ToPs: Ensemble Learning with Trees of Predictors

Jinsung Yoon, William R. Zame, and Mihaela van der Schaar, Fellow, IEEE

Abstract—We present a new approach to ensemble learning. Our approach constructs a tree of subsets of the feature space and associates a predictor (predictive model) - determined by training one of a given family of base learners on an endogenously determined training set - to each node of the tree; we call the resulting object a tree of predictors. The (locally) optimal tree of predictors is derived recursively; each step involves jointly optimizing the split of the terminal nodes of the previous tree and the choice of learner and training set (hence predictor) for each set in the split. The feature vector of a new instance determines a unique path through the optimal tree of predictors; the final prediction aggregates the predictions of the predictors along this path. We derive loss bounds for the final predictor in terms of the Rademacher complexity of the base learners. We report the results of a number of experiments on a variety of datasets, showing that our approach provides statistically significant improvements over state-of-the-art machine learning algorithms, including various ensemble learning methods. Our approach works because it allows us to endogenously create more complex learners - when needed - and endogenously match both the learner and the training set to the characteristics of the dataset while still avoiding over-fitting.

Index Terms—Ensemble learning, Model tree, Personalized predictive models

I. INTRODUCTION

ENSEMBLE methods [1], [2], [3], [4] are general techniques in machine learning that combine several learners to create a more accurate learner (such as bagging [4], [6], boosting [8], [9] and stacking [10]). Ensemble methods frequently improve performance. We develop a novel approach to ensemble learning that chooses the learners to be used (from a given set of base learners), the way in which these learners should be trained to create predictors (predictive models), and the way in which the predictions of these predictors should be combined according to the features of an instance for which a prediction is desired. By jointly deciding which features, training sets and learners to use we provide a novel method to grow complex predictors; by deciding how to aggregate these predictors we control overfitting. We derive loss bounds and present a variety of experiments demonstrating that our algorithm achieves substantial and statistically significant improvements over state-of-the-art methods.

Given a feature space $X$, a label set $Y$, a dataset $D = \{(x', y')\}$ of instances (assumed to be drawn i.i.d. from a true distribution $\mathcal{D}$), and a set $\mathcal{A}$ of algorithms (hypothesis classes, learners), our procedure partitions the dataset $D = S \cup V^1 \cup V^2$ into a training set and two validation sets, and constructs a tree of predictors; i.e. a tree $T$ of subsets of $X$ and an assignment of a predictor (predictive model) $C \rightarrow h_C$ to each set $C \in T$. The locally optimal tree of predictors is constructed for each terminal node $C$ of the previous tree, we choose a feature and a threshold to split $C = C^- \cup C^+$ and choose algorithms $A^-, A^+$ and training sets $S^-, S^+$ to obtain predictors $h^-, h^+$; we jointly choose the feature, threshold, algorithms and training sets in order to minimize the total empirical loss. After constructing the locally optimal tree of predictors, we construct the overall prediction for each feature $x$ by aggregating the predictions along the (unique) path $\Pi(x)$ from the initial node $X$ to the (unique) terminal node that contains $x$: $H(x) = \sum_{C \in \Pi(x)} w^*(C, \Pi(x)) h_C(x)$, where the weights $w^*(C, \Pi)$ are computed by linear regression using the second validation set $V^2$. (The weights depend on the path $\Pi(x)$ but not on the particular feature vector $x$.) Importantly, note that if $x, x'$ belong to the same terminal node then they determine the same path $\Pi(x) = \Pi(x')$ and hence the same predictors $\{h_C\}_{C \in \Pi(x)} = \{h_C\}_{C \in \Pi(x')}$, the same weights $w^*(C, \Pi(x)) = w^*(C, \Pi(x'))$ and hence the same overall predictor $H = \sum_{C \in \Pi(x)} w^*(C, \Pi(x)) h_C = \sum_{C \in \Pi(x)} w^*(C, \Pi(x')) h_C$ - but, in general, not the same predictions: $H(x) \neq H(x')$. This is because the predictors $h_C$ are not constant (on the nodes to which they are associated) and so the predictions $h_C(x), h_C(x')$ - and a fortiori the aggregate predictions $H(x), H(x')$ - will depend on the entire array of features and not just the nodes to which these features belong.

One of our experiments – prediction of survival while wait-listed for a heart transplant – provides a good illustration of our approach. (For more discussion, see Section [V] and [V].) In that setting features $X$ are patient characteristics and labels $Y$ are survival times. The data set $D$ consists of records of actual patients; a single data point $= (x^t, y^t)$ records that a patient with features $x^t$ survived for time $y^t$. The construction of our algorithm demonstrates that the best predictor of survival for males is different than the best predictor of survival for females. In particular, predictions of survival for a male and a female with otherwise similar features may be quite different – because the features that influence survival have different importance and interact differently for males and females. Using a gender-specific predictor leads to significant improvement in prediction accuracy.

Section [III] provides a full description of our method. Section [IV] derives loss bounds. Section [V] compares the performance of our method with that of many other methods on a variety of datasets; we demonstrate that our method provides substantial and statistically significant improvement. Section [V] details the operation of our algorithm for one of the datasets to reveal why our method works. Section [V] highlights the differences between our method and related machine learning methods. Section [VII] concludes. All the proofs can be found in the
Appendix (at the end of the manuscript), and parameters of the experiments and additional figures can be found in the Supplementary Materials.

II. ToPs

We work in a supervised setting so data is presented as a pair \((x, y)\) consisting of a feature and a label. We are presented with a (finite) dataset \(D = \{(x^i, y^i)\}\), assumed to be drawn iid from the true distribution \(D\), and seek to learn a model that predicts, for a new instance drawn from \(D\) and for which we observe the feature vector \(x\), the true label \(y\). We assume the space of features is \(X = X_1 \times \cdots \times X_d\); if \(x \in X\) then \(x_i\) is the \(i\)-th feature. Some features are categorical, others are continuous. For convenience (and without much loss of generality) we assume categorical features are binary and represented as \(0, 1\) and that continuous features are normalized between \(0, 1\); hence \(X_i \subset [0, 1]\) for every \(i\) and \(X \subset [0, 1]^d\). We also take as given a set \(Y \subset \mathbb{R}\) of labels. For \(Z \subset X\), a predictor (predictive model) on \(Z\) is a map \(h : Z \to Y\); we interpret \(h(z)\) as the predicted expectation of \(y\) given \(z\). (We suppress \(Z\) when \(Z = X\) or when \(Z\) is understood.) If \(h_1 : Z_1 \to Y, h_2 : Z_2 \to Y\) are predictors and \(Z_1 \cap Z_2 = \emptyset\) we define \(h_1 \vee h_2 : Z_1 \cup Z_2 \to Y\) by \(h_1 \vee h_2(z) = h_i(z)\) if \(z \in Z_i\).

