FORESTPRUNE: Compact Depth-Controlled Tree Ensembles

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ABSTRACT
Tree ensembles are versatile supervised learning algorithms that achieve state-of-the-art performance. These models are extremely powerful but can grow to enormous sizes. As a result, tree ensembles are often post-processed to reduce memory footprint and improve interpretability. In this paper, we present FORESTPRUNE, a novel optimization framework that can post-process tree ensembles by pruning depth layers from individual trees. We also develop a new block coordinate descent method to efficiently obtain high-quality solutions to optimization problems under this framework.

The number of nodes in a decision tree increases exponentially with tree depth, so pruning deep trees can drastically improve model parsimony. FORESTPRUNE can substantially reduce the space complexity of an ensemble for a minimal cost to performance. The framework supports various weighting schemes and contains just a single hyperparameter to tune. In our experiments, we observe that FORESTPRUNE can reduce model size 20-fold with negligible performance loss.

1 INTRODUCTION
Tree ensembles are highly popular in machine learning for their predictive accuracy and interpretability. These ensembles combine weak decision trees by either averaging independently grown trees (bagging) or by adding trees grown sequentially (boosting) [3, 6]. The resulting model is more accurate and generalizes better than any single decision tree, but is much more complex. In bagging, thousands of trees are often grown to full depth, and the number of nodes increases exponentially per layer. Boosting typically uses shallower trees, however, the boosting sequence can be long and may overfit. The complexity of tree ensembles raises several issues. Tree ensembles can grow to massive sizes and require substantial memory to store. In addition, computing the predictions of large ensembles is slow, since each observation in the test dataset must pass through each tree. Large ensembles with deep trees are also difficult to interpret since the structures of deep trees are impossible to visualize. Finally, complex tree ensembles can overfit, and tuning large ensembles to improve performance is incredibly time-consuming.

To reduce tree ensembles to a more parsimonious form, ensembles can be processed after training. Cutting ensemble size vastly improves memory footprint, prediction speed, and interpretability.

In this paper, we present FORESTPRUNE, a novel optimization framework for post-processing tree ensembles. Compared to traditional methods that encourage compactness through removing trees, FORESTPRUNE trims individual trees in the ensemble. Trees can be reduced in depth or eliminated altogether. FORESTPRUNE regularizes ensemble complexity and can directly penalize the number of nodes in the ensemble so that the post-processed model is compacted with minimal performance loss. The optimization problems in FORESTPRUNE scale; good solutions can be obtained by using coordinate descent methods to minimize regularized loss.

As a by-product of our framework, we observe that FORESTPRUNE can serve as an alternative to hyperparameter tuning. By growing a long sequence of boosted trees and pruning that sequence, FORESTPRUNE can produce a pruned model that performs comparably to a tuned ensemble, for a fraction of the computational cost.

1.1 Applications
Online prediction. In machine learning pipelines designed to predict in real-time, prediction speed is of critical importance. Milliseconds of delay per prediction can contribute to unacceptable latency for the end-user. By reducing the number of nodes in a tree ensemble, FORESTPRUNE can greatly reduce prediction time.

On-device learning. On-device learning improves the privacy and latency of machine learning workflows but requires models to be small. FORESTPRUNE can trim large tree ensembles to fit on a local device without substantially reducing performance.

Interpretable ML. In highly regulated fields such as banking and insurance, machine learning models are strictly audited. For models such as boosted trees and random forests to pass an audit, it may be necessary to examine the structure of each tree in the ensemble [4]. This is infeasible when trees are deep and contain thousands of nodes. By pruning the depths of trees in the ensemble, FORESTPRUNE can improve interpretability and transparency.

1.2 Main Contributions
- We present FORESTPRUNE, a novel optimization framework that can post-process tree ensembles by pruning depth layers from trees.
- We develop a new algorithm based on cyclic block coordinate descent to efficiently find good solutions to optimization problems formulated in FORESTPRUNE.

2 BACKGROUND
The following section provides an overview of tree ensembles and post-processing algorithms.

2.1 Tree Ensembles
2.1.1 Decision trees. Decision trees form the base learners used in tree ensembles. We give a quick overview of regression trees below. A regression tree of depth \(d\) partitions a dataset into at most \(2^d\) non-overlapping partitions (leaf nodes). Within each leaf node, the prediction rule is the mean response of the training samples in that partition. Regression trees are grown greedily, at each interior node, splits are selected to minimize the error of the directly resulting partitions. Decision trees are not necessarily balanced, but the number of nodes generally increases exponentially as the tree grows.
deeper. More information on decision trees can be found in Hastie (2009, chapter 9) [9].

2.1.2 Bagging. Bagging averages the predictions of many weakly correlated decision trees to reduce variance [3]. A dataset is sampled with replacement to create multiple bags, and decision trees are fit on each bag. Through averaging the predictions of almost uncorrelated trees, bagging improves the performance of the ensemble. To reduce the correlation between trees, limit the number of features considered per split, the number of features considered per tree, or the amount of training data used in each bag. Bagging generally does not overfit with respect to the number of features used, the number of trees grown, or the depth of each tree [17]. Typically each tree is grown to full depth, where each leaf node only contains instances with the same response, and at least 100 trees are grown. The resulting ensembles are large but can in principle be trained with sufficient computational resources. More information on bagging ensembles can be found in Hastie (2009, chapter 15) [9].

