Acceleration of a Dynamically Packed Oblique Sparse Projection Random Forest

by

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Abstract

The proliferation of scientific and industrial sensors is causing an accelerating deluge of data, the processing of which into actionable knowledge requires fast and accurate machine learning methods. A class of algorithms suited to process these large amounts of data is decision forests, widely used methods known for their versatility, state of the art inference, and fast model training. Oblique Sparse Projection Forests — OSPFs — are a subset of decision forests, which provide data inference superior to other methods. Despite providing state of the art inference and having a computational complexity similar to other popular decision forests, there are no OSPF implementations that scale beyond trivially sized datasets.

We explore whether OSPF training and inference speeds can compete with other popular decision forest variants despite an algorithmic incompatibility which prevent OSPFs from using traditional forest training optimizations. First, using R, we implement a highly extensible proof of concept version of a recently conceived OSPF, Randomer Forest, shown to provide state of the art results on many datasets and provide this system for general use via CRAN. We then develop and implement a postprocessing method, Forest Packing, to pack the nodes of a trained forest into a novel data structure and modify the ensemble traversal method to accelerate forest based inferences. Finally, we develop FastRerF, an optimized version of Randomer Forest which dynamically performs forest packing during training.

The initial implementation in R provided training speeds inline with other decision forest systems and scaled better with additional resources, but used an excessive amount of memory and provided slow inference speeds. The development of Forest Packing increased inference throughput by almost an order of magnitude as compared to other systems while greatly reducing prediction latency. FastRerF model training is faster than other popular decision forest systems when using similar parameters and trains Random Forests faster than the current state of the art. Overall, we provide data scientists a novel OSPF system with R and Python front ends, which trains and predicts faster than other decision forest implementations.

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Chapter 1

Introduction

In order to leverage the growing amount of data being created today, researchers are continuously developing machine learning techniques and systems to process data faster and better. For example, deep networks classify gravitational waves more accurately and orders of magnitude faster than matched filtering in LIGO simulations [1]. Using reinforcement learning to drive parameter exploration has transformed mapping protein-ligand interactions, reducing simulation time from hours to minutes [2]. On smaller scales, suites of tools like Scikit-learn and MLkit provide scalable implementations of many machine learning tools including neural nets, SVMs, and decision forests [3, 4].

Decision forests are a popular group of ensemble machine learning techniques which provide superior accuracy, interpretable models, and are robust to parameter selection. It can be shown that decision forests are equivalent to weighted nearest neighbor classifiers and, as such, continually improve with additional training observations [5] and the use of multiple weak learners further improves accuracy by reducing variance. Good results are normally obtainable with default parameter settings, but, when optimized, decision forests can provide state of the art accuracy which has made them a dominant tool used to win multiple Kaggle competitions [6, 7]. Another positive aspect of decision forests are their easily interpreted and visualized dimension partitioning hyper-planes [8].

Of the many decision forest variants, many prior works have shown that oblique hyper-planes are capable of superior predictive performance [9, 10, 11, 12]. The non-axial splits of these forests are able to model the boundaries between classes more accurately, which allows them to perform better than other forest variants. The drawback to these oblique forests are their long training times. A recent framework — Oblique Sparse Projection Forests (OSPF) — overcomes this limitation by using sparse oblique projections, thereby allowing oblique forests to have computational complexities similar to other forest variants.

This work explores the evolution of the first scalable OSPF implementation. We start with a scalable system written in R, which suffered from poor training and inference speeds. We describe and implement a post-training process to reduce inference latency, call Forest Packing. And we finish with an OSPF that rivals traditional forest training times, while simultaneously packing a forest for reduced inference latency.

1.1 Random Forest IO

Decision tree variants all share the same slow IO bound properties, with over 80% of typical implementation training time spent determining node splits. Node splitting is a difficult task to optimize because of erratic memory accesses compounded with runtime characteristics that change from the top of the tree to the leaf nodes. We analyze several node splitting optimizations and determine they are not practical for many oblique forest techniques including OSPFs.

1.2 R-RerF

Breiman first hypothesized that oblique forests could provide superior inference as compared to forests relying solely on axial splits. Subsequent studies have agreed with Breiman's hypothesis, showing obliqe forests are capable of outperforming the current state of the art on many datasets. Despite the benefits, there was no scalable system that produces oblique forests. We created R-RerF, an implementation of Randomer Forest in R, a scalable and easily modifiable OSPF system and test it using several popular large datasets. R-RerF training times are comparable to other forest variants, but is able to scale more efficiently with additional resources. Two weaknesses are identified in the system, which motivates the subsequent chapters.

1.3 Forest Packing

A negative aspect of decision forests, and an untenable property for many real time applications, is their high inference latency caused by the combination of large model sizes with random memory access patterns. We present memory packing techniques and a novel tree traversal method to overcome this deficiency. The result of our system is a grouping of trees into a hierarchical structure. At low levels, we pack the nodes of multiple trees into contiguous memory blocks so that each memory access fetches data for multiple trees. At higher levels, we use leaf cardinality to identify the most popular paths through a tree and collocate those paths in contiguous cache lines. We extend this layout with a re-ordering of the tree traversal algorithm to take advantage of the increased memory throughput provided by out-of-order execution and cache-line prefetching. Together, these optimizations increase the performance and parallel scalability of classification in ensembles by a factor of ten over an optimized C++ implementation and a popular R-language implementation.

1.4 Dynamic Forest Packing

The idea for most machine learning techniques is to train on a test set of data once and perform inference on new data for the life time of the system. There is often a disconnect between training a model and the ideal format to use the model. For this reason there are several post training systems which will rearrange a decision forest model to optimize the inference stage of the models use [13, 14, 15]. These optimizations can perform inference an order of magnitude or more faster than naive models. We show that we can pack the nodes of a decision forest during model training in a manner that optimizes inference with minimal effect on training times. The resulting system uses the OSPF framework to quickly train oblique forests, packs nodes for fast inference speeds, and provides extensibility for future sparse forest implementations.