We take as given a finite family \(A = \{A_1, \ldots, A_M\}\) of algorithms or hypothesis classes or learners. We interpret an algorithm as including the parameters of that algorithm (if any); thus Random Forest with 100 trees is a different algorithm than Random Forest with 200 trees. Given an algorithm \(A \in A\) and a set \(E \subset D\) to be used to train \(A\), we write \(A(E)\) for the resulting predictor. If \(E\) is a family of subsets of \(D\) then we write \(A(E) = \{A(E) : A \in A, E \in \mathcal{E}\}\) for the set of predictors that can arise from training some algorithm \(A\) on some set in \(\mathcal{E}\).

A tree of predictors is a pair \((\mathcal{T}, \{h_C\})\) consisting of a family \(\mathcal{T}\) of non-empty subsets of \(X\) together with an assignment \(C \mapsto h_C\) of a predictor \(h_C : C \to Y\) to each element of \(\mathcal{T}\) such that:

(i) \(X \in \mathcal{T}\).

(ii) With respect to the ordering induced by set inclusion, \(\mathcal{T}\) forms a tree; i.e., \(\mathcal{T}\) is partially ordered in such a way that each \(C \in \mathcal{T}\), \(C \neq X\) has a unique immediate predecessor. As usual, we refer to the elements of \(\mathcal{T}\) as nodes. Note that \(X\) is the initial node.

(iii) If \(C \in \mathcal{T}\) is not a terminal node then the set \(C^{\text{succ}}\) of immediate successors of \(C\) is a partition of \(C\).

(iv) For each node \(C \in \mathcal{T}\) there is an algorithm \(A_C \in A\) and a node \(C^* \in \mathcal{T}\) such that \(C \subset C^*\) (so that either \(C = C^*\) or \(C^*\) precedes \(C\) in \(\mathcal{T}\)) such that \(h_C = A_C(C^*)\) is the predictor formed by training the algorithm \(A_C\) on the training set \(C^*\).

It follows from these requirements that for any two nodes \(C_1, C_2 \in \mathcal{T}\) exactly one of the following must hold: \(C_1 \subset C_2\) or \(C_2 \subset C_1\) or \(C_1 \cap C_2 = \emptyset\). It also follows that the set of terminal nodes forms a partition of \(X\). For any node \(C\) we write \(C^+\) for the set consisting of \(C\) and all its predecessors. For \(C \in \mathcal{T}\) we write \(C(x)\) for the unique terminal node that contains \(x\) and \(\Pi(x) = \Pi(C(x))\) for the unique path in \(\mathcal{T}\) from the initial node \(X\) to the terminal node \(C(x)\). We write \(\mathcal{T}\) for the set of all terminal nodes.

We fix a partition of the given dataset as \(D = S \cup V^1 \cup V^2\); we view \(S\) as the (global) training set and \(V^1, V^2\) as (global) validation sets. In practice, the partition of \(D\) into training and validation sets will be chosen randomly. Given a set \(C \subset X\) of feature vectors and a subset \(Z \subset D\), we write \(Z(C) = \{(x^i, y^i) \in D : x^i \in C\}\).

We express performance in terms of loss. For many problems, an appropriate measure of performance is the Area Under the (receiver operating characteristic) Curve (AUC); for a given set of data \(Z \subset D\) and predictor \(h : Z(X) \to Y\) the loss is \(L(h, Z) = 1 - \text{AUC}\). For other problems, an appropriate measure of loss is the sample mean error \(L(h, Z) = \frac{1}{|Z|} \sum_{(x^i, y^i) \in Z} |h(x^i) - y^i|\). For our general model, we allow for an arbitrary loss function. Given disjoint sets \(Z_1, \ldots, Z_N\) and predictors \(h_i\) on \(Z_i\), we measure the total (joint) loss as \(L(\bigvee h_i, \bigcup Z_i)\). Note that the loss function need not be additive, so in general \(L(\bigvee h_i, \bigcup Z_i) \neq \sum L(h_i, Z_i)\).

A. Growing the (Locally) Optimal Tree of Predictors

We begin with the tree of predictors \(\{\{X\}, \{X\}\}\) where \(h_X\) is the predictor \(h \in A(S)\) that minimizes the loss \(L(h, V^1(X))\). Note that we are training \(h\) globally – on the entire training set – and evaluating/validating it globally – on the entire (first) validation set – because the initial node consists of the entire feature space. We now grow the tree of predictors by a recursive splitting process. Fix the tree of predictors \((\mathcal{T}, \{h_C\})\) constructed to this point. For each terminal node \(C \in \mathcal{T}\) with its associated predictor \(h_C\), choose a feature \(i\) and a threshold \(\tau_i \in [0, 1]\). (In practice, this involves discretizing each feature space; we assume this to have been done.) Write

\[
C^-(\tau_i) = \{x \in C : x_i < \tau_i\} \\
C^+(\tau_i) = \{x \in C : x_i \geq \tau_i\}
\]

Evidently \(C^-(\tau_i), C^+(\tau_i)\) are disjoint and \(C = C^-(\tau_i) \cup C^+(\tau_i)\), so we are splitting \(C\) according to the feature \(i\) and the threshold \(\tau_i\). Note that \(C^-(\tau_i) = \emptyset\) if \(\tau_i = 0\); in this case we are not properly splitting \(C\). For each of \(C^-(\tau_i), C^+(\tau_i)\) we choose predictors \(h_i \in A(C^-(\tau_i)), h_i^* \in A(C^+(\tau_i))\).

(That is, we choose predictors that arise from one of the learners \(A \in A\), trained on some node that (weakly) precedes the given node.) We then choose the feature \(i^*\), the threshold \(\tau_i^*\), and the predictors \(h_{C^-(\tau_i^*)}, h_{C^+(\tau_i^*)}\) to minimize the total loss on \(V^1\); i.e. we choose them to solve the minimization problem

\[
\arg \min_{i, \tau_i, h^-, h^+} L\left(h_i \vee h_i^*, V^1(C^-(\tau_i)) \cup V^1(C^+(\tau_i))\right)
\]

subject to the requirement that this total loss should be strictly less than \(L(h_C, V^1(C))\). Note that because choosing the threshold \(\tau_i = 0\) does not properly split \(C\), the loss \(L(h_C, V^1(C))\) can always be achieved by setting \(\tau_i = 0\) and

---

1In principle, the predictive model \(h_C\) and/or the algorithm \(A_C\) and the node \(C^*\) might not be unique. In that case, we can randomly choose randomly among the possibilities. Because this seems an unusual situation, we shall ignore it and similar indeterminacies that may occur at other points of the construction.
Algorithm 1 Growing the Optimal Tree of Predictors

Input: Feature space $X$, a set of algorithms $A$, training set $S$, the first validation set $V^1$

First step:
Initial tree of predictors $= (X, h_X)$, where $h_X = \arg \min_{A \in A} L(A(S), V^1)$

Recursive step:
Input: Current tree of predictors $= (\cal T, \{h_C\})$

For each terminal node $C \in \cal T$

For a feature $i$ and a threshold $\tau_i \in [0,1]$

Set $C^-(\tau_i) = \{ x \in C : x_i < \tau_i \}$

$C^+(\tau_i) = \{ x \in C : x_i \geq \tau_i \}$

Then, $\{i^*, \tau_i^*, h_C^-(\tau_i), h_C^+(\tau_i)\} = \arg \min L(h^\top \lor h^+, V^1(C^-(\tau_i)) \lor V^1(C^+(\tau_i)))$

Output: Locally optimal tree of predictors $= (\cal T, \{h_C\})$

End For

End For

Stopping criterion:
$L(h_C, V^1(C)) \leq \min L(h^- \lor h^+, V^1(C^-(\tau_i)) \lor V^1(C^+(\tau_i)))$

Output: Locally optimal tree of predictors $= (\cal T, \{h_C\})$

$w^+ = h_C$. If there is no proper splitting that yields a total loss smaller than $L(h_C, V^1(C))$ we do not split this node. This yields a new tree of predictors. We stop the entire process when no terminal node is further split; we refer to the final object as the locally optimal tree of predictors. (We use the adjective “locally” because we have restricted the splitting to be by a single feature and a single threshold and because the optimization process employs a greedy algorithm – it does not look ahead.)

B. Weights on the Path

Fix the locally optimal tree of predictors $= (\cal T, \{h_C\})$ and a terminal node $C$, let $\Pi$ be the path from $X$ to $C$. We consider vectors $w = (w(\Pi, C))_{C \in \Pi}$ of non-negative weights summing to one; for each such weight vector we form the predictor $H_w = \sum_{C \in \Pi} w(C, \Pi) h_C$. We choose the weight vector $w^*(\Pi)$ that minimizes the empirical loss of $H_w$ on the second validation set $V^2$; i.e.:

$w^*(\Pi) = \arg \min_w L(H_w, V^2(C))$

By definition, the weights depend on the path and not just on the node; the weights assigned to a node $C$ along different paths may be different.

C. Overall Predictor

Given the locally optimal tree of predictors $= (\cal T, \{h_C\})$ and the optimal weights $= \{w^*(\Pi)\}$ for each path, we define the overall predictor $H : X \rightarrow \mathbb{R}$ as follows: Given a feature $x$, we define

$H(x) = \sum_{C \in \Pi(x)} w^*(\Pi(x), C) h_C(x)$

Algorithm 2 Weights on the Path

Input: Locally optimal tree of predictors $= (\cal T, \{h_C\})$, second validation set $V^2$

For each terminal node $C$ and the corresponding path $\Pi$ from $X$ to $C$

For each weight vector $w = (w_C)$,

Define $H_w = \sum_{C \in \Pi} w(C) h_C$. Then,

$w^*(\Pi) = \arg \min \ L(H_w, V^2(C))$

End For

Output: Optimized weights $w^*(\Pi)$ for each terminal node $C$ and corresponding path $\Pi$

Algorithm 3 Overall Predictor

Input: Locally optimal tree of predictions $= (\cal T, \{h_C\})$, optimized weights $= \{w^*(\Pi)\}$, and testing set $T$

Given a feature vector $x$,

Find unique path $\Pi(x)$ from $X$ to terminal node containing $x$;

Then

$H(x) = \sum_{C \in \Pi(x)} w^*(\Pi, C) h_C(x)$

Output: The final prediction $H(x)$

That is, we compute the weighted sum of all predictions along the path $\Pi(x)$ from the initial node to the terminal node that contains $x$.

Note that we construct predictors by training algorithms on (subsets of) $S$ but we construct the locally optimal tree by minimizing losses with respect to (subsets of) the validation set $V^1$; this avoids overfitting to the training set $S$. We then construct the weights, hence the overall predictor, by minimizing losses with respect to (subsets of) the validation set $V^2$; this avoids overfitting to the validation set $V^1$. The pseudo-codes of the entire ToPs algorithms are in Algorithm 1, 2 and 3.

D. Instantiations

It is important to keep in mind that we take as given a family $A$ of base learners (algorithms). Our method is independent of the particular family we use, but of course, the final overall predictor is not. We use ToPs to refer to our general method and to ToPs/A to refer to a particular instantiation of the method, built on top of the family $A$ of base learners; e.g., ToPs/LR is the instantiation build on Linear Regression as the sole base learner. In our experiments, we compare the performance of two different instantiations of ToPs.

E. Computational Complexity

The computational complexity of constructing the tree of predictors is $\sum_{i=1}^{M} O(N^2 D \times T_i(N, D))$ where $N$ is the number of instances, $D$ is the number of features, $M$ is the number of algorithms and $O(T_i(N, D))$ is the computational complexity of the $i$-th algorithm. (The proof is in the Appendix.) For instance, the computational complexity of ToPs/LR is $O(N^3 D^3)$. The computational complexity of finding the weights is low in comparision with constructing the tree of
predic tators because it is just a linear regression. In all our simulations, the entire training time was less than 12 hours using an Intel 3.2GHz i7 CPU with 32GB RAM. Testing can be done in real-time without any delay.

III. LOSS BOUNDS

In this Section, we show how the Rademacher complexity of the base learners can be used to provide loss bounds for our overall predictor. Throughout this section we assume the loss function is the sample mean of individual losses: \( L(h, Z) = \frac{1}{|\mathcal{Z}|} \sum_{z \in \mathcal{Z}} \ell(h(z), z) \), and that the individual loss is a convex function of the difference \( \ell(h, z) = \ell(h(x) - z) \) where \( \ell \) is convex. Note that mean loss and mean square loss satisfy these assumptions. Recall that for each node \( C \), \( A_C \) is the base learner (hypothesis class) used to construct the predictor \( h_C \) associated to the node \( C \) and that for a terminal node \( \overline{C} \) we write \( \Pi(\overline{C}) \) for the path from \( X \) to \( \overline{C} \). We first present an error bound for each individual terminal node and then derive an overall error bound. (Proofs are in the Appendix.) We write \( \mathcal{R}(A_C, S(\overline{C})) \) for the Rademacher complexity of \( A_C \) with respect to the portion of the training set \( S(\overline{C}) \) and \( \mathbb{E}[L(H)] \) for the expected loss of the overall predictor \( H \) with respect to the true distribution when features are restricted to lie in \( \overline{C} \) and \( \mathbb{E}[L(H)] \) for the expected loss of the overall predictor \( H \) with respect to the true distribution.

**Theorem 1.** Let \( H \) be the overall predictor and let \( \overline{C} \) be a terminal node of the locally optimal tree. For each \( \delta > 0 \), with probability at least \( 1 - \delta \) we have

\[
\mathbb{E}[L(H)] \leq L(H, S(\overline{C})) + 2 \max_{C \in \Pi(\overline{C})} \mathcal{R}(A_C, S(\overline{C})) + 4 \sqrt{\frac{2 \log(4/\delta)}{|S(\overline{C})|}}
\]

Note that the Rademacher complexity term is at most the maximum of the Rademacher complexities of the learners used along the path from \( X \) to \( \overline{C} \).

**Corollary 1.1.** Let \( H \) be the overall predictor. For each \( \delta > 0 \), with probability at least \( 1 - \delta \),

\[
\mathbb{E}[L(H)] \leq \frac{1}{n} \sum_{\overline{C} \in \mathcal{T}} |S(\overline{C})| \times \left[ L(H, S(\overline{C})) + 2 \max_{C \in \Pi(\overline{C})} \mathcal{R}(A_C, S(\overline{C})) + 4 \sqrt{\frac{2 \log(4/\delta)}{|S(\overline{C})|}} \right]
\]

where \( n = \sum_{\overline{C} \in \mathcal{T}} |S(\overline{C})| \).

IV. EXPERIMENTS

In this Section, we compare the performance of two instantiations of ToPs – ToPs/LR (built on Linear Regression as the single base learner) and ToPs/B (built on the set \( B = \{ \text{AdaBoost, Linear Regression, Logistic Regression, Logit Boost, Random Forest} \} \) of base learners) – against the performance of state-of-the-art algorithms on four publicly available data sets: MNIST, Bank Marketing and Popularity of Online News datasets from UCI, and publicly available medical dataset (survival while waitlisted for a transplant). Considering two instantiations of ToPs allows us to explore the source of the improvement yielded by our method over other algorithms. In the following subsections, we describe the datasets and the performance comparisons; the exploration of the source of improvement is in Section V.

A. MNIST

Here we use the MNIST OCR-49 dataset [13]. The entire MNIST dataset consists of 70,000 samples with 400 continuous features which represent the image of a hand-written number from 0 to 9. Among 70,000 samples, we only use the 13,782 samples which represent 4 and 9; we treat 4 as label 0 (42.4%) and 9 as label 1 (57.6%). Each sample records all 400 features of a hand-written number image and the label of the image. There is no missing information. The objective is to classify, from the hand-written image features, whether the image represents 4 or 9. For ToPs we further divided the training samples into a training set \( S \) and validation sets \( V^1, V^2 \) in the proportions 75%-15%-10% (same with all datasets). For comparisons, we use the results given in [13] for various instantiations of DeepBoost, AdaBoost and LogitBoost and two model trees [12], [11] as benchmarks. To be consistent with [14], we use the error rate as the loss function. Table I presents the performance comparisons: the column Gain1 shows the performance gain of ToPs/B over all the other algorithms; the column Gain2 shows the performance gain of ToPs/LR over all the other algorithms except ToPs/B (The table is exactly as in [14] with ToPs/B and ToPs/LR added). ToPs and ToPs/LR have 14.1% and 5.6% gains from the best benchmark (DeepBoost with Stump) and these are statistically significant improvements \((p < 0.01)\). We also compared the performance of ToPs on the entire MNIST dataset using a depth 6 CNN (AlexNet with 3 convolution nets and 3 max pooling nets). The loss of ToPs is 0.0081; this is slightly worse than CNN (0.0068) but much
better than the best ensemble learning benchmark, XgBoost (0.0103). Keep in mind that CNN’s are designed for spatial tasks such as character recognition, while ToPs is a general-purpose method; as we shall see in later subsections, ToPs outperforms neural networks for other tasks.

B. Bank Marketing

For this comparison, we use the UCI Bank Marketing dataset [13]. This dataset consists of 41,188 samples with 62 features; 10 of these features are continuous, and 52 are binary. Each sample records all 62 features of a particular client and whether the client accepted a bank marketing offer (a particular term deposit account). There is no missing information. In this case, the objective is to predict, from the client features, whether or not the client would accept the offer. (In the dataset 11.3% of the clients accepted and the remaining 88.7% declined.) To evaluate performance, we conduct 10 iterations of 5-fold cross-validation. Because the dataset is unbalanced, we use 1 – AUC as the loss function.

Table II shows the overall performance of the our two instantiations of ToPs and 13 comparison machine-learning algorithms: Model trees [12], AdaBoost [9], Decision Trees (DT), Deep Boost [14], LASSO, Linear Regression (LR), Logistic Regression (Logit), LogitBoost [16], Neural Networks [17], Random Forest (RF) [5], Support Vector Machines (SVM) and XGBoost [18]. ToPs/LR outperforms all of the benchmarks by more than 10% and ToPs/B outperforms all of the benchmarks by more than 20%. (Significance levels p < 0.01.) In Section V, we show the locally optimal trees of predictors for this setting (Figures 1 and 2) and discuss the source of performance gain of ToPs.

C. Popularity of Online News

Here we use the UCI Online News Popularity dataset [15]. This dataset consists of 39,397 samples with 57 features (43 continuous, 14 binary). Each sample records all 57 features of a particular news item and the number of times the item was shared. There is no missing information. The objective is to predict, from the news features, whether or not the item would be popular – defined to be “shared more than 5,000 times.” (In the dataset 12.8% of the items are popular; the remaining 87.2% are not popular.) To evaluate performance of all algorithms, we conduct 10 iterations of 5-fold cross-validation. As it can be seen in Table III, ToPs/LR and ToPs/B both outperform all the other machine learning algorithms: ToPs/B achieves a loss (measured as 1 − AUC) of 0.2689, which is 7.2% lower than the loss achieved by the best competing benchmark. (p-value< 0.01 for all benchmarks.)

D. Heart Transplants

The UNOS (United Network for Organ Transplantation) dataset (available at https://www.unos.org/data/) provides information about the entire cohort of 36,329 patients (in the U.S.) who were on a waiting list to receive a heart transplant but did not receive one, during the period 1985-2015. Patients in the dataset are described by a total of 334 clinical features, but much of the feature information is missing, so we discarded 301 features for which more than 10% of the information was missing, leaving us with 33 features – 14 continuous and 19 binary. To deal with the missing information, we used 10 multiple imputations using Multiple Imputation by Chained Equations (MICE) [19]. In this setting, the objective(s) are to predict survival for time horizons of 3 months, 1 year, 3 years and 10 years. (In the dataset, 68.3% survived for 3 months, 49.5% survived for 1 year, 28.3% survived for 3 years, and 6.9% survived for 10 years.) To evaluate performance, we divided the patient data based on the admission year: we took patients admitted to a waiting list in 1985-1999 as the training sample and patients admitted in 2000-2015 as the testing sample. In this case, we compared the performance of ToPs with the same machine-learning algorithms as before and also against the three most widely-employed medical scoring methods: Heart Failure Survival Score (HFSS) [20], Meta-Analysis Global Group in Chronic Heart Failure (MAGGIC) [21] and Seattle Heart Failure Model (SHFM) [22]. Once again, both ToPs/LR and ToPs/B outperform all the other machine learning algorithms; as we shall see in later subsections, ToPs outperforms neural networks for other tasks.

| Algorithms | Loss | Gain1 | Gain2 |
|------------|------|-------|-------|
| ToPs/LR    | 0.4028* | -     | -     |
| ToPs/B     | 0.3081 | -     | -     |

*: p-value < 0.01

| Algorithms | Loss | Gain1 | Gain2 |
|------------|------|-------|-------|
| ToPs/LR    | 0.2801 | -     | -     |
| ToPs/B     | 0.2689 | -     | -     |

*: p-value < 0.01
### Table IV

| Algorithms | 3-month mortality | 1-year mortality |
|------------|-------------------|------------------|
|            | Loss | Gain1 | Gain2 | Loss | Gain1 | Gain2 |
| ToPs/B     | 0.207 | - | 0.181 | 0.207 | - | - |
| ToPs/LR    | 0.231 | 10.4% | - | - | 12.6% | - |

### Table V

| Algorithms | 3-year mortality | 10-year mortality |
|------------|-------------------|-------------------|
|            | Loss | Gain1 | Gain2 | Loss | Gain1 | Gain2 |
| ToPs/B     | 0.177 | - | - | 0.175 | - | - |
| ToPs/LR    | 0.201 | 11.9% | - | - | 13.8% | - |

|            | Loss | Gain1 | Gain2 | Loss | Gain1 | Gain2 |
|------------|-------------------|------------------|
| AdaBoost   | 0.229 * | 22.7% | 12.2% | 0.237 * | 26.2% | 14.3% |
| DTrees     | 0.287 * | 38.3% | 30.0% | 0.249 * | 29.7% | 18.5% |
| DeepBoost  | 0.219 * | 19.2% | 8.2% | 0.213 * | 17.8% | 4.7% |
| LASSO      | 0.248 * | 28.6% | 19.0% | 0.228 * | 23.2% | 11.0% |
| LR         | 0.264 * | 33.0% | 23.9% | 0.285 * | 38.6% | 28.8% |
| Logit      | 0.249 * | 28.9% | 19.3% | 0.236 * | 25.8% | 14.0% |
| LogitBoost | 0.221 * | 19.9% | 9.0% | 0.229 * | 23.6% | 11.4% |
| NeuralNets | 0.225 * | 21.3% | 10.7% | 0.221 * | 20.8% | 8.1% |
| Random Forest | 0.217 * | 18.4% | 7.4% | 0.225 * | 22.2% | 9.8% |
| SVM        | 0.218 * | 18.8% | 7.8% | 0.284 * | 38.4% | 28.5% |
| XGBoost    | 0.223 * | 20.6% | 9.9% | 0.226 * | 22.6% | 10.2% |
| HFSS       | 0.377 * | 53.1% | 46.7% | 0.381 * | 54.1% | 46.7% |
| MAGGIC     | 0.352 * | 49.7% | 42.9% | 0.351 * | 50.1% | 42.2% |
| SHFM       | 0.376 * | 52.9% | 46.5% | 0.388 * | 54.9% | 47.7% |

*: p-value < 0.01

As the experiments show, our method yields significant performance gains over a large variety of existing machine learning algorithms. More specifically, as it can be seen in Table IV and V, ToPs/B achieves losses (measured as 1 – AUC) between 0.175 and 0.207; these improve by 17.9% to 22.3% over the best machine learning benchmarks and by 43.4% to 50.1% over the best medical score (p-value < 0.01). The figures for locally optimal trees of predictors for ToPs can be found in the Supplementary Materials.

V. Discussion

As the experiments show, our method yields significant performance gains over a large variety of existing machine learning algorithms. These performance gains come from the concatenation of a number of different factors. To aid in the discussion, we focus on the Bank Dataset and refer to Figures 1 and 2, which show the locally optimal trees of predictors grown by ToPs/LR and ToPs/B, respectively. For ToPs/B, which uses multiple learners, we show, in each node, the learner assigned to that node; for both ToPs/LR and ToPs/B we indicate the training set assigned to that node: For instance, in Figure 2 Random Forest is the learner assigned to the initial node; the training set is necessarily the entire feature space X. In subsequent nodes, the training set is either the given node (if there is no marker) or the immediately preceding node (if the node is marked with a single up arrow) or the node preceding that (if the node is marked with two up arrows), and so forth. Note that different base learners and/or different training sets are used in various nodes. In each non-terminal node we also show the improvement Δv in loss (computed with respect to V1) obtained in splitting into the two immediate successor nodes. (By construction, we split exactly when improvement...
is possible so $\Delta_v > 0$ at every non-terminal node and $\Delta_v = 0$ at terminal nodes.) At the terminal nodes (shaded), we show the loss improvement $\Delta_t$ achieved on that node (that set of features) that is obtained by using the overall predictor rather than the initial predictor. Finally, for one particular path through the tree (indicated by heavy blue arrows), we show the weights assigned to the nodes along that path in computing the overall predictor. Note that the deeper nodes do not necessarily get greater weight: using the second validation set to optimize the weights compensates for overfitting deeper in the tree.

The first key feature of our construction is that it identifies a family of subsets of the feature space – the nodes of the locally optimal tree – and optimally matches training sets to the nodes. Moreover, as Figures 1 and 2 make clear, the optimal training set at the node $C$ need not be the node $C$ itself, but might be one of its predecessor nodes. For ToPs/LR it is this matching of training sets to nodes that gives our method its power: if we were to use the entire training set $S$ at every node, our final predictor would reduce to simple Linear Regression – and as Table I shows, Linear Regression performs. However, because we do match training sets to nodes, the performance of ToPs/LR is 27.1% better than that of Linear Regression.

The second key feature of our construction is that it also optimally matches learners to the nodes. For ToPs/LR, there is only a single base learner, so the matching is trivial (LR is matched to every node) – but for ToPs/B there are five base learners and the matching is not trivial. Indeed, as can be seen in Figure 2 of the five available base learners, four are actually used in the locally optimal tree. This explains why ToPs/B improves on ToPs/LR. Note the performance of ToPs/B might be further improved by enlarging the set of base learners. More generally it seems clear that the performance of ToPs/A depends to some extent on the set of base learners $A$.

Our recursive construction leads, in every stage, to a (potential) increase in the complexity of the predictors that can be used. For example, Linear Regression fits a linear

---

Fig. 1. The locally optimal tree of predictors for ToPs/LR applied to the Bank Marketing dataset

Fig. 2. The locally optimal tree of predictors for ToPs/B applied to the Bank Marketing dataset
function to the data; ToPs/LR fits a piecewise linear function to the data. This additional complexity raises the problem of overfitting. However, because we train on the training set $S$ and evaluate on the first validation set $V^1$, we avoid overfitting to the training set. As can be seen from Figures 1 and 2, this avoidance of overfitting is reflected in the way it limits the depth of the locally optimal tree: the growth of the tree stops when splitting no longer yields improvement on the validation set $V^1$. Although training on $S$ and evaluating on $V^1$ avoids overfitting to $S$, it leaves open the possibility of overfitting to $V^1$. We avoid this problem by using the second validation set $V^2$ to construct optimal weights and aggregating predictors along paths.

ToPs performs significantly better than the previous model trees as well. In comparison with previous model trees, the performance improvements of ToPs arise from the reasons given above: ToPs allows the learners to train either on the current node or parent nodes; ToPs allows for splitting when only one side of the split improves performance; ToPs constructs the final prediction as the weighted average of predictions along the path.

VI. METHODOLOGICAL COMPARISONS

ToPs is most naturally compared with four previous bodies of work: model trees, other tree-based methods, ensemble methods, and non-parametric regression.

A. Model trees

There are similarities between ToPs and model trees but also very substantial differences. The first works on model trees [23], [24] first construct a tree using a splitting criterion that depends on labels but not on predictions, then prunes the tree, using linear regression at a node to replace subtrees from that node. [25] constructs the tree in the same way but allows for more general learners when replacing subtrees from a node. Note that ToPs operates quite differently from all of these: it constructs the tree using a splitting criterion that depends on labels and on predictions of its base learners, and it does not prune its tree nor replace any subtrees with learners (use top-down approach).

ToPs is a very general framework that allows for an arbitrary set of base learners; ToPs/LR is the particular instantiation of ToPs for which linear regression is the only base learner used. The construction of ToPs differs in a number of important ways from the construction in all of the cited papers. [12], [11] split the tree by jointly optimizing the linear predictive model and the splits that minimize the loss or maximize the statistical differences between two splits. However, in ToPs, the potential split of a node is evaluated by training each base learner on the current node and on all parent nodes - not just the current node, as in [12], [11] - and choosing the split and the predictor that yield best overall performance (most reduce loss). This approach is important for several reasons: (1) It avoids the problem of small training sets and reduces overfitting. (2) At allows splits even when only one side of the split yields an improved performance. (3) It allows for choosing the base learner among multiple learners that best capture interactions among features. Moreover, ToPs constructs the final prediction as a weighted average of predictions along the path (with weights chosen by linear regression). Weighted averaging is important because it smooths the prediction, from the least biased model to the most biased model. Choosing the weights by linear regression is important because it is an optimizing procedure and allows the weights to depend on the data and on the accuracy of the predictors constructed. [11] also smooths by weighted averaging but they choose the weights according to the number of samples and number of features. This makes sense only with a single base learner and hence a single model complexity. With multiple models of different model complexities, it is impossible to find the appropriate aggregation weights using only the number of features and number of samples. Finally, the construction of ToPs allows for arbitrary loss functions, including loss functions such as AUC that are not sample means. This is important because loss functions such as AUC are especially appropriate for unbalanced datasets; e.g. survival in the heart transplant dataset.

B. Other tree-based methods

[Decisions trees, regression trees [26], tree bagging, random forest [5]]. These methods follow a recursive procedure, growing a tree by using features to create tentative splits and labels to choose among the tentative splits. Eventually, these methods create a final partition (the terminal nodes of the tree) and make a single uniform prediction within each set of this partition. Some of these methods construct multiple trees and hence multiple partitions and aggregate the predictions arising from each partition. Our method also follows a recursive procedure, growing a tree by using features to create tentative splits, but we then use features and labels and predictors to choose the optimal split and associated predictors. Eventually, we produce a locally optimal tree of predictors. However, the final prediction for a given new instance is not computed solely by the predictor associated with the terminal node to which the feature vector of that instance belongs, but rather by aggregating the predictions along with a path in this tree of predictors. Crucially: instances that have very different feature vectors may give rise to the same paths and hence be predicted by the same aggregate predictor but may still have very different predictions because each predictor incorporates the entire feature vector to provide the prediction.

C. Ensemble methods

[Bagging [27], boosting [9], [14], [16], [18], stacking [10], [28]]. These methods construct multiple predictive models using different training sets and then aggregate the predictions of these models according to endogenously determined weights. Bagging methods use a single base learner and choose random training sets (ignoring both features and labels). Boosting methods use a single base learner and choose a sequence of training sets to create a sequence of predictive models; the sequence of training sets is created recursively according to random draws from the entire training set but weighted by the errors of the previous predictive model. Stacking uses multiple
base learners with a single training set to construct multiple predictive models and then aggregates the predictions of these multiple predictive models. Our method uses a recursive construction to construct a locally optimal tree of predictors, using both multiple base learners and multiple training sets and constructs optimal weights to aggregate the predictions of these predictors.

D. Non-parametric regressions

[Kernel regression [29], [30], Gaussian process regression [31]]. These have in common that given a feature \( x \), they choose a training set and use that set to determine the coefficients of a linear learner/model to predict the label \( y \). Kernel regression begins with a parametrized family of kernels \( \{K_\theta\} \). For a specific vector \( \theta \) of parameters and a specific bandwidth \( b \), the regression considers the set \( B \) of data points \( (x^i, y^i) \) whose feature \( x^i \) are within the specified bandwidth \( b \) of \( x \); the predicted value of the corresponding label \( y \) is the weighted sum \( \sum_B K_\theta(x, x^i) y^i \). The optimal parameter \( \theta^* \) and bandwidth \( b^* \) can be set by training, typically using least square error as the optimization criterion. Gaussian process regression begins by assuming a Gaussian form for the kernel but with unknown mean and variance. It first uses a maximum likelihood estimator based on the entire data set to determine the mean and variance (and perhaps a bandwidth), and then uses that the Gaussian kernel to carry out a kernel regression. In both kernel regression and Gaussian process regression, the prediction for a new instance is formed by aggregating the labels associated to nearby features. In our method, the prediction for a new instance is formed by carefully aggregating the predictions of a carefully constructed family of predictors.

VII. Conclusion

In this paper, we developed a new approach to ensemble learning. We construct a locally optimal tree of predictors and construct an overall predictor by patching together weighted averages of predictors along the paths from the initial node to the various terminal nodes. Our approach allows us to endogenously match both the learner and the training set to the characteristics of the data sets while still avoiding overfitting using ensemble approach. Experiments on a variety of datasets show that this approach yields statistically significant improvements over state-of-the-art methods.

APPENDIX A

PROOF OF THEOREM 1 (BOUNDS FOR THE PREDICTIVE MODEL OF EACH TERMINAL NODE)

Proof. The definition of \( \mathcal{R}(A, S) \) is

\[
\mathcal{R}(A, S) = \frac{1}{|S|} \mathbb{E}_{\sigma = \{\pm 1\}^{|S|}} \left[ \sup_{h \in A} \sum_{z \in S} \sigma_i \times l(h, z) \right]
\]

where \( P(\sigma_i = 1) = P(\sigma_i = -1) = 0.5 \).

Let us define \( \{A_1, ..., A_p\} \) as the set of all hypothesis classes that ToPs uses.

Then, let us define hypothesis class \( A \) as follow.

\[
A = \{ h = \sum_{i=1}^p w_i \times h_i | w \in \text{simplex}, h_i \in A_i \} \]

Then,

\[
\mathcal{R}(A, S) = \frac{1}{|S|} \mathbb{E}_{\sigma = \{\pm 1\}^{|S|}} \left[ \sup_{h \in A} \sum_{z \in S} \sigma_i \times l(h, z) \right]
\]

\[
= \frac{1}{|S|} \mathbb{E}_{\sigma = \{\pm 1\}^{|S|}} \left[ \sup_{h \in A} \sum_{z \in S} \sigma_i \times \left( \sum_{j=1}^p w_j h_{j, z} \right) \right]
\]

\[
= \frac{1}{|S|} \mathbb{E}_{\sigma = \{\pm 1\}^{|S|}} \left[ \sup_{h \in A} \sum_{z \in S} \sigma_i \times \left( \sum_{j=1}^p w_j h_{j, z} \right) \right]
\]

Therefore, using the Radamacher Complexity Theorem,

\[
\mathbb{E}_D[L(h)] \leq L(h, S) + 2 \max_i \mathcal{R}(A_i, S) + 4 \sqrt{\frac{2 \log(4/\delta)}{|S|}}
\]

For each terminal node \( \bar{C} \), the predictive model is \( H = \sum_{C \in \Pi(\bar{C})} w^*(\Pi(\bar{C}), C) \times h_C \). Therefore, the upper bound of the expected loss for each terminal node \( \bar{C} \) is

\[
\mathbb{E}_{D_C}[L(H)] \leq L(H, S(\bar{C})) + 2 \max_{C \in \Pi(\bar{C})} \mathcal{R}(A_C, S(\bar{C})) + 4 \sqrt{\frac{2 \log(4/\delta)}{m}}
\]

where \( m = |S| \).

APPENDIX B

PROOF OF THE COROLLARY 1.1 (BOUNDS FOR THE ENTIRE PREDICTIVE MODEL)

Proof. Based on the assumption,

\[
L(h, Z) = \frac{1}{m} \sum_{z \in Z} l(h, z)
\]

where \( m = |Z| \). Then

\[
\mathbb{E}_D[L(H)] = \sum_{C \in T} P(\bar{C}) \times \mathbb{E}_{D_C}[L(H)]
\]

Based on the Theorem 1, with probability at least \( (1 - \delta)^{1/|T|} \), each terminal node \( \bar{C} \) satisfied the following condition.

\[
\mathbb{E}_{D_C}[L(H)] \leq L(H, S(\bar{C})) + 2 \max_{C \in \Pi(\bar{C})} \mathcal{R}(A_C, S(\bar{C})) + 4 \sqrt{\frac{2 \log(4/1 - (1 - \delta)^{1/|T|})}{m}}
\]

where \( m = |S| \).

Because the definition of the \( L(h, Z) \) is the sample mean of
each loss $l(h, z)$, the entire loss is the weighted average of each terminal node. (weight is the number of samples $S([C])$ in each terminal node).

Furthermore, if each terminal node satisfies the above condition with probability at least $(1 - \delta)^{1/|\mathcal{T}|}$, it means that the probability that all terminal nodes satisfy the following condition is at least $((1 - \delta)^{1/|\mathcal{T}|})^{|\mathcal{T}|} = (1 - \delta)$

Therefore, with at least $1 - \delta$ probability,

$$
\mathbb{E}_D[L(H)] \leq \sum_{C \in \mathcal{T}} \frac{|S(C)|}{n} L(H, S(C)) + 2 \sum_{C \in \mathcal{T}} |S(C)| \max_{C \in \Pi(C)} R(A_C, S(C)) + 4 \sum_{C \in \mathcal{T}} |S(C)| \sqrt{\frac{2 \log(4/(1 - \delta)^{1/|\mathcal{T}|})}{|S(C)|}}
$$

Furthermore, $1 - (1 - \delta)^{1/|\mathcal{T}|} \geq \frac{\delta}{|\mathcal{T}|}$. Thus, we can switch $1 - (1 - \delta)^{1/|\mathcal{T}|}$ to $\frac{\delta}{|\mathcal{T}|}$ in this inequality. (Using Binomial Series Theorem, the inequality is easily proved.) Therefore, with at least $1 - \delta$ probability,

$$
\mathbb{E}_D[L(H)] \leq \frac{1}{n} \sum_{C \in \mathcal{T}} |S(C)| \times 
\left[L(H, S(C)) + 2 \max_{C \in \Pi(C)} R(A_C, S(C)) + 4 \sqrt{\frac{2 \log(4|\mathcal{T}|/\delta)}{|S(C)|}} \right]
$$

APPENDIX C
PROOF OF THE COMPUTATIONAL COMPLEXITY

A. Proof of computational complexity of one recursive step:

Statement: The computational complexity of one recursive step for constructing tree of predictors grows as $\sum_{i=1}^{M} \mathcal{O}(ND \times T_i(N, D))$.

Proof. There are two procedures in one recursive steps of constructing a tree of predictors. (1) Greedy search for the division point, (2) Construct the predictive model for each division.

First, the possible combinations of dividing the feature space into two subspaces using one feature with the threshold are at most $N \times D$ where $N$ is the total number of samples, and $D$ is the number of dimensions. Because, in each subspace, there should be at least one sample.

Second, for each division, we need to construct $M$ predictive models. The computational complexity to construct the $M$ number of predictive models for each division is trivially computed as $\sum_{i=1}^{M} \mathcal{O}(T_i(N, D))$ where $\mathcal{O}(T_i(N, D))$ is the computational complexity of $i$-th learner to construct the predictive model with $N$ samples and $D$ dimensional features.

Therefore, the computational complexity of one recursive step with $M$ learner can be written as follow.

$$
ND \times \sum_{i=1}^{M} \mathcal{O}(T_i(N, D)) = \sum_{i=1}^{M} \mathcal{O}(ND \times T_i(N, D))
$$

Because, there are $ND$ possibilities of division and for each division, the computational complexity is $\sum_{i=1}^{M} \mathcal{O}(T_i(N, D))$.

B. Proof of computational complexity of constructing the entire tree of predictors

Statement: The computational complexity of constructing the entire tree of predictors is $\sum_{i=1}^{M} \mathcal{O}(N^2D \times T_i(N, D))$.

Proof. By the previous statement, we know that the computational complexity of one recursive step of constructing the tree of predictors is $\sum_{i=1}^{M} \mathcal{O}(ND \times T_i(N, D))$. Therefore, now, we need to figure out the maximum number of recursive steps with $N$ samples.

For each recursive step, the number of clusters is stepwise increased. Furthermore, in each cluster, there should be at least one sample. Therefore, we can easily figure out that the maximum number of recursive steps are at most $N$. (Note that the recursive steps are much less needed in practice because ToPs does not divide all the samples into different clusters)

Therefore, the computational complexity of the entire construction tree of predictors is as follow.

$$
N \times \sum_{i=1}^{M} \mathcal{O}(ND \times T_i(N, D)) = \sum_{i=1}^{M} \mathcal{O}(N^2D \times T_i(N, D))
$$

For instance, if we only use the linear regression as the learner of ToPs (ToPs/LR), the computational complexity of ToPs is $\mathcal{O}(N^3D^3)$. This is because, the computational complexity of linear regression is $\mathcal{O}(ND^2)$. Therefore, the entire computational complexity of ToPs/LR is $\sum_{i=1}^{M} \mathcal{O}(N^2DT_i(n, D)) = \mathcal{O}(N^3D^3)$

ACKNOWLEDGMENT

This work was supported by the Office of Naval Research (ONR) and the NSF (Grant number: ECCS1462245).

REFERENCES

[1] D. J. Miller and L. Yan, “Critic-driven ensemble classification,” IEEE Transactions on Signal Processing, vol. 47, no. 10, pp. 2833–2844, 1999.
[2] C. Tekin, J. Yoon, and M. van der Schaar, “Adaptive ensemble learning with confidence bounds,” IEEE Transactions on Signal Processing, vol. 65, no. 4, pp. 888–903, 2016.
[3] N. Asadi, A. Mirmoezri, and E. Haghshenas, “Multiple observations hmm learning by aggregating ensemble models,” IEEE Transactions on Signal Processing, vol. 61, no. 22, pp. 5767–5776, 2013.
[4] L. Canzian, Y. Zhang, and M. van der Schaar, “Ensemble of distributed learners for online classification of dynamic data streams,” IEEE Transactions on Signal and Information Processing over Networks, vol. 1, no. 3, pp. 180–194, 2015.
[5] L. Breiman, “Random forests,” Machine learning, vol. 45, no. 1, pp. 5–32, 2001.
[6] Y. Freund, Y. Mansour, and R. E. Schapire, “Generalization bounds for averaged classifiers,” Annals of Statistics, pp. 1698–1722, 2004.
[7] D. J. MacKay, “Bayesian methods for adaptive models,” Ph.D. dissertation, California Institute of Technology, 1992.
[8] V. Y. Tan, S. Sanghavi, J. W. Fisher, and A. S. Willsky, “Learning graphical models for hypothesis testing and classification,” IEEE Transactions on Signal Processing, vol. 58, no. 11, pp. 5481–5495, 2010.
[9] Y. Freund and R. E. Schapire, “A decision-theoretic generalization of on-line learning and an application to boosting,” in European conference on computational learning theory. Springer, 1995, pp. 23–37.
[10] P. Smyth and D. Wolpert, “Linearly combining density estimators via stacking,” Machine Learning, vol. 36, no. 1-2, pp. 59–83, 1999.
[11] D. Malerba, F. Esposito, M. Ceci, and A. Appice, “Top-down induction of model trees with regression and splitting nodes,” IEEE Transactions on Pattern Analysis and Machine Intelligence, vol. 26, no. 5, pp. 612–625, 2004.
[12] D. Potts and C. Sammut, “Incremental learning of linear model trees,” Machine Learning, vol. 61, no. 1-3, pp. 5–48, 2005.
[13] Y. LeCun, “The mnist database,” 2016. [Online]. Available: http://yann.lecun.com/exdb/mnist/
[14] C. Cortes, M. Mohri, and U. Syed, “Deep boosting,” in 31st International Conference on Machine Learning, ICML 2014. International Machine Learning Society (IMLS), 2014.
[15] M. Lichman, “UCI machine learning repository,” 2013. [Online]. Available: http://archive.ics.uci.edu/ml
[16] J. Friedman, T. Hastie, R. Tibshirani et al., “Additive logistic regression: a statistical view of boosting (with discussion and a rejoinder by the authors),” The annals of statistics, vol. 28, no. 2, pp. 337–407, 2000.
[17] S. Fritsch, F. Guenther, and M. F. Guenther, “Package ‘neuralnet’,” 2016.
[18] T. Chen and C. Guestrin, “Xgboost: A scalable tree boosting system,” in Proceedings of the 22Nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining. ACM, 2016, pp. 785–794.
[19] S. Buuren and K. Groothuis-Oudshoorn, “mice: Multivariate imputation by chained equations in R,” Journal of statistical software, vol. 45, no. 3, 2011.
[20] K. D. Aaronson, J. S. Schwartz, T.-M. Chen, K.-L. Wong, J. E. Goin, and D. M. Mancini, “Development and prospective validation of a clinical index to predict survival in ambulatory patients referred for cardiac transplant evaluation,” Circulation, vol. 95, no. 12, pp. 2660–2667, 1997.
[21] S. J. Pocock, C. A. Ariti, J. J. McMurray, A. Maggioni, L. Kaber, I. B. Squire, K. Swedberg, J. Dobson, K. K. Poppe, G. A. Whalley et al., “Predicting survival in heart failure: a risk score based on 39 372 patients from 30 studies,” European heart journal, p. ehs337, 2012.
[22] W. C. Levy, D. Mozaffarian, D. T. Linker, S. C. Sutradhar, S. D. Anker, A. B. Cropp, I. Anand, A. Maggioni, P. Burton, M. D. Sullivan et al., “The seattle heart failure model,” Circulation, vol. 113, no. 11, pp. 1424–1433, 2006.
[23] J. R. Quinlan et al., “Learning with continuous classes,” in 5th Australian joint conference on artificial intelligence, vol. 92. Singapore, 1992, pp. 343–348.
[24] Y. Wang and I. H. Witten, “Induction of model trees for predicting continuous classes,” 1996.
[25] L. Torgo, “Functional models for regression tree leaves,” in ICML, vol. 97. Citeseer, 1997, pp. 385–393.
[26] L. Breiman, J. Friedman, C. J. Stone, and R. A. Olshen, Classification and regression trees. CRC press, 1984.
[27] L. Breiman, “Bagging predictors,” Machine learning, vol. 24, no. 2, pp. 123–140, 1996.
[28] P. Smyth and D. Wolpert, “Linearly combining density estimators via stacking,” Machine Learning, vol. 36, no. 1-2, pp. 59–83, 1999.
[29] E. A. Nadaraya, “On estimating regression,” Theory of Probability & Its Applications, vol. 9, no. 1, pp. 141–142, 1964.
[30] G. S. Watson, “Smooth regression analysis,” Sankhyā: The Indian Journal of Statistics, Series A, pp. 359–372, 1964.
[31] C. K. Williams, “Prediction with gaussian processes: From linear regression to linear prediction and beyond,” in Learning in graphical models. Springer, 1998, pp. 599–621.