2.1.3 Boosting. Boosting sums the predictions of a sequence of decision trees, where each tree in the sequence is fit on the residuals of the earlier ensemble. At each boosting iteration, the predictions of the current tree are dampened by the learning rate \( \gamma \). This parameter controls the effect that each tree has on the ensemble as well as the similarity between trees adjacent in the boosting sequence. Boosting can overfit if the learning rate is too high, if too many trees are grown, or if trees are grown very deep. Tuning these parameters can improve performance. In addition, randomized variants such as stochastic gradient boosting can improve runtime and ensemble variance [7]. More information on boosting ensembles can be found in Hastie (2009, chapter 10) [9].

2.2 Ensemble Post-Processing

In the following section, we overview existing literature on processing tree ensembles to improve compactness. Friedman (2003) introduces the importance sampled learning ensemble (ISLE) framework [8]. This framework involves growing a tree ensemble using various sampling techniques and post-processing the ensemble in the following manner. Assign each tree \( \ell \) in the ensemble coefficient \( \beta_\ell \). Incorporate an \( \ell \)-penalty on the weights, \( \sum_\ell |\beta_\ell| \), to encourage shrinkage and sparsity. The ensemble produced is compactified and often performs comparably to the full model. ISLE regularizes the number of trees in the ensemble as a proxy for ensemble size, the framework can not trim individual trees in the ensemble.

Joly (2012) extends this approach by proposing \( \ell \)-regularization over the node space [14]. Indicator variables \( \mathbb{I}(i,j) \) are introduced to represent if observation \( i \) reaches node \( j \), for each observation in the data and node in the ensemble. While this approach is interesting, the number of nodes in a tree increases exponentially with depth, so the total number of nodes in an ensemble is enormous. As a result, it is often infeasible to minimize \( \ell \)-regularized loss over the node space.

Besides regularization, various selection heuristics can be used to decide which trees to remove from an ensemble [16, 18]. These heuristics select a compact subset of estimators with respect to some target such as performance, diversity, or interpretability.

3 FORESTPRUNE FRAMEWORK

We detail FORESTPRUNE for regression ensembles and assume without loss of generality that all trees in the ensemble are grown to the same maximum depth. Our main goal is to introduce an optimization framework to prune depth layers from trees in a trained ensemble. Using so-called depth-difference matrices, we show that this framework can be expressed as a regularized least-squares criteria, where the penalty controls which layers to prune.

3.1 Notation

Given dataset \( X \) with \( m \) rows and \( p \) columns, \( X \in \mathbb{R}^{m \times p} \), and response \( y \in \mathbb{R}^m \), decision tree \( T_i \) maps \( T_i(X) : \mathbb{R}^{m \times p} \to \mathbb{R}^m \). Let the prediction of \( T_i(X) = \hat{y}_i \). A tree ensemble is a collection of \( n \) decision trees \( T_i, i \in [n] \) grown via bagging or boosting, and the prediction of the ensemble is given by \( \hat{y} = \sum_{i=1}^n y T_i(X) \). In the context of bagging, \( y = \frac{1}{n} \) and in the context of boosting \( y \) is the learning rate. Let \( d \) denote the maximum depth of decision trees in the ensemble.

3.2 Depth-Difference Matrix

For decision tree \( T_i(X) \), depth-difference matrix \( D_i \in \mathbb{R}^{m \times d} \) encodes the decision path of each observation in \( X \), with respect to the depth layers that the observations traverse. To initialize FORESTPRUNE compute \( D_i \) for each tree in the ensemble.

Algorithm 1 presents the procedure for constructing \( D_i \). Consider a single decision tree, \( T_i(X) \) of depth \( d \). For each observation \( x_j \), find the sequence of nodes in the tree traversed by \( x_j \), \( N_1 \rightarrow N_2 \rightarrow \ldots \rightarrow N_k \). For each node in this sequence, compute the mean of the observations found in the node, \( \mu_1 \rightarrow \mu_2 \rightarrow \ldots \rightarrow \mu_k \). The last element of this sequence \( \mu_k \) is the prediction for observation \( x_j \), \( T_i(x_j) \). Take the rolling difference of values in this sequence of means and store these differences in vector \( v_j \) where,

\[
\mathbb{v}_j = [\mu_1, \mu_2 - \mu_1, \mu_3 - \mu_2, \ldots, \mu_k - \mu_{k-1}].
\]

Pad the tail end of \( \mathbb{v}_j \) with zeros so that \( \mathbb{v}_j \in \mathbb{R}^d \). The vector \( \mathbb{v}_j \) has the property that \( \mathbb{v}_j, 1 \) = \( T_i(x_j) \), i.e., the elements of \( \mathbb{v}_j \) sum to the prediction of tree \( T_i \) for observation \( x_j \). Repeat this procedure for \( j \in [m] \) and store the results \( \mathbb{v}_j \) as the rows of \( D_i \in \mathbb{R}^{m \times d} \).

Algorithm 1: Computing Depth-Difference Matrices

| Input: Tree \( T_i \) of depth \( d \), \( X \in \mathbb{R}^{m \times p} \), \( y \in \mathbb{R}^m \) |
|-------------|
| 1 \( D_i \leftarrow \{} \) |
| 2 for \( x_j \in X \) do |
| 3 Find sequence of nodes in \( T_i \) traversed by \( x_j \), \( N_1 \rightarrow N_2 \rightarrow \ldots \rightarrow N_k \) |
| 4 Compute the mean of \( y \) partitioned by each node, \( \mu_1 \rightarrow \mu_2 \rightarrow \ldots \rightarrow \mu_k \) |
| 5 Difference the sequence of means and store in vector \( \mathbb{v}_j = [\mu_1, \mu_2 - \mu_1, \ldots, \mu_k - \mu_{k-1}] \) |
| 6 Pad the tail of \( \mathbb{v}_j \) with zeros, \( \mathbb{v}_j \in \mathbb{R}^d \) |
| 7 Append \( \mathbb{v}_j \) as a row to \( D_i \) |
| end |
| Output: \( D_i \in \mathbb{R}^{m \times d} \) |
3.2.1 Pruning Trees. Given depth-difference matrix $D_t$, the predictions of the full tree $T_t(X) = y_t$ can be obtained by summing over all the columns of $D_t$. $y_t = \text{colsum}(D_t)$. This can be equivalently expressed as $y_t = D_t \cdot 1$, where $1$ is a $d$-dimensional vector of all ones.

Consider the case where we want to prune the deepest layer of tree $T_t(X)$, where $d > 1$. The predictions of this new tree, of depth $d - 1$, can be obtained by summing over all but the last column of $D_t$. Let $z_t$ be a vector in $\{0, 1\}^d$ with $d - 1$ ones followed by a single zero, $z_t = [1, 1, \ldots, 1, 0]$. The predictions of the pruned tree equal $D_t z_t$.

To prune tree $T_t(X)$ to depth $d - k$, set $z_t \in \{0, 1\}^d$ as a vector of $d - k$ ones followed by $k$ zeros. Note that setting $z_t = 0$ removes tree $T_t(X)$ from the ensemble.

3.2.2 Ensemble Predictions. Given tree ensemble $T_i, i \in [n]$, compute depth-difference matrices $D_t, i \in [n]$ for each tree. The predictions of the original ensemble can be represented by

$$\hat{y} = \sum_{i=1}^{n} y_D z_t,$$

where $z_t = 1 \; \forall \; i \in [n]$.

To prune the ensemble, modify the $z_t$ vectors. For example, setting $z_t = [1, 0, \ldots, 0]$ prunes the first tree in the ensemble to depth 1 and setting $z_t = 0$ removes the second tree entirely.

3.3 Ensemble Optimization Problem

Notationally, let $(z_t)_k$ represent the $k$-th element of vector $z_t$. FORESTPRUNE uses the following optimization problem to prune depth layers from an ensemble:

$$\min_{z_1, \ldots, z_n} \frac{1}{m} \|y - \gamma \sum_{i} D_t z_t\|^2 + \frac{\alpha}{K} \sum_{i=1}^{n} \|W_i z_t\|_1 \tag{1a}$$

s.t. $(z_t)_k \in \{0, 1\} \; \forall \; i \in [n], \; k \in [d], \tag{1b}$

$(z_t)_k \geq (z_t)_{k+1} \; \forall \; i \in [n], \; k_1 > k_2, \tag{1c}$

$z_t \in \{0, 1\}^d \; \forall \; i \in [n]. \tag{1d}$

$s_i \in R^{d \times d}$ is a diagonal weight matrix assigned to each tree $T_i$, of the form $s_i = \text{diag}(w_{i1}, \ldots, w_{id})$. These weights are prespecified, and we discuss weighting schemes in §3.4. Normalization constant $K$ is computed from $W_i, i \in [n]$, and regularization parameter $\alpha$ is prespecified as well.

Each decision variable $(z_t)_k$ is binary (1b) and represents whether to include the $k$-th layer of tree $T_t$ in the processed ensemble. Each tree $T_t$ has a corresponding decision vector $z_t \in \{0, 1\}^d$ that contains $d$ decision variables (1d). The goal of FORESTPRUNE is to minimize regularized loss (1a) with respect to decision vectors $z_t, i \in [n]$. Constraint (1c) ensures that the pruned trees are contiguous, since trees should not be able skip depth layers. The solution $z_t = [1, 0, \ldots, 0]$ is infeasible since a tree cannot skip depth layer 2 and proceed to depth layer 3; trees can only be pruned from the bottom up.

Consider the regularized loss function in objective (1a). The first term of the function is least-squares loss and the second term is the regularization penalty. The parameter $\alpha$ controls regularization; larger values of $\alpha$ encourage shallower trees in the processed ensemble. Each entry of $W_t, w_{i,k}$ for $k \in [d]$, is nonnegative and represents the weight associated with including depth layer $k$ of tree $T_t$ into the processed ensemble. Since $W_t$ and $z_t$ are both nonnegative, the norm $\|W_t z_t\|_1$ is equivalent to summing the elements of vector $W_t z_t$. Finally, $K$ is a normalization constant set such that $K = \sum_{i=1}^{n} \sum_{k=1}^{d} w_{i,k}$. This constant ensures that $\alpha$ remains within a reasonable range.

3.4 Weighting Schemes

FORESTPRUNE is a general framework that can accommodate different forms of regularizers. We can specify weight matrices $W_t, i \in [n]$ to produce post-processed ensembles with different parsimony properties. Three such weighting schemes are presented below.

3.4.1 Depth-Weighting. We assign $w_{i,k} = 1$ if the depth of decision tree $T_i$ is less than or equal to $k$, otherwise we assign $w_{i,k} = 0$. The normalization constant $K = n \cdot d$. This weighting scheme directly penalizes the total number of layers in the ensemble and produces ensembles with fewer trees.

3.4.2 Node-Weighting. We assign $w_{i,k}$ equal to the number of nodes in layer $k$ of tree $i$. The normalization constant $K$ is equal to the total number of nodes in the ensemble. This weighting scheme directly penalizes ensemble size and produces the most compact processed ensemble, with the shallowest trees.

3.4.3 Balanced Node-Weighting. We assign $w_{i,k}$ equal to the absolute difference in the number of nodes between the right side and left side of layer $k$ of tree $i$. This weighting scheme penalizes tree imbalance and produces ensembles with more balanced trees.

3.5 Depth vs. Node-Weighting

The left plot in Figure 1 compares the effect of depth vs. node-weighted FORESTPRUNE on the Moneyball dataset (appx. A). Node-weighting produces shallower trees compared to depth-weighting. In addition, the total size of the node-weighted pruned ensemble is approximately three times smaller than the depth-weighted one, 7247 vs. 21588 nodes. However, the ensemble processed by node-weighted FORESTPRUNE contains more trees than the depth-weighted one, 95 vs. 62 trees. The test errors of the post-processed ensembles are comparable under both weighting schemes.

![Figure 1: Effects of node-weighting and polishing when using FORESTPRUNE on the Moneyball dataset. Node-weighting encourages shallower trees and the polishing heuristic improves test performance.](image-url)
produces an ensemble with fewer estimators. Figure 2 presents the distribution of nodes per layer for trees grown to full depth in a bagging ensemble. The proportion of nodes contained in layer \( k \) of the full model, the plot in blue, increases exponentially to a peak and then rapidly declines. The layer at which this peak occurs depends on the size of the dataset. Node-weighting encourages the optimization problem to prune the peak layers, and as a result, all layers deeper than the peak layers are pruned as well. The orange plot in Figure 2 shows that node-weighted ForestPrune, with \( \alpha = 0.1 \), produces an ensemble much shallower than the full model.

Note that after the peak in the blue plot, the proportion of nodes contained per layer decreases. This suggests that the deeper layers of full-depth trees are imbalanced.

Figure 2: Distribution of nodes by depth layer for a bagging ensemble. The proportion of nodes contained in each layer of the full model increases exponentially to a peak that depends on dataset size. Node-weighting ForestPrune encourages shallower trees.

3.6 Polishing Weights of Pruned Trees

Solving Problem 1 with respect to \( z_i, i \in [n] \) yields solution vectors \( z^*_i, i \in [n] \). These vectors, combined with depth-difference matrices \( D_i, i \in [n] \) represent the processed ensemble, with trees \( T^*_i(x) = D_i z^*_i, i \in [n] \).

We can adjust the weights of trees in this processed ensemble to better fit the model to \( y \). This especially helps for boosting, where trees are grown sequentially, since pruning a tree breaks the boosting sequence. The following polishing heuristic reweights the processed ensemble by following optimization criterion:

\[
\min_{\beta_1 \ldots \beta_n} \frac{1}{m} \| y - y \sum_{i=1}^{n} \beta_i D_i z^*_i \|^2_2 + \alpha_2 \sum_{i=1}^{n} \beta_i^2 \quad (2a)
\]

where coefficients \( \beta_i, i \in [n] \) are the weights assigned to each tree. The first term in objective (2a) is least-squares loss and the second term is a ridge penalty, with regularization parameter \( \alpha_2 \). The squared \( L_2 \) penalty serves two purposes. First, when the number of trees in the ensemble is larger than the number of rows in the dataset, \( n > m \), the ridge penalty ensures a unique estimator in \( \beta \). Second, the ridge penalty offers stability when the bases elements \( D_i z^*_i \) are correlated.

We observe empirically that a small value of the ridge parameter, between \( 10^{-4} \) and \( 10^{-1} \), appears to work well in terms of producing a polished model with good test performance. The parameter is not very sensitive, so we recommend using a default of \( \alpha_2 = 10^{-2} \).

The right plot in Figure 1 shows the effect of the polishing heuristic when ForestPrune is used on the Moneyball dataset (appx. A). The original tree ensemble is grown using stochastic gradient boosting with a learning rate of \( \gamma = 0.01 \). The polishing heuristic substantially improves test performance across all sizes of the pruned ensemble.

3.7 Putting Together the Pieces

Algorithm 2 presents the overall framework of ForestPrune. We recommend using both node-weighting and the polishing heuristic to compactify ensembles.

Ensemble optimization Problem 1 can be expressed as a mixed-integer optimization problem [21], which can be computationally challenging for large problems [1, 2, 12]. Here we propose a novel algorithm based on block coordinate descent to obtain good quality solutions for Problem 1, that appear to work well for the problems we study.

Problem 2 is equivalent to ridge regression using the predictions of the pruned trees \( D_i z^*_i, i \in [n] \) as features. The problem has a closed-form solution and can be quickly solved [13].

Algorithm 2: ForestPrune Framework

Input: \( T_i \) for \( i \in [n] \), \( X \in \mathbb{R}^{m \times p} \), \( y \in \mathbb{R}^m \), \( \alpha \)
1. Compute \( D_i, i \in [n] \).
2. Choose weighting scheme \( W_i, i \in [n] \).
3. Solve Problem 1 for \( z^*_i, i \in [n] \).
4. if polish = True then
5. | Solve Problem 2 for \( \beta^*_i, i \in [n] \).
6. else
7. | \( \beta^* = 1 \).
8. end

Output: \( z^*, \beta^* \)

4 OPTIMIZATION ALGORITHM

Note that Problem 1 can be written as:

\[
\min z_1 \ldots z_n \quad L(z_1 \ldots z_n) + \sum_{i=1}^{n} g_i(z_i) \quad (3a)
\]

\[
\text{s.t.} \quad z_i \in C_i \quad \forall i \in [n] \quad (3b)
\]

where

\[
L(z_1 \ldots z_n) = \frac{1}{m} \| y - y \sum_{i=1}^{n} D_i z_i \|^2_2
\]

is a smooth function and

\[
\sum_{i=1}^{n} g_i(z_i) = \alpha \sum_{i=1}^{n} \| W_i z_i \|_1
\]

is separable across blocks \( z_i, i \in [n] \). Constraints (1b) and (1c) can be represented by constraint (3b), where \( C_i \) is the set of vectors in \( \{0, 1\}^d \) that satisfy the condition \( (z_i)_{k_2} \geq (z_i)_{k_1} \), \( \forall z_i \in C_i, k_1 > k_2 \).

The non-smooth part of the objective in (3a) and the constraint (3b) are both separable across \( z_i \)’s. Motivated by the success of cyclic block coordinate descent methods (CBCD) for large-scale sparse regression problems [10, 22], we apply CBCD methods to
We consider a partition of the decision variables in Problem 3 into the blocks $z_i$, $i \in [n]$ with $z_i \in C_i$.

A drawback of this local search procedure is that it can be expensive to update block $\omega \in \mathcal{S}$ and let $\omega_i = \omega(S)$. Selecting a random index $\omega_i$ for which $\omega_i$ is the smallest index, i.e., let $i^* = \min(i \mid \hat{z}_i \in \mathcal{S})$. In boosting ensembles, trees grown early in the boosting sequence are more directly correlated with the response. This smallest index rule ensures that the local search heuristic always swaps in the earliest grown tree, for negligible computational cost.

The complete CBCD algorithm with local search is presented in Algorithm 3.

Algorithm 3: ForestPrune CBCD

| Input: $D_i, W_i$ for $i \in [n], y \in \mathbb{R}^m, \alpha$ |
| repeat |
| $\omega = \omega \mod n$ |
| Solve Problem 4 to update $\omega_i$ |
| $\omega = \omega + 1$ |
| until converged |
| Local search §4.1.3. |
| until objective no longer improves |
| Output: $z_i, i \in [n]$ |

4.2 Regularization Paths

We use warm start continuation with Algorithm 3 to efficiently compute the entire regularization path of $z_i$’s, across tuning parameter $\alpha$. This provides a sequence of solutions with varying ensemble sizes, that a practitioner can use to quickly select a suitable model. This procedure is similar to computing regularization paths for sparse regression [5, 11].

We select a value of $\alpha$ large enough to guarantee that $z_i = 0$ for $i \in [n]$. Decrement $\alpha$ and for each value of $\alpha$, use the previous solution $\alpha^*$ as a warm start to initialize CBCD. We compute a sequence of solutions till $\alpha$ is sufficiently small, so that we obtain the full model with $z_i = 1, i \in [n]$.

When warm start continuation is used without local search, CBCD tends to get stuck at local minima. This can be seen in the middle plot of Figure 3. In this example, CBCD with warm start continuation is used to compute the entire regularization path of ForestPrune on the Moneyball dataset. The scatter plot presents the test error of the processed ensemble with respect to the regularization parameter $\alpha$. The plot is nearly piecewise and the histogram shows that with warm starts, CBCD often terminates immediately after initialization.

Combining warm start continuation with local search resolves this issue. In the right most plot of Figure 3 the regularization path computed using CBCD with warm start continuation and local search is very similar to the path computed using the base CBCD algorithm, where CBCD is always initialized with $z_i = 0, i \in [n]$. From the histograms in the second row of Figure 3 it is apparent that CBCD with warm start continuation and local search requires to find the best swap-coordinate $i^* \in \mathcal{S}$ that would result in the largest improvement in the current objective. In fact, this would require computing the correlation coefficient between each block in $\mathcal{S}$ and $y$. We present a heuristic that we found to work quite well for our problem in the context of boosting, always select the block in $\mathcal{S}$ with the smallest index, i.e., let $i^* = \min(i \mid \hat{z}_i \in \mathcal{S})$. In boosting ensembles, trees grown early in the boosting sequence are more directly correlated with the response. This smallest index rule ensures that the local search heuristic always swaps in the earliest grown tree, for negligible computational cost.
how well ForestPrune performs in compactifying bagging ensembles, we fix a threshold for acceptable performance loss and find the smallest pruned ensemble within this threshold. We compare the performance of the pruned ensemble against the full model. We describe the procedure below.

**Procedure.** Split a given dataset into a training, validation, and test set, and scale and center each set. On the training set, fit a bagging ensemble of 500 trees, where each tree is grown to depth \( d = 20 \) and a subsample of \( \sqrt{p} \) features is considered at each split. This bagging ensemble is a random forest [3].

Evaluate the validation error of the full ensemble, \( e_f \), and fix a threshold for acceptable performance loss, \( \phi \in \{0.01, 0.025, 0.05\} \). Compute the entire regularization path for ForestPrune. Select the largest value of \( \alpha \) such that the validation error of the pruned ensemble, \( e_p \), is within \( \phi \) of the full ensemble, i.e., \( |e_p - e_f| \leq \phi \). The pruned ensemble is the most compact ensemble within performance threshold \( \phi \).

Compare the reduction in ensemble size, as well as the percent difference in test error, between the pruned ensemble and the original. Use the baseline and LASSO methods described above to find the best performing model not larger than the ensemble pruned by ForestPrune. Compare the test performance of the models produced by all three methods.

### 5.2 Compact Boosting Ensembles

Large boosting ensembles can overfit, so post-processing can potentially improve performance. To evaluate how well ForestPrune compactifies boosting ensembles, we compute the entire regularization path for ForestPrune and compare the performance of the path against other methods. This procedure was used to compare LASSO vs. baseline post-processing in Hastie (2009, chapter 16) [9]. We present our approach below.

**Procedure.** Split a given dataset into a training and test set, and center and scale both sets. On the training set, fit a stochastic gradient boosting regressor with 1000 trees and a learning rate of \( \gamma = 0.01 \). Subsample 10 percent of the training data when fitting each tree and grow each tree to depth \( d = 5 \). Compare the following.

- Compute the entire regularization path for ForestPrune. Evaluate test error and ensemble size for each value of \( \alpha \) (ForestPrune).
- Compute the entire LASSO regularization path and evaluate test error and ensemble size for each value of \( \lambda \) (LASSO).
- Repeatedly trim trees from the tail of the boosting sequence in multiples of 5 and evaluate test error and ensemble size at each iteration (Baseline).

Compare test errors across the entire regularization path for each of the three methods.

### 5.3 Parameter Tuning for Boosting Ensembles

Hyperparameters tree depth \( d \), number of trees \( n \), and learning rate \( \gamma \) are commonly tuned to improve the performance of boosting ensembles. This tuning process is computationally expensive since the ensemble must be retrained to evaluate each parameter combination. We observe that ForestPrune can be a potentially useful alternative to expensive hyperparameter tuning.
Start by growing a large ensemble, of many deep trees, with a slow learning rate. Use FORESTPRUNE to prune this overparameterized ensemble; compute the entire regularization path and select $\alpha$ to minimize validation loss. Empirically, we observe that this pruned ensemble performs comparably to a tuned ensemble, and can be obtained for a fraction of the computational cost. The following experiment evaluates how well FORESTPRUNE performs as an alternative to random search tuning.

Procedure. Split a given dataset into a training, validation, and test set, and center and scale each set. Fit a stochastic gradient boosting ensemble on the training set with 1000 trees of depth 10 and a learning rate of $\gamma = 0.01$. Train each tree on a 10 percent subsample of the training data. Compute the entire regularization path for FORESTPRUNE and select $\alpha$ to minimize validation loss. Evaluate the test error of the pruned ensemble.

Compare the test error of the ensemble processed by FORESTPRUNE against the following tuning procedure. Define the following parameter ranges: $d \in \{1, 4, 7, 10\}$, $n \in \{10, 250, 500, \ldots, 1000\}$, and $\gamma \in \{0.01, 0.02, 0.05, 0.07, 0.14, 0.27, 0.5, 1\}$. These parameter ranges form 288 parameter combinations. Random search through these combinations and select the parameters that minimize validation loss. At each tuning iteration, evaluate the test error of the best model found so far. Compare the number of tuning iterations required for random search to beat FORESTPRUNE and the gap in performance between the fully tuned model and the best model produced by FORESTPRUNE.

5.4 Data
We conduct the experiments detailed above on a selection of 25 regression benchmark datasets from OpenML [20]. The full list of selected datasets, with metadata, can be found in Appendix A. All experiments are conducted using 5-fold cross-validation.

5.5 Implementation
FORESTPRUNE is implemented in Python with just-in-time compilation provided by Numba [15]. All tree ensembles in the experiments are built using Scikit-learn [19].

6 RESULTS
6.1 Compact Bagging
FORESTPRUNE compactifies bagging ensembles remarkably well with nominal performance loss. Figure 4 presents the results of the compact bagging experiment detailed in §5.1. The top left plot shows the percent increase in test error between the model pruned by FORESTPRUNE and the full model, where

$$\text{% increase error} = \frac{\text{MSE pruned model} - \text{MSE full model}}{\text{MSE full model}}.$$  

As the threshold for acceptable performance loss $\phi$ increases, the percent increase in test error rises correspondingly.

The top right plot in Figure 4 presents the compactness ratio, i.e., the ratio of the number of nodes in the pruned model over the number of nodes in the full model. The compactness ratio decreases as $\phi$ increases; if the threshold for acceptable performance loss is increased, the model can be made much smaller.

The bottom left plot in Figure 4 presents the distribution of tree depths in the pruned ensemble. Originally all trees in the bagging ensemble are grown deep, to depth $d = 20$. Node-weighted FORESTPRUNE produces much shallower trees, across all levels of $\phi$; the average tree depth in the pruned ensemble is 5.

Consider using FORESTPRUNE to compactify bagging ensembles with $\phi = 0.01$. The pruned ensembles perform nearly the same as the full ensembles, with only a 1-5% increase in test error, and are reduced 10-20 fold in size. The average depth of trees in the pruned ensemble is also reduced by a factor of 4. On the other hand, FORESTPRUNE with $\phi = 0.05$ produces pruned ensembles two orders of magnitude smaller than the original, for around a 10-20% increase in test error. By varying the threshold $\phi$, FORESTPRUNE can be tuned to balance performance and compactness. Across all levels of $\phi$ considered, FORESTPRUNE produces a substantially smaller ensemble for a modest increase in test error.

FORESTPRUNE also performs substantially better than LASSO and baseline methods at producing compact bagging ensembles. The bottom right plot in Figure 4 shows the percent increase in test error between the model produced by baseline/LASSO pruning and the model produced by FORESTPRUNE. The baseline/LASSO model is constrained to be no larger in size than the FORESTPRUNE model. Across all values of $\phi$, the distributions of the percent increase in test error between baseline/LASSO and FORESTPRUNE are almost entirely positive, with medians around 300% and 100% respectively. Baseline and LASSO methods are only capable of excluding or selecting trees, and when deep trees are grown, the size of a single tree may be larger than the ensemble produced by FORESTPRUNE. As a result, these regularization methods are unable to produce a model similar in size to FORESTPRUNE with comparable test performance.

6.2 Compact Boosting
FORESTPRUNE can effectively compactify boosting ensembles and prevent overfitting compared to baseline and LASSO post-processing.
Each optimization iteration in ForestPrune (Problem 4) is not restricted by the shape of $D_i$. For sparse models, models with less than 1000 nodes, ForestPrune consistently outperforms LASSO as well. ForestPrune directly penalizes the number of nodes in the ensemble, while LASSO penalizes the number of trees as a proxy for ensemble size. LASSO can only include or exclude entire trees, while ForestPrune can trim deep layers that contain many nodes. When given a tight budget for ensemble size, LASSO can often only select a single tree while ForestPrune can produce an ensemble of shallower ones.

The bottom right plot in Figure 5 presents the percent difference in test error between models processed by ForestPrune and LASSO, for both sparse and dense models. This distribution is obtained by evaluating both methods across all datasets in the experiment. In both the sparse and dense cases, the entire distribution is negative. This shows that ForestPrune consistently performs better than LASSO in these two scenarios. ForestPrune produces a considerably more compact model than baseline pruning and outperforms LASSO at producing both sparse and dense models.

### 6.3 Tuning Boosting

![Figure 5: Results using ForestPrune to prune boosting ensembles. ForestPrune outperforms LASSO pruning for obtaining very sparse or dense models.](image)

Figure 5 presents the results of the boosting compactness experiment described in §5.2. The plots in the top row of the figure show examples of the experiment on the no2 and autoMpg datasets. The x-axes show the number of nodes in the pruned ensemble and the y-axes show test error.

For these datasets, the best models produced by each of the methods, ForestPrune, LASSO, and baseline, have similar test errors. This result is consistent across all datasets in the experiment. However, ForestPrune and LASSO produce substantially more compact processed models compared to the baseline method. The bottom left plot in Figure 5 compares the distribution of model sizes of the best model produced by each method, across all datasets in the experiment. On average, the best model produced by the baseline method is twice as large as the best model produced by ForestPrune or LASSO.

We also observe that ForestPrune outperforms LASSO in two scenarios. For dense models, models that are similar in size to the full ensemble, the test error of ensembles produced by LASSO post-processing is very large. This can be observed in the autoMPG plot in Figure 5; as the number of nodes in the processed ensemble increases, the test error of the LASSO-processed ensemble rises rapidly. This phenomenon was also observed by Hastie (2009, chapter 16) [9]. LASSO overfits when the regularization parameter $\lambda$ is small. Additionally, in the autoMPG example, the number of observations in the dataset is smaller than the number of trees in the full ensemble. LASSO does not select more trees than the number of observations, so when $\lambda$ is reduced, the weights on the small subset of selected trees are inflated.

ForestPrune is robust to overfitting compared to LASSO. The regularization parameter $\alpha$ only controls sparsity, so setting $\alpha = 0$ simply yields the original model. In addition, ForestPrune can select the full ensemble even if the number of trees in the ensemble is greater than the number of observations in the training data.

The numerical results discussed here suggest that ForestPrune can potentially serve as an efficient alternative to expensive parameter tuning for boosting ensembles. Figure 6 presents a representative subset of results from the tuning boosting ensembles experiment detailed in §5.3. In each plot, the x-axis presents the number of random search tuning iterations conducted and the y-axis presents test error. The dashed orange line shows the test error of the ensemble produced by ForestPrune. The solid blue line shows the test error of the best ensemble found via random search tuning (i.e., selecting hyperparameters uniformly at random), with respect to the number of tuning iterations. All error bands are generated from 5-fold CV.

For the Mercedes and no2 datasets, random search tuning beats ForestPrune after roughly 25 iterations. After around 75 iterations, the tuned ensemble always outperforms ForestPrune. For
the kin8nm dataset, it takes roughly 50 tuning iterations for random search to approach ForestPrune. The test errors of the models produced by both methods converge to similar values. For the socmob dataset, random search rapidly approaches ForestPrune, but as the number of tuning iterations increases, the model produced by ForestPrune performs marginally better.

Across all 25 datasets in the experiment, it takes on average 129 tuning iterations for random search to consistently outperform ForestPrune. In addition, the test error of the fully tuned model is on average 15% lower compared to the model produced by ForestPrune, at the expense of higher computational cost incurred from training across multiple tuning parameters.

Compared to random search, tuning with ForestPrune sacrifices a marginal amount of predictive performance for computational efficiency. In random search tuning, the tree ensemble must be retrained in each iteration, while in ForestPrune the ensemble is only trained once. Tuning $\alpha$ for ForestPrune can be done very efficiently via §4.2. In practice, we observe that the time needed to compute the entire regularization path for ForestPrune is roughly the same as training a gradient boosting ensemble 10 times. For a time budget of 10 iterations, ForestPrune produces a substantially better performing model compared to random search tuning.

7 CONCLUSION

In this work, we develop ForestPrune an optimization framework to prune depth layers from trees in an ensemble. We propose a cyclic block coordinate descent method with local search to compute high-quality solutions to the optimization problems formulated under this framework. The per iteration cost of this method is linear in the number of training samples. ForestPrune is flexible and can accommodate various weighting schemes to produce post-processed ensembles with different parsimony properties. The framework only contains a single hyperparameter to tune, the regularization parameter $\alpha$, and we can leverage warm start continuation to efficiently compute the entire regularization path.

Our results show that ForestPrune can reduce the size of bagging and boosting ensembles drastically with nominal performance loss. In addition, ForestPrune outperforms traditional ensemble post-processing methods across a wide range of scenarios. Finally, we observe that ForestPrune can serve as an alternative to parameter tuning, and can produce high-performing models for a fraction of the computational cost.

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A OPENML DATASETS

| Dataset Name                              | Rows | Features |
|-------------------------------------------|------|----------|
| humanevel                                 | 130  | 2        |
| triazines                                 | 186  | 61       |
| tecator                                   | 240  | 125      |
| autoMpg                                   | 398  | 8        |
| no2                                       | 500  | 8        |
| boston                                    | 506  | 14       |
| stock                                     | 950  | 10       |
| socmob                                    | 1156 | 6        |
| Moneyball                                  | 1232 | 15       |
| balloon                                   | 2001 | 2        |
| space_ga                                  | 3107 | 7        |
| abalone                                   | 4177 | 9        |
| Mercedes_Benz_Greener_Manufacturing       | 4209 | 377      |
| mtp                                       | 4450 | 203      |
| wine_quality                              | 6497 | 12       |
| wind                                      | 6574 | 15       |
| kin8nm                                    | 8192 | 9        |
| cpu_small                                 | 8192 | 13       |
| puma32H                                   | 8192 | 33       |
| bank32nh                                  | 8192 | 33       |
| pol                                       | 15000| 49       |
| elevators                                 | 16599| 19       |
| houses                                    | 20640| 9        |
| house_16H                                 | 22784| 17       |
| 2dplanes                                  | 40768| 11       |

Table 1: OpenML Datasets with metadata.