1.5 List of contributions

This work explores techniques to overcome the poor computational properties of oblique forest ensembles and extends the findings to improve the performance of a well performing but, until now, poorly scaling machine learning class, oblique decision forests. We show that oblique forests using sparse projections, OSPFs, are similar to the training times and scalability of other forest variants and provide the system through CRAN. Traditional optimizations are incompatible with oblique forests including OSPFs so we provide several forest optimizations that reduce IO and greatly improve the scalability of these oblique forests. We describe and implement Forest Packing, a post processing method that re-arranges forest models to greatly reduce inference latencies. We describe a method to grow forests so the resulting forest models closely conform to the models produced via Forest Packing post processing. Together these contributions result in the creation of fastRerF, an OSPF with training speeds and inference latencies superior to the current state of the art.

Chapter 2

Background

Forest ensemble training and use have several inherent challenges that limit the practical dataset size used to create a model. The choice of specific ensembles, such as the focus of this document on supervised sparse projection forests, further exacerbates these challenges. This chapter briefly describes the following: decision forest overview, the general training and inference algorithms used by these ensembles, and the data access pattern design choices typical of these algorithms.

2.1 Decision Trees

A decision tree is a collection of hyperplanes that partition a dataset into informative cells. The root of each tree symbolizes the whole of the training set and each subsequent level of the tree is a partitioning of the data into subsets. Leaf nodes represent cells in the dataset space where observations have similar properties. The properties of unlabeled data can then be inferred by traversing the observation from root to leaf and assuming properties are shared among all observations in the leaf node.

2.2 Decision Forests

Decision Forests are a popular category of machine learning techniques, popular for their discriminating properties and natural extensions. These forests are composed of multiple decision trees each of which contribute to the inference provided by the model. By combining these multiple weak learners, the forests are able to reduce inference variance without affecting model bias. Devroye and Gyiorfi show the isometry of Random Forests with nearest neighbor classification, a universally consistent classifier [16]. Simple extensions of the forest ensembles can provide popular machine learning goals such as feature importance, model accuracy estimates, regression, nearest neighbor search, unsupervised Learning, and many others [10, 8]

2.2.1 Forest Growing

Forest models consist of one or more decision trees, which are independently grown from their roots to their leaves in a recursive process. Although the process itself is independent, initial input of a tree can be influenced by previously grown trees and a tree's output may be considered by subsequent trees [17].

2.2.2 Inference

The purpose of a supervised decision forest is to infer properties of observations not present in the training set. It is assumed that the properties of a new observation will be similar to the closest observations in the training set. The nearest neighbors of an observation are determined by traversing the observation through a decision tree from the root to a leaf, where, either the nearest neighbor indices or their properties are stored. This work only considers classification forests which store class labels in leaf nodes. A forest uses multiple decision trees and combines their predictions to come up with an overall prediction.

2.3 Forest Variants

The many decision forest variants typically differ by input — how to populate the root node, splitting criteria — how to determine the best split at each node, and stopping criteria — when to make an internal node a leaf. Random Forests and Boosted Forests are popular variants with many implementations [6, 7, 18, 19, 3]. Oblique forests are a less studied and used variant lauded for providing superior class discrimination, but has no scalable implementation.

2.3.1 Random Forest

Random Forest is the prototypical forest variant first described by Leo Breiman in 1999 [10]. Independent decision trees are grown with multiple forms of randomness in order to de-correlate trees, leading to a lower variance in predictions. The first form of randomness comes from bagging where each tree is grown with a subset of the N training observations. The second form of randomness comes from choosing a random subset of features to explore at each node. The feature used to split a node and the value at which to split is chosen by the minimization of impurity or the maximization of information gain. When performing inference on a test observation, each individual tree infers a class label for the observation and the final prediction is the class that receives a plurality of votes.

2.3.2 Boosted Forests

Boosted forests consist of sequentially grown trees where each subsequent tree learns from the error induced by the previously grown tree. There are two main types of boosted forest: Adaptive and Gradient. Adaptive boosted forests give more credence to trees that do well on held out samples and is more likely to use mislabeled data in subsequent tree growing iterations. Gradient boosted forests use the prediction error of all observations in the current tree to refine predictions of the subsequent tree. Inference in boosted forests is performed by summing the predictions of all trees rather than using the plurality vote used by many forest variants. This forest variant is popular due to its accuracy and efficient training implementations.

2.3.3 Oblique Forests

Oblique forests consist of decision trees that create non axis aligned splits. Compared to axis split decision forests, forests using oblique splits are capable of better defining class boundaries, resulting in superior inference performance [20]. This can be seen in Fig. 2.1 where an axis aligned decision tree creates a stair step like boundary between classes, whereas an oblique decision tree can create a perfectly discriminating non-axis aligned boundary, Fig. 2.2.

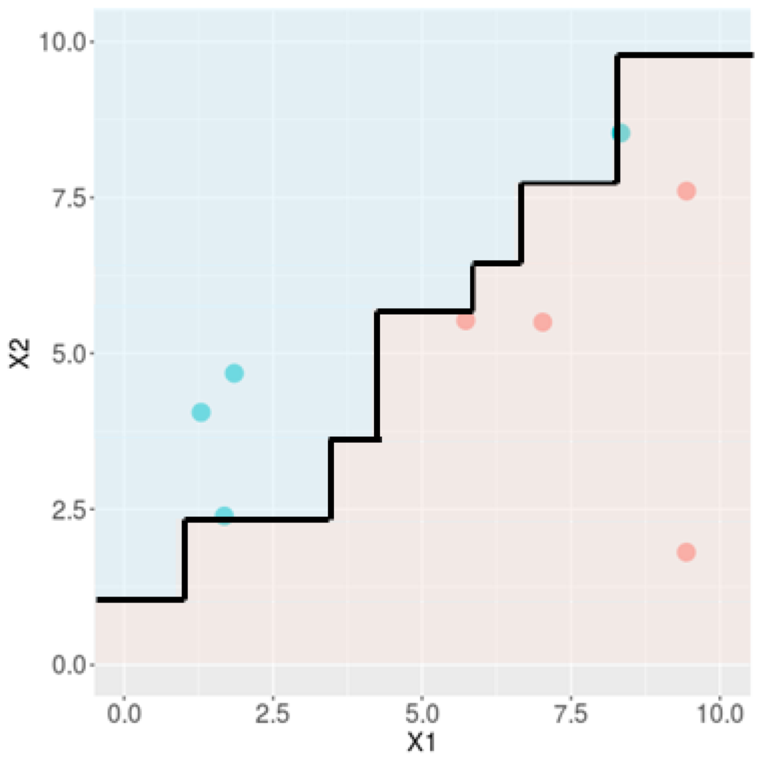


Figure 2.1: Stair step boundary between classes is characteristic of axis aligned splits.

The downside of these forests are their increased training times and storage requirements, sensitivity to noise, and reduced interpretability [9, 21]. So, despite producing superior results, at the time of this writing there are no other oblique forest implementations that scale beyond trivially sized datasets.

2.3.4 Oblique Sparse Projections Forest

Sparse Projections Forests — a subset of oblique forests — use oblique splits at each node in a manner that reduces the drawbacks found in other oblique forests. Leo Breiman first describes such a forest, Forest-RC, in his seminal work on Random Forests [10]. The sparse projections of Forest-RC are created by linearly combining multiple weighted features to create a single new feature. Many of these features are created at each node and searched for an impurity minimizing split.

Randomer Forest (RerF) is an oblique sparse projection forest that limits feature weights to $+1$ and -1 resulting in $d!$ possible feature combinations, where d is the number of features in a dataset. Using sparse projections, rather than completely rotated data, allows RerF to reduce training times, sensitivity to noise, and model complexity as compared to other oblique techniques. RerF outperforms other forest variants including Random Forest, XGBoost, and Random-Rotation Random Forests on a large proportion of the UCI datasets [22].

2.4 Discussion

Decision forests are a broad class of robust machine learning algorithms composed of ensembles of weak learners. Two of the most widely used and studied variants are Random Forests and gradient boosted forests. Another variant, oblique forests, provides class discrimination superior to other decision forests. Despite this highly beneficial quality, oblique forests have not been widely adopted and there are currently no implementations that scale beyond small datasets.

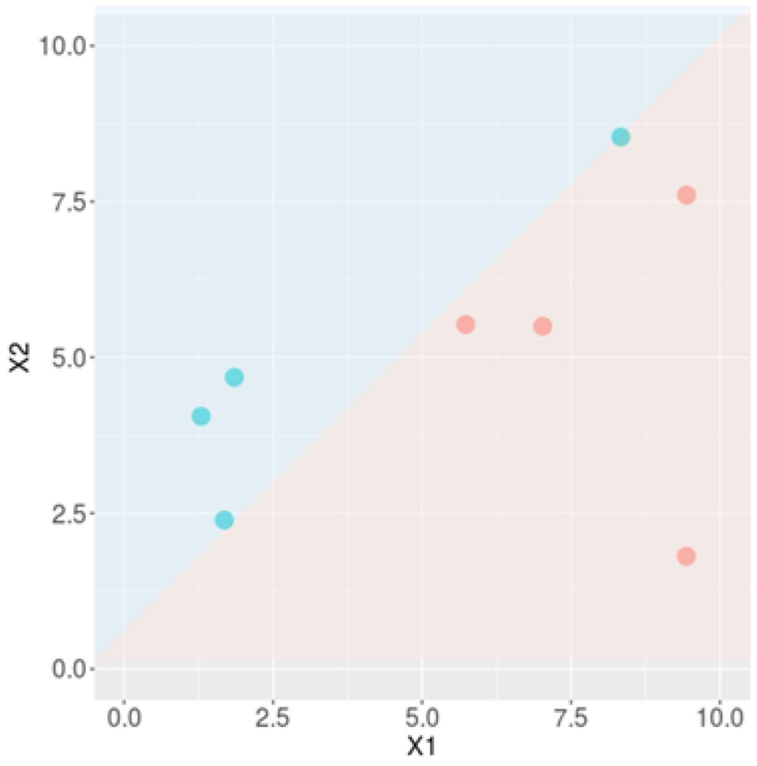


Figure 2.2: Sparse Oblique boundary is able to better discriminate between class boundaries.

Chapter 3

Decision Forest IO

The random nature of decision forests and their applicability to many dataset types makes optimization difficult. Often, optimizing techniques will benefit node splitting either near the tops of trees or for nodes near the base of trees, but not both. We detail here the various methods to grow trees and their implications on memory use and processing time. Several methods to accelerate forest growing are described, followed by a discussion on why these methods are incompatible with oblique sparse projection forests.

3.1 Memory Access Patterns of Random Forests

3.1.1 Node Processing Order

There are two methods to recursively grow a tree structure: breadth first and depth first. In breadth first traversal, all nodes at level L are processed before processing any nodes at level $L + 1$. This requires the storage of 2^L unprocessed nodes at each level, with a maximum of 2^D nodes at maximum depth D. The use of breadth first traversal when growing forests is widely recommended [23, 8, 24] because it allows for several space-time trade-off optimizations, see 3.3.

In depth first traversal, child nodes are placed on a stack as they are created. Nodes are popped from the stack and processed, either placing resulting child nodes on the stack or creating new leaf nodes. This method requires the storage of at most D unprocessed nodes at any time. Depth first traversal requires less memory than breadth first traversal.

3.1.2 Data Traversal: Training

Data consisting of N observations each with d features is an Nxd structure, stored in memory either in row major or column major formats. Each of the N observations are placed contiguously in memory when using the row major format. This format is useful when multiple features in a single observation are accessed closely in time. This is contrasted by the column major format, which stores each of the d features contiguously, a useful method when the same feature in multiple observations are accessed closely in time.

The choice of which format to prefer depends on a system's cache size and the algorithm's data access pattern. In Random Forest, when $\widetilde{N}$ is large, typically near the top of a tree, it is beneficial to use the column major format, where $\widetilde{N}$ is the number of observations in a node. As tree growing progresses, $\widetilde{N}$ shrinks and the row major format becomes preferable. This switch over occurs when cache pollution is unlikely to evict required data ($\widetilde{N} \times cachelinesize < cachesize$) and when a cache load is likely to fetch multiple useful data elements ($\widetilde{N}/N < mtry/d$).

3.1.3 Data Traversal: Inference

Like training data, the data presented to a decision forest model for classification can be formatted in either row major — where an observation's features are contiguous in memory — or column major — where features are stored contiguously. The choice of which to use depends on whether inference is performed on individual observations or on multiple observations in a batch. The row major format is preferable when performing inference on single observations because each cache line request of the inference data provides data potentially useful by subsequently traversed nodes in the forest. This is contrasted by column major storage where each cache line request is only guaranteed to provide one useful data element and all other elements in the remainder of the cache line will be cache pollution. Contrarily, batched processing can benefit from a column major formatting because, at each node, a single feature of multiple observations is tested, allowing a single cache line request to potentially load multiple useful data elements. When batching inferences a row major format guarantees a load of one useful element and multiple cache pollution elements.

3.2 Multithreaded Forest Training

There are multiple locations within the decision forest training process where multiple threads can be used to accelerate training. The most fine grained parallelism will process each feature using multiple threads to find the best split. Both the sorting and best split searching sub-tasks are cache efficient and not easily divisible, so neither would benefit from multithreading. In the case where histogram bins are well defined, multiple threads could populate thread specific bins — a slow random read process — then merge bin tallies with other threads prior to the exhaustive split search sub-task. This form of parallelism is typical of histogram accelerated decision forests.

Another location within the forest training process where multiple threads could be employed is over each of the *mtry* features in a node. This method would be inefficient when *mtry* is less than the number of threads and when $\tilde{N}$ is small because little work would be done by each thread. A third location for parallelism is at each node. This form of parallelism is easily implemented but is inefficient when the number of nodes waiting to be processed is less than the number of threads (i.e. at the tops of trees) and when $\tilde{N}$ is small because little work would be done by each thread. The final location to perform parallelism is at the tree level, where a single thread processes an entire tree. This method duplicates all tree growing structures, thereby resulting in a per thread $O(N)$ memory increase roughly equivalent to the size of a single feature. This method is also inefficient when the number of trees to process is less than the available number of threads.

3.3 Decision Forest Training Acceleration

Testing shows many forest implementations spend greater than 80% of forest growing time determining the cut feature and cut value for each node, making this sub-task the target for most optimizations in decision forest systems. The most simplest way to reduce node splitting time is using hyper-parameter selection to reduce the number of nodes a tree creates or reduce the number of features explored at each node. Three parameters are typically available in decision forests to reduce the number of nodes created in each tree: minimum parent size, maximum depth, and maximum number of nodes. There is also a parameter to change the number of features explored at each node, mtry, which ranges from 1 to d, where d is the number of features in a dataset. Reducing training time through parameter selection can reduce model efficacy, so it is important to make the node splitting function, see Alg. 1, as efficient as possible.

The sub-tasks of the node split algorithm, Alg. 1, which require the most time are: feature loading (line 6), feature sorting (line 7), and the exhaustive split search (line 8). The complexities of these sub-tasks are respectively $O(\tilde{N})$, $O(\tilde{N}log(\tilde{(}N))$, and $O(\tilde{N}C$, where C is the number of unique labels in the dataset. Run time analysis shows each of the sub-tasks take nearly the same operating time despite the range of complexities.

3.3.1 Feature Loading Optimization

Feature loading consists of loading the target feature from each of a node's $\tilde{N}$ resident observations into a temporary vector. This is an inherently inefficient gather operation, which suffers from cache misses due to the random memory reads induced by the splitting of observations at each node. Thus, at the top of a tree each gather operation tends to be efficient because the bagging of observations results in roughly 63% of the training set observations being resident in the root node. The efficiency at this level of a tree is realized because each cache load is likely to result in multiple cache hits. At each level

Algorithm 1 Basic Find Best Split Location

```
1:  ▷ $n$: a set of observations
2:  ▷ $mtry$: the number of features to consider for each split
3:  procedure FIND BEST SPLIT($n$)
4:      $testfeatures \leftarrow$ randomly select $mtry$ features to test
5:      for all $i$ in $testFeatures$ do
6:          load all $n_i$ into tempFeature vector
7:          sort(tempFeature)
8:          $splitInfo \leftarrow exhaustiveSplitSeach(tempFeature)$
9:          if $splitInfo.Score > bestSplit.Score$ then
10:             $bestSplit.Score \leftarrow splitInfo.Score$
11:             $bestSplit.Feature \leftarrow i$
12:             $bestSplit.Value \leftarrow splitInfo.Value$
13:         end if
14:     end for
15:     return $bestSplit$
16: end procedure
```

of the tree, $\tilde{N}$ is reduced by half, which reduces the chance the loading of a feature into cache will result in subsequent cache hits.

The typical means to accelerate the feature loading sub-task is through software prefetching. Modern Processors perform hardware prefetching when memory accesses form a simple pattern (e.g. loading every fourth memory location) and so is unlikely to be triggered when training forests due to the random splitting of observations. The software prefetcher is able to inform the processor to load memory locations regardless of access pattern, thereby reducing the load latency that would otherwise be experienced.

3.3.2 Sorting Optimization

Feature sorting entails sorting a vector of feature values while maintaining a mapping between each observation's feature value and class label. The typical alternative to per node feature sorting is to sort all features prior to forest training, maintaining a two way mapping between feature values and observation indices, and rearranging the training data in memory as observations are split between children nodes [25, 19]. In addition to removing the need to sort, this technique also removes the need to gather feature values at each node. The algorithm instead searches for the best split point by streaming over each of the *mtry* features. The downside of this method is a large memory footprint and the need to relocate observations in memory after each node split, which requires accessing every feature of every resident observation in a random manner. The number of memory accesses grows linearly with d, the number of features in a dataset, irrespective of hyper-parameter settings.

Another method to remove per node sorting is to define sorted accumulation bins. Some systems define bins based on the unique values of each feature [18], whereas other systems implement a histogram method [6], or a similar reduced precision method [7]. The predefinition of the number and size of bins is a trade-off between processing time and best split accuracy. When using bins, the gathering step of the splitting function changes to incrementing a bin's tally when its specific feature value is encountered. An added benefit of this technique is the possible reduction of split locations when the number of bins is smaller than $\tilde{N}$. A downside of this method is the increase of split locations when the number of bins is greater than $\tilde{N}$.

Each of these binning optimizations requires increased memory usage due to the storage of bin properties and mappings between features and bins. In addition, the determination of value to bin can become a costly function due to a random read pattern.

3.3.3 Split Search Optimization

The exhaustive search for an optimal split entails traversing the ordered feature vector from least to greatest value and calculating the impurity of each side assuming all values less than the current traversal location would go to the left node and all greater values would go to the right node. Splits between equal feature values are not possible and need not be considered. Thus a weighted bin for each unique feature value reduces the possible split points from $\tilde{N}$ to U, where U is the number of unique feature values. This is beneficial when U is less than $\tilde{N}$ and detrimental otherwise. When using histogram bins split are only possible between bins. This reduces the required search space, but, as a heuristic method, does not guarantee the best possible split and so may affect model efficacy.

3.4 Conclusion

Decision Forests algorithms are difficult to efficiently process because the random IO of the algorithm is a product of the random splits that occur in each node of the forest. Optimizations in sorting and searching have been developed to minimize this lack of cache coherence, but are not practical for sparse projection forests. For OSPFs to realize the gains of these optimizations all potential oblique features would need to be materialized, which is unfeasible. Thus, implementations of oblique sparse projection forests cannot rely on many of the optimizations employed by axis aligned forests.

Chapter 4

R-RerF

4.1 Introduction

Randomer Forest (RerF) is a recently conceived decision forest variant with superior accuracy and complexities, both training and inference, similar to those of Random Forest. RerF and Random forest are both considered sparse random projection forests. The algorithms differ by their choice of sparse projections, Random Forest node splitting only considers very sparse projections, whereas RerF node splitting also considers linear combinations of sparse projections.

At each node in a Random Forest a random subset of features are exhaustively tested to determine which feature and cut value minimizes impurity when resident observations are split into two subsets. When class boundaries are not axis aligned this splitting method potentially leads to deep trees, increased variance, and over-fitting. This is contrasted by RerF, which, considers oblique features created by linearly combining multiple features in addition to the axial splits considered by Random Forest.

We implement R-RerF in the R programming language using the Oblique Sparse Projection Forest (OSPF) framework. Including this framework in the system allows for easy extension of R-RerF to other oblique sparse projection forests.

4.2 R-RerF Implementation

RerF was originally implemented in matlab and was ported to R in order to increase speed and flexibility. This new system was branded R-RerF. Acceleration of R-RerF was accomplished through multithreading and execution analysis. Multithreading in R is realized by forking the R process, which limits the fine grained interactions possible with threads. To overcome this limitation, R-RerF processes a single tree per forked process, thereby trading memory efficiency for processing efficiency. Execution profiling was used to further improve processing efficiency, helping us avoid slow R functions and identifying the slowest portions of our system: sorting and split finding. We were unable to improve upon R's c++ optimized quick sort function. The splitting function was rewritten in C++, but still remained our function with the highest execution time.

Writing the code in R allowed for quick modification and testing of implementation details and allowed for custom tailoring of the algorithm to suit novel problems. To accomplish this level of extensibility required two key insights. First, we realized that the rotation of training data need not be completely materialized, instead the sparse projections can be materialized as needed in a computationally efficient sparse vector multiplication. The second realization was that by allowing a data scientist to provide their own sparse rotation matrix would allow for easily implementable data specific custom projections. Thus, at the core of R-RerF's novelty is a sparse projection matrix which efficiently rotates the data at each node to increase the number of potential split features, thereby facilitating the rapid integration of other forest variants such as patch detectors, random forest, Random Rotation Random Forest, and Forest-RC. This ease of code manipulation coupled with the package management system provided in R, CRAN, minimizes the effort required by data scientists to use and contribute to the system.

4.3 System Complexity

The complexity of a system shows how a runtime characteristic of an algorithm changes with input size.

4.3.1 Theoretical Time Complexity

The time complexity of an algorithm characterizes how the theoretical processing time for a given input relies on both the hyper-parameters of the algorithm and the characteristics of the input. Let T be the number of trees, N the number of training samples, d the number of features in the training data, and $mtry$ the number of features sampled at each split node. The average case time complexity of constructing a Random Forest is $\mathcal{O}(mtryTN\log^2 N)$ [24]. The $mtryN\log N$ accounts for the sorting of $mtry$ features at each node. The additional $\log N$ accounts for both the reduction in node size at lower levels of the tree and the average number of nodes produced. Random Forest's near linear complexity shows that a good implementation will scale nicely with large input sizes, making it a suitable algorithm to process big data. RerF's average case time complexity is similar to Random Forest's, the only difference being the addition of a term representing a sparse matrix multiplication which is required in each node. This makes RerF's complexity $\mathcal{O}(mtryT \log N(N \log N + \lambda d))$, where λ is the fraction of nonzeros in the $d \times mtry$ random projection matrix. We generally let λ be close to $1/d$, giving a complexity of $\mathcal{O}(mtryTN \log^2 N)$, which is the same as for Random Forest. Of note, in Random Forest $mtry$ is constrained to be no greater than d, the dimensionality of the data. RerF, on the other hand, does not have this restriction on $mtry$. Therefore, if $mtry$ is selected to be greater than d, RerF may take longer to train. However, $mtry > d$ often results in improved classification performance.

4.3.2 Theoretical Space Complexity

The space complexity of an algorithm describes how the theoretical maximum memory usage during runtime scales with the inputs and hyperparameters. Let C be the number of classes and T, d, and N be defined as in Section 4.3.1. Building a single tree requires the data matrix to be kept in memory, which is $\mathcal{O}(Nd)$. During an attempt to split a node, two C-length arrays store the counts of each class to the left and to the right of the candidate split point. These arrays are used to evaluate the decrease in Gini impurity or entropy. Additionally, a series of random sparse projection vectors are sequentially assessed. Each vector has less than d nonzeros. Therefore this term is dominated by the Nd term. Assuming trees are fully grown, meaning each leaf node contains a single data point, the tree has $2N$ nodes in total. This term gets dominated by the Nd term as well. Therefore, the space complexity to build a RerF model is $\mathcal{O}(T(Nd + C))$. This is the same as that of Random Forest.

4.3.3 Theoretical Storage Complexity

We define storage complexity as the dependency of disk space required to store a forest on the inputs and hyperparameters. Assume that trees are fully grown. For each leaf node, only the class label of the training data point contained within the node is stored, which is $\mathcal{O}(1)$. For each split node, the split dimension index and threshold are stored, which are also both $\mathcal{O}(1)$. Therefore, the storage complexity of a RF is $\mathcal{O}(TN)$.

For RerF, the only aspect that differs is that a (sparse) vector projection along which to split is stored at each split node rather than a single split dimension index. Let z denote the number of nonzero entries in a vector projection stored at each split node. Storage of this vector at each split node requires $\mathcal{O}(z)$ memory. Therefore the storage complexity of a RerF model is $\mathcal{O}(TNz)$. z is a random variable whose prior is governed by λ, which is typically set to $1/d$. The posterior mean of z is determined also by the data; empirically it is close to $z = 1$. Therefore, in practice, the storage complexity of RerF is close to that of Random Forest.

4.4 Experimental Results

The performance of decision tree implementations typically entail a thorough exploration of accuracy – how well models classify test data – and training times; inference speed is another important measure but is not commonly discussed for many popular systems. The measure of performance used here is training time, scalability, and inference throughput; system performance as it relates to accuracy can be found in other RerF literature [22]. We test our system with three datasets commonly used to measure training time performance: MNIST consists of 60000 images of digits (0-9) each containing 784 features; Higgs consists of 250,000 observations of two classes, either signal or background, each containing 28 features; and p53 consists of 16,772 observations of protein mutations, either active or inactive, each containing 5409 features. We compare our system to what we consider the most popular decision forest implementation, XGBoost, and the fastest Random Forest implementation, Ranger. All experiments were run on a 64-bit Ubuntu 16.04 platform with four Intel Xeon E7-4860V2 2.6 GHz processors, with 1TB RAM.

Initially it was assumed that an implementation primarily written in R would be significantly slower than its C++ counterparts. Surprisingly, R-RerF outperformed XGBoost in two of three experiments, Fig. 4.1. R-RerF performs worst on Higgs, the largest dataset, because the size of resulting trees in R combined with memory inefficiencies inherent in R exacerbates the memory bottleneck. As resources are added, the additional cache and separation of growing trees into separate processes allows R-RerF to more efficiently use memory resulting in improved scalability on the Higgs dataset, Fig. 4.2.

When performing inference, R-RerF batches test observations in order to accelerate the process. Batching allows for a regular traversal of trees and multiple reuse of fetched memory. This inference technique is found in most decision forest implementations including Ranger and XGBoost. It can be seen in Fig. 4.3 that R-RerF's inference speed is far slower than XGBoost. R-RerF's inference speed is slow when compared to traditional decision forests because determining a traversal path requires combining multiple features, requiring an additional memory indirection. Despite this penalty, R-RerF is still able to outperform Ranger in two out of three tests.

4.5 Conclusion

R-RerF is the first scalable and easily accessible, via CRAN, oblique forest implementation. The system provides state of the art discriminating performance and scales well with additional resources. In addition, because it is written in R, R-RerF can easily be tailored to a given dataset through its use of an easily modifiable sparse projection matrix or by taking advantage of R packages of popular enhancements such as external memory, distributed computing, or sparse processing. Unfortunately, R-RerF suffers from a large memory footprint, poor single core performance, large model size, and poor inference speeds; deficiencies we address in subsequent chapters. Despite these shortcomings R-RerF's performance remains competitive with other highly optimized decision forest variants.

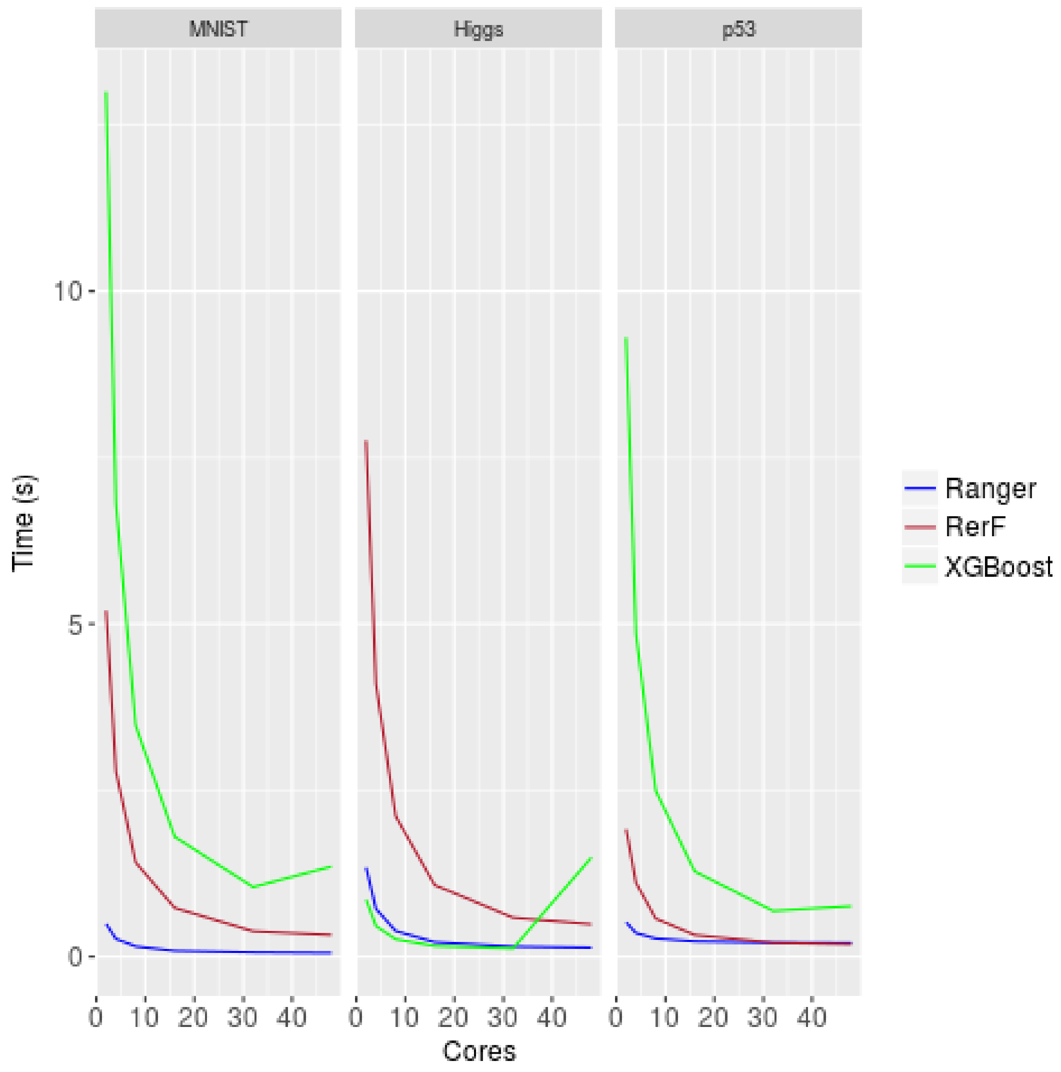


Figure 4.1: R-RerF Training Time as a function of cores used as compared to similar systems. Three datasets were used: MNIST, Higgs, and p53.

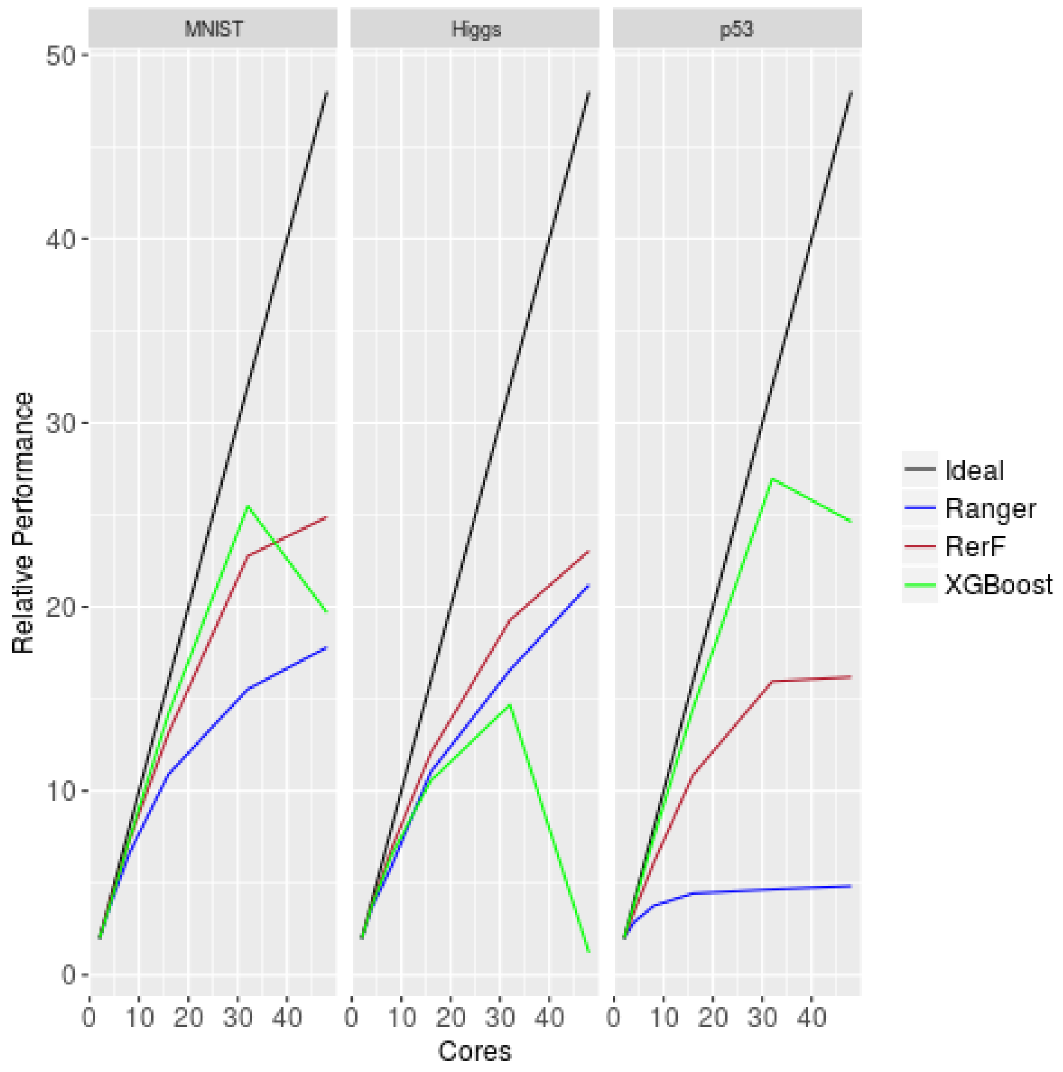


Figure 4.2: R-RerF Strong Scaling compared to similar systems. Three datasets were used: MNIST, Higgs, and p53.

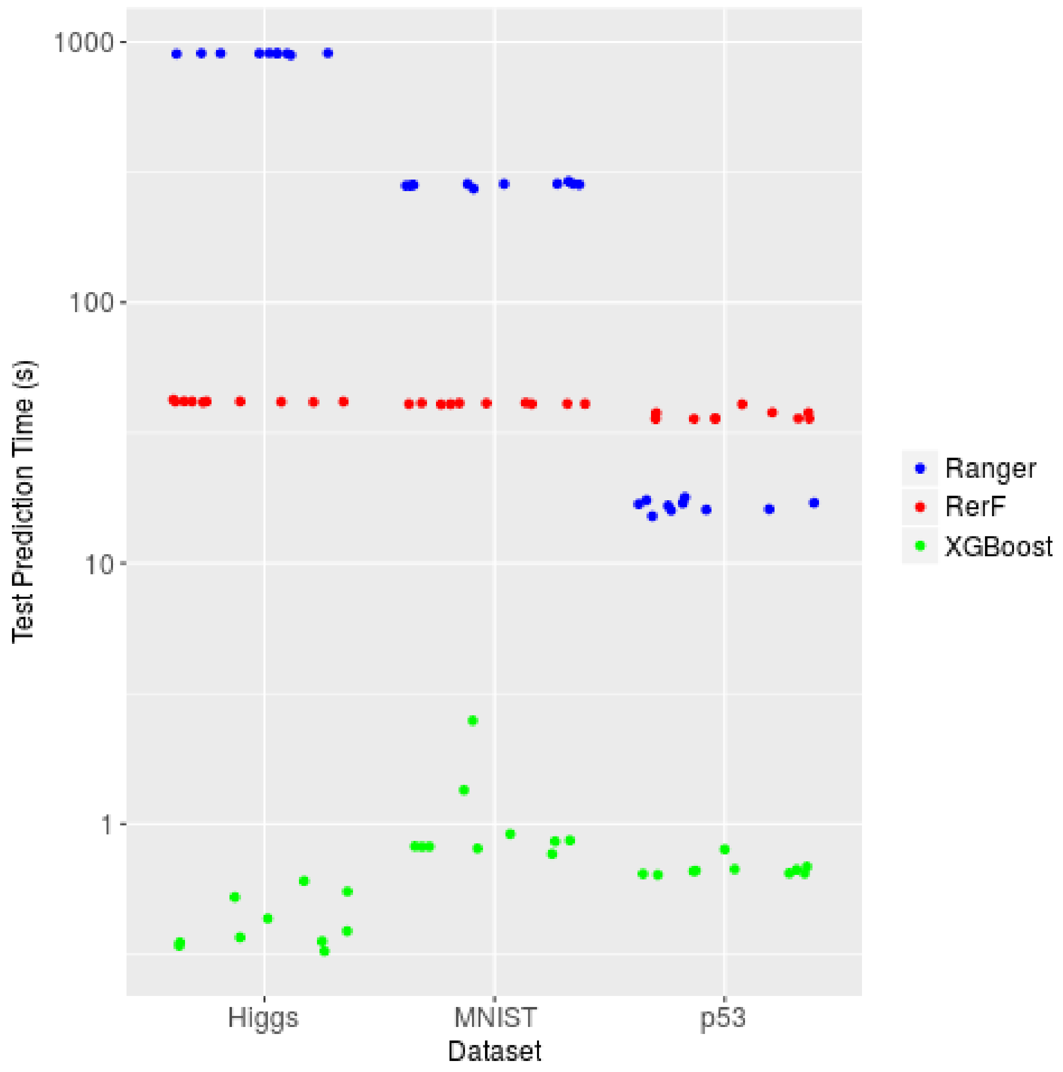


Figure 4.3: R-RerF Inference Times on hold-out test observations compared to similar systems. Test set sizes: Higgs 25,000; MNIST 10,000; p53 400.

Chapter 5

Forest Packing

5.1 Introduction

R-RerF was the first scalable oblