	0.0019±0.0012	0.0489±0.0118 •
18	0.0387±0.0073	0.0377±0.0082	0.0372±0.0072 ◦	0.1272±0.02 •
20	0.0015±0.0011	0.0015±0.001	0.0011±0.0008	0.0325±0.0105 •
22	0.0209±0.003	0.0207±0.0042	0.0242±0.0036 •	0.0863±0.0397 •
9942	0.0±0.0	0.0±0.0	0.0±0.0	0.0013±0.0042
9955	0.016±0.0033	0.0167±0.0042	0.0145±0.0025 ◦	0.0787±0.0112 •
9964	0.0038±0.0015	0.0039±0.0017	0.0032±0.001	0.0586±0.0166 •
9979	0.0±0.0	0.0±0.0	0.0±0.0	0.0±0.0

Logistic Regression in three instances, we note that Logistic Regression slightly surpasses PTE-LR on five datasets. A similar pattern of degraded performance is observed when comparing ToP-LR to Logistic Regression. These observations suggest that both tree-based ensemble methods might be overfitting the training data, thereby offering an avenue for further investigation and optimisation of these methods.

In Table 4, we present the outcomes derived from PTE-ALL, ToP-ALL, Random Forest, and AdaBoost. Exploiting a broader set of base learners, we note outcomes akin to those observed when using solely Logistic Regression. Specifically, PTE-ALL outperforms ToP-ALL in five scenarios, while the reverse occurs in two instances, with no statistically significant differences in these comparisons. However, PTE-ALL exceeds the performance of Random Forest in three cases and falls behind in four, with one instance of statistically significant improvement and two cases of statistically significant degradation. Meanwhile PTE-ALL consistantly outperforms AdaBoost. Taking into account these results, we can assert that for the AUC-Loss function, incorporating Class Dichotomies into tree-based ensembling is indeed advantageous. Nevertheless, the comparison to Random Forest raises doubts about the merits of attempting to enhance Random Forest by employing it as a base learner in PTEs or ToPs.

Evaluating the performance of the three distinct base learners, we find that Random Forest is the most proficient in capturing the underlying distribution of the datasets we explored. Given that its base learners—Decision Trees—have an intrinsic ability to partition the feature space, we hypothesise that they might not obtain significant advantages from the tree-based partitioning characteristic of our ensemble methods.

Table 5: Runtime of PTE-ALL and baselines optimised for ROC-AUC.

Task ID	PTE-ALL	ToP-ALL	PTE-LR	ToP-LR	RF	AdaBoost	LR
14	171.6819±58.8443	77.7228±19.3721 ○	1.0283±0.0362 ○	0.5091±0.0336 ○	31.272±6.8324 ○	3.5745±0.2582 ○	0.1625±0.0078 ○
16	176.6548±72.4138	59.2395±24.3352 ○	1.1891±0.6958 ○	0.4631±0.0257 ○	27.6619±11.8803 ○	2.951±0.2188 ○	0.1332±0.0067 ○
18	55.1±44.2909	31.1692±20.3078	2.351±0.6888 ○	0.3143±0.0415 ○	2.0931±1.7565 ○	0.1606±0.1092 ○	0.1049±0.0019 ○
20	147.4708±61.4661	60.185±15.4995 ○	19.8405±10.0204 ○	12.1076±1.5598 ○	3.2289±1.1929 ○	9.7781±1.0633 ○	0.7686±0.4613 ○
22	89.3503±18.7013	42.5977±6.5014 ○	0.9597±0.2382 ○	0.4143±0.0595 ○	25.8293±2.9524 ○	2.3192±0.1968 ○	0.1253±0.0027 ○
9942	771.8217±519.4681	688.7455±305.1365	15.7081±3.163 ○	14.4876±2.9639 ○	0.7687±1.1615 ○	0.6253±0.04 ○	0.119±0.0068 ○
9955	171.4221±47.3616	69.4383±9.6315 ○	31.0588±11.3884 ○	10.0724±0.5299 ○	22.2991±25.0351 ○	3.4312±0.7699 ○	0.5485±0.0541 ○
9964	98.5397±45.7543	38.8915±7.974 ○	2.0098±0.628 ○	0.6526±0.0767 ○	2.4775±0.5695 ○	1.2225±0.0923 ○	0.2283±0.0333 ○
9979	31.1584±2.2996	15.5143±0.26 ○	4.0713±0.6113 ○	0.4265±0.0843 ○	0.5081±0.7243 ○	0.5961±0.0134 ○	0.126±0.005 ○

Table 5 displays the average runtime of each method and dataset. We observe that PTEs exhibit significantly longer runtimes compared to ToPs for both families of base learners. The increased runtime can range from two-fold to almost ten-fold in some cases.

5.2 Experiments Using F1-Loss

This section outlines the results from our experiments using the F1-Loss. F1 is a metric that reflects a classifier's precision and recall, thereby providing a balanced evaluation of the model's performance.

5.2.1 Motivation

The F1-Measure is a widely-used evaluation metric, due to its ability to better manage class imbalances compared to accuracy. In situations where the dataset is unbalanced accuracy tends to become an unreliable measure because it often gives an overly optimistic estimation based on the classifier's performance on the majority class, thereby obscuring its potential shortcomings in predicting minority classes (Chicco and Jurman, 2020). Conversely, the F1-Measure represents the harmonic mean of Precision and Recall. Given that the harmonic mean of two numbers tends to be closer to the smaller one, a high F1-Measure signifies a strong Recall and Precision, thus providing a more appropriate measure of the classifier's performance in the presence of class imbalances (Gu et al., 2009).

5.2.2 Multi-Class F1

In our multi-class classification experiments we use the Macro F1-Score described in (Grandini et al., 2020). The Macro F1-Score is calculated based on the Macro Average Precision (MVP) and Recall (MVR). We calculate the macro average of a measure by applying it to all classes individually and taking the arithmetic mean of the results.

Table 6: Loss of PTE-LR and baselines optimised for F1-Score.

Task ID	PTE-LR	ToP-LR	LR
14	0.1687±0.0302	0.1788±0.0301 ●	0.1739±0.0232
16	0.0457±0.0176	0.0425±0.0145	0.0421±0.0162 ○
18	0.3851±0.1047	0.5287±0.0391 ●	0.533±0.032 ●
20	0.0285±0.0111	0.0325±0.012	0.029±0.0113
22	0.2003±0.0148	0.1837±0.0366	0.1928±0.0183
9942	0.0174±0.0143	0.0158±0.007	0.0312±0.009 ●
9955	0.5356±0.0337	0.5344±0.0314	0.5433±0.0332
9964	0.083±0.0192	0.079±0.0167	0.085±0.0244
9979	0.3761±0.0839	0.645±0.038 ●	0.6192±0.0414 ●

5.2.3 Experimental Results

In Table 6, we present the mean loss obtained for each dataset using PTE-LR, ToP-LR, and individual Logistic Regression when optimising for multi-class F1-Loss.

Figure 5 provides a visual representation of the results obtained.

We observe that PTE-LR outperforms ToP-LR in four cases, with three of them showing statistically significant differences. Conversely, ToP-LR achieves better results in five instances, although none of these differences are statistically significant. This pattern, characterised by slight performance degradation on some datasets and significant gains on others, mirrors what we previously observed in our experiments with AUC-Loss.

In Section 5.1.3 we hypothesised that these variations in performance can be attributed to certain datasets possessing intrinsic characteristics that make them more amenable to the application of Class Dichotomies. Interestingly, all three datasets that exhibited significant improvements in F1-Loss also showed significant improvements in AUC-Loss, reinforcing our conjecture that, regardless of the loss function employed, there exists a property in the underlying distribution that can be more effectively captured when utilising Class Dichotomies.

On the other hand, the minor performance degradations observed on datasets where this property is not apparent may again be attributed to factors such as noise and overfitting, which can pose challenges for the PTEs.

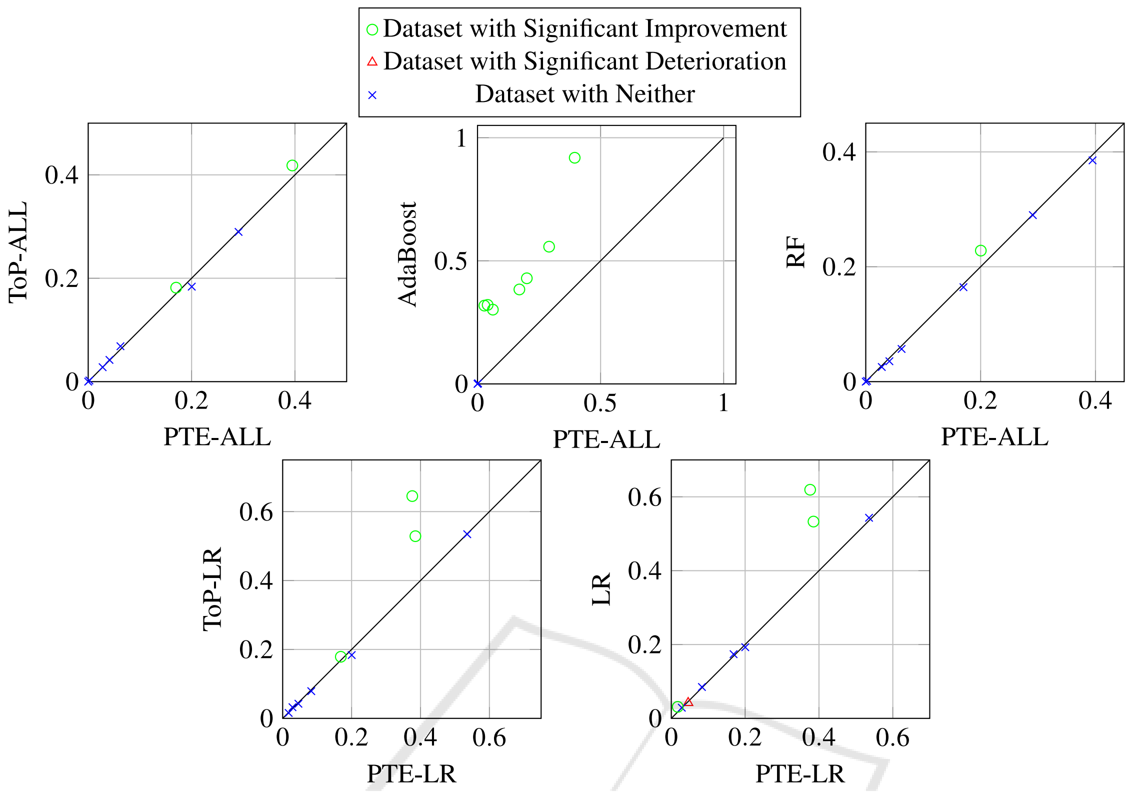


Figure 5: Scatter plots contrasting the F1-Loss of PTE-ALL with baselines ToP-ALL, Random Forest, and AdaBoost, as well as the F1-Loss of PTE-LR compared to ToP-LR and Logistic Regression.

When comparing PTE-LR with simple Logistic Regression, we continue to observe a similar pattern as in the previous experiments. PTE-LR outperforms Logistic Regression in seven cases, with three of them showing statistically significant improvements. Conversely, Logistic Regression outperforms PTE-LR in two cases, with one of them being statistically significant. Based on the observed results, it is evident that overfitting is a significant challenge for both ToP-LR and PTE-LR, with the more flexible PTE-LR model being particularly susceptible. This conclusion is supported by the fact that, in datasets where individual Logistic Regression outperforms PTE-LR, ToP-LR also demonstrates performance superior to PTE-LR. Therefore, in future research it will be essential to address the issue of overfitting in order to enhance the performance of our ensemble method further.

The outcomes of PTE-ALL, ToP-ALL, Random Forest, and AdaBoost optimised for F1-Loss are presented in Table 7.

Consistent with previous findings, PTE-ALL outperforms ToP-ALL in the majority of cases, with two instances demonstrating statistical significance. Furthermore, there is one case where PTE-ALL exhibits a significant improvement over Random Forest. We observe that the runtime for optimising F1-Loss is comparable to that of AUC-Loss.

Table 7: Loss of PTE-ALL and baselines optimised for F1-Score.

Task ID	PTE-ALL	ToP-ALL	RF	AdaBoost
14	0.1701±0.0209	0.1818±0.0246 •	0.1644±0.0235	0.3836±0.0634 •
16	0.0411±0.0152	0.0421±0.0114	0.0355±0.0137	0.321±0.1003 •
18	0.2909±0.0233	0.2896±0.0283	0.2899±0.0291	0.5574±0.0789 •
20	0.0279±0.0101	0.028±0.0088	0.0255±0.005	0.318±0.2167 •
22	0.2003±0.0148	0.1837±0.0366	0.2281±0.0291 •	0.4291±0.0626 •
9942	0.0023±0.0074	0.0023±0.0072	0.0014±0.0043	0.0023±0.0074
9955	0.3949±0.049	0.4181±0.0438 •	0.3852±0.0412	0.9187±0.0181 •
9964	0.0624±0.0132	0.0685±0.0114	0.0569±0.0097	0.3017±0.0583 •
9979	0.0±0.0	0.0±0.0	0.0±0.0	0.0±0.0

6 CONCLUSION

This paper introduced Partition Tree Ensembles, a tree-based ensemble method that incorporates ideas from Nested Dichotomies and Trees of Predictors to improve multi-class classification performance. Through an extensive experimental evaluation, we demonstrated that our approach achieves significant performance gains over its predecessor Tree of Predictors across various datasets and loss functions. Furthermore, we observed significant improvements over Random Forest on several datasets. In comparison with AdaBoost, our method demonstrated significantly higher performance in nearly all cases. However, this comes at the cost of a significantly increased runtime.

There are several avenues for future research that stand to be explored. Firstly, we intend to apply PTEs to other families of base learners. Recent studies have shown that well-tuned neural networks exhibit state-of-the-art performance on tabular data (Kadra et al., 2021), and it would be interesting to investigate whether ensembling using our Partition Tree Method can further improve their performance.

Secondly, we suspect that there is potential for enhancing performance by employing alternative strategies for selecting and weighting the base learners. In the current algorithm, the subtrees of each class dichotomy allocate a portion of the training data to replace the second validation set. Future work could explore using greedy forward selection, proposed in (Caruana et al., 2004), to determine the optimal weight for each base learner and the best possible split using only a single validation set. Furthermore, it might be valuable to investigate the benefits of retaining base learners in the final ensemble that were trained but not selected as optimal.

Finally, an interesting avenue for future research would be to explore the strategy of sampling a subset of attributes to evaluate for each split in the tree construction process. This approach has the potential to mitigate overfitting and improve runtime efficiency.

In conclusion, the development of Partition Tree Ensembles presents a promising approach for enhancing multi-class classification performance. By leveraging ideas from Nested Dichotomies and Trees of Predictors, our method offers significant performance gains over the Trees of Predictors method.

ACKNOWLEDGMENTS

This work was performed using resources provided by the Cambridge Service for Data Driven Discovery (CSD3) operated by the University of Cambridge Research Computing Service (www.csd3.cam.ac.uk), provided by Dell EMC and Intel using Tier-2 funding from the Engineering and Physical Sciences Research Council (capital grant EP/T022159/1), and DiRAC funding from the Science and Technology Facilities Council (www.dirac.ac.uk). For the purpose of open access, the author has applied a Creative Commons Attribution (CC BY) licence to any Author Accepted Manuscript version arising from this submission.

REFERENCES

Beneke, M., König, M., and Link, M. (2023). The inverted pendulum as a classical analog of the eft paradigm.

Beygelzimer, A., Langford, J., and Ravikumar, P. (2007). Multiclass classification with filter trees, 2007. *Preprint, available at http://hunch.net/jl/projects/reductions/mc_to_b/invertedTree. pdf.*

Breiman, L. (2001). Random forests. *Machine Learning*, 45(1):5–32.

Breiman, L., Friedman, J., Stone, C., and Olshen, R. (1984). *Classification and Regression Trees*. Taylor & Francis.

Caruana, R., Niculescu-Mizil, A., Crew, G., and Ksikes, A. (2004). Ensemble selection from libraries of models. In *Proceedings of the Twenty-First International Conference on Machine Learning*, ICML '04, page 18, New York, NY, USA. Association for Computing Machinery.

Chicco, D. and Jurman, G. (2020). The advantages of the matthews correlation coefficient (MCC) over F1 score and accuracy in binary classification evaluation. *BMC Genomics*, 21(1):6.

Cortes, C. and Mohri, M. (2003). Auc optimization vs. error rate minimization. In Thrun, S., Saul, L., and Schölkopf, B., editors, *Advances in Neural Information Processing Systems*, volume 16. MIT Press.

Dua, D. and Graff, C. (2017). UCI machine learning repository.

Fox, J. (2016). *Applied Regression Analysis and Generalized Linear Models*. SAGE, London.

Frank, E. and Kramer, S. (2004). Ensembles of nested dichotomies for multi-class problems. In Brodley, C. E., editor, *Machine Learning, Proceedings of the Twenty-first International Conference (ICML 2004), Banff, Alberta, Canada, July 4-8, 2004*, volume 69 of *ACM International Conference Proceeding Series*. ACM.

Freund, Y., Schapire, R., and Abe, N. (1999). A short introduction to boosting. *Journal-Japanese Society For Artificial Intelligence*, 14(771-780):1612.

Grandini, M., Bagli, E., and Visani, G. (2020). Metrics for multi-class classification: an overview. *arXiv preprint arXiv:2008.05756*.

Gu, Q., Zhu, L., and Cai, Z. (2009). Evaluation measures of the classification performance of imbalanced data sets. In Cai, Z., Li, Z., Kang, Z., and Liu, Y., editors, *Computational Intelligence and Intelligent Systems*, pages 461–471, Berlin, Heidelberg. Springer Berlin Heidelberg.

Hand, D. J. and Till, R. J. (2001). A simple generalisation of the area under the roc curve for multiple class classification problems. *Machine Learning*, 45(2):171–186.

Kadra, A., Lindauer, M., Hutter, F., and Grabocka, J. (2021). Well-tuned simple nets excel on tabular datasets. *Advances in neural information processing systems*, 34:23928–23941.

Leathart, T., Pfahringer, B., and Frank, E. (2016). Building ensembles of adaptive nested dichotomies with random-pair selection. In Frasconi, P., Landwehr, N., Manco, G., and Vreeken, J., editors, *Machine Learning and Knowledge Discovery in Databases -*

European Conference, ECML PKDD 2016, Riva del Garda, Italy, September 19-23, 2016, Proceedings, Part II, volume 9852 of *Lecture Notes in Computer Science*, pages 179–194. Springer.

Leathart, T. M. (2019). *Tree-structured multiclass probability estimators*. PhD thesis, The University of Waikato, Hamilton, New Zealand. Doctoral.

Lindauer, M., Eggensperger, K., Feurer, M., Biedenkapp, A., Deng, D., Benjamins, C., Ruhkopf, T., Sass, R., and Hutter, F. (2022). Smac3: A versatile bayesian optimization package for hyperparameter optimization. *Journal of Machine Learning Research*, 23(54):1–9.

Malerba, D., Appice, A., Bellino, A., Ceci, M., and Pallotta, D. (2001). Stepwise induction of model trees. In Esposito, F., editor, *AI*IA 2001: Advances in Artificial Intelligence*, pages 20–32, Berlin, Heidelberg. Springer Berlin Heidelberg.

Maso, G., Businelli, C., Piccoli, M., Montico, M., De Seta, F., Sartore, A., and Alberico, S. (2012). The clinical interpretation and significance of electronic fetal heart rate patterns 2 h before delivery: an institutional observational study. *Archives of Gynecology and Obstetrics*, 286(5):1153–1159.

Mohr, F., Wever, M., and Hüllermeier, E. (2018). Reduction stumps for multi-class classification. In Duivesteijn, W., Siebes, A., and Ukkonen, A., editors, *Advances in Intelligent Data Analysis XVII*, pages 225–237, Cham. Springer International Publishing.

Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., Blondel, M., Prettenhofer, P., Weiss, R., Dubourg, V., Vanderplas, J., Passos, A., Cournapeau, D., Brucher, M., Perrot, M., and Duchesnay, E. (2011). Scikit-learn: Machine learning in Python. *Journal of Machine Learning Research*, 12:2825–2830.

Quinlan, J. R. (1986). Induction of decision trees. *Machine Learning*, 1(1):81–106.

Quinlan, J. R. et al. (1992). Learning with continuous classes. In *5th Australian joint conference on artificial intelligence*, volume 92, pages 343–348. World Scientific.

Rey, D. and Neuhäuser, M. (2011). *Wilcoxon-Signed-Rank Test*, pages 1658–1659. Springer Berlin Heidelberg, Berlin, Heidelberg.

Singh, J. (2023). Computational complexity and analysis of supervised machine learning algorithms. In Kumar, R., Pattnaik, P. K., and R. S. Tavares, J. M., editors, *Next Generation of Internet of Things*, pages 195–206, Singapore. Springer Nature Singapore.

Torgo, L. (1997a). Functional models for regression tree leaves. In *ICML*, volume 97, pages 385–393. Citeseer.

Torgo, L. (1997b). Kernel regression trees. In *Poster papers of the 9th European conference on machine learning (ECML 97)*, pages 118–127. Prague, Czech Republic.

Wang, Y. and Witten, I. (1997). Induction of model trees for predicting continuous classes. *Induction of Model Trees for Predicting Continuous Classes*.

Wever, M., Mohr, F., and Hüllermeier, E. (2018). Ensembles of evolved nested dichotomies for classification. In Aguirre, H. E. and Takadama, K., editors, *Proceedings of the Genetic and Evolutionary Computation Conference, GECCO 2018, Kyoto, Japan, July 15-19, 2018*, pages 561–568. ACM.

Wever, M., Özdogan, M., and Hüllermeier, E. (2023). Cooperative co-evolution for ensembles of nested dichotomies for multi-class classification. In *Proceedings of the Genetic and Evolutionary Computation Conference*, pages 597–605.

Wolpert, D. H. (1992). Stacked generalization. *Neural Networks*, 5(2):241–259.

Yoon, J., Zame, W. R., Banerjee, A., Cadeiras, M., Alaa, A. M., and van der Schaar, M. (2018a). Personalized survival predictions via trees of predictors: An application to cardiac transplantation. *PLOS ONE*, 13(3):e0194985.

Yoon, J., Zame, W. R., and van der Schaar, M. (2018b). ToPs: Ensemble learning with trees of predictors. *IEEE Transactions on Signal Processing*, 66(8):2141–2152.

APPENDIX

Hyperparameter Tuning

In this Appendix, we outline the hyperparameter tuning procedure employed to optimise our predictors. It is important to note that we perform hyperparameter tuning for each cross-validation split and loss function evaluated.

We implement our hyperparameter tuning procedure using the state-of-the-art Bayesian Optimisation framework SMAC3 (Lindauer et al., 2022). We employ the Hyperparameter Tuning facade, which uses Random Forest as a surrogate model.

However, due to their substantial runtime, conducting a comprehensive hyperparameter tuning procedure is not feasible within our constraints for both PTEs and ToPs. Instead, we focus on tuning the hyperparameters of their respective base learners on the specific dataset at hand. Although the optimal base learner parameters for standalone use may differ from those for ensemble methods, we assume that they are a reasonable approximation.

Furthermore, we choose $\texttt{min\_leaf\_samples} = 100$, slightly higher than (Torgo, 1997a) to mitigate overfitting. As done in (Yoon et al., 2018b), we set $\texttt{val1\_size} = 0.15$ and $\texttt{val2\_size} = 0.1$.

In Table 8 we present the search space we set for hyperparameter optimisation. For hyperparameters not mentioned in this table, we rely on the default values as provided by the scikit-learn library.

Table 8: Hyperparameter search spaces.

Classifier	Hyperparameter	Search Space
Random Forest	*n_estimators*	$\{i \mid i \in \mathbb{N} \wedge 10 \leq i \leq 1000\}$
	criterion	$\{$"*gini*", "*log_loss*"$\}$
	max_depth	$\{i \mid i \in \mathbb{N} \wedge 3 \leq i \leq 10\}$
AdaBoost	*n_estimators*	$\{i \mid i \in \mathbb{N} \wedge 25 \leq i \leq 200\}$
	learning_rate	$[0.5, 2.0]$
Logistic Regression	*penalty*	$\{$"*l2*", "*none*"$\}$
	C	$[0.5, 5.0]$

Proof of the Computational Complexity

Proof of Computational Complexity for One Recursive Step

Statement: For a single recursive step of our method the computational complexity is given by

$$O\left(nd\sum_{i=1}^{m}\left(T_i\left(n,d\right)\right) + \sum_{j=1}^{m_{CD}}\left(T_j^{CD}\left(n,d\right)+\sum_{i=1}^{m}\left(T_i\left(n,d\right)\right)\right)\right) \quad (5)$$

Proof. Each recursive step consists of two main parts. First, we create candidate splits of the feature space as in ToPs. Second, we create candidate Class Dichotomies.

The computational complexity of the splitting of the feature space is shown in (Yoon et al., 2018b) to be

$$O\left(nd\sum_{i=1}^{m}T_i\left(n,d\right)\right). \quad (6)$$

When creating a candidate Class Dichotomy for an algorithm $A_j \in \mathcal{A}_{CD}$, we use the Random Pair method to obtain the two meta-classes. In this process, we require one execution of A_j to obtain h_{c^-,c^+}, which is used to determine the meta-classes. Subsequently, another execution of A_j is required to obtain the meta-classifier $h_{\mathcal{Y}^-,\mathcal{Y}^+}$. Additionally, we need to select the classifiers $h_{\mathcal{Y}^-}$ and $h_{\mathcal{Y}^+}$. Both of these require one execution each of every algorithm $A \in \mathcal{A}$. In total, we arrive at a complexity of

$$O\left(2\cdot T_j^{CD}\left(n,d\right)+2\cdot\sum_{i=1}^{m}\left(T_i\left(n,d\right)\right)\right) = O\left(T_j^{CD}\left(n,d\right)+\sum_{i=1}^{m}\left(T_i\left(n,d\right)\right)\right) \quad (7)$$

for the creation of a single Class Dichotomy. Since we repeat this procedure for every $A_j \in \mathcal{A}_{CD}$ we obtain the complexity

$$O\left(\sum_{j=1}^{m_{CD}}\left(T_j^{CD}\left(n,d\right)+\sum_{i=1}^{m}\left(T_i\left(n,d\right)\right)\right)\right). \quad (8)$$

Adding the complexity $O\left(nd\sum_{i=1}^{m}\left(T_i\left(n,d\right)\right)\right)$ of splitting the feature space we obtain

$$O\left(nd\sum_{i=1}^{m}\left(T_i\left(n,d\right)\right) + \sum_{j=1}^{m_{CD}}\left(T_j^{CD}\left(n,d\right)+\sum_{i=1}^{m}\left(T_i\left(n,d\right)\right)\right)\right). \quad (9)$$

Proof of Computational Complexity for an Entire Partition Tree Ensemble

Statement: For constructing an entire Partition Tree Ensemble the computational complexity is given by

$$O\left(n\left(nd\sum_{i=1}^{m}\left(T_i\left(n,d\right)\right) + \sum_{j=1}^{m_{CD}}\left(T_j^{CD}\left(n,d\right)+\sum_{i=1}^{m}\left(T_i\left(n,d\right)\right)\right)\right)\right). \quad (10)$$

Proof. To prove this, we must consider the maximum number of possible recursions. We know that there cannot be more recursive calls than the number of nodes in the tree. Furthermore, we understand that every leaf node of our Partition Tree contains at least one sample. Since there are n samples in total, the tree can have at most n leaves. In Partition Trees, a node only has children if we split it, in which case it has two children. Therefore, Partition Trees are full binary trees. Consequently, the number of recursive calls is at most $2n-1$. This leads us to the overall computational complexity of

$$\begin{aligned} &O(2n-1(nd\sum_{i=1}^{m}T_i(n,d)+\sum_{j=1}^{m_{CD}}(T_j^{CD}(n,d) + \sum_{i=1}^{m}T_i(n,d)))) \\ &= O\Big(n\Big(nd\sum_{i=1}^{m}T_i(n,d)+\sum_{j=1}^{m_{CD}}\Big(T_j^{CD}(n,d) + \sum_{i=1}^{m}T_i(n,d)\Big)\Big)\Big). \end{aligned} \quad (11)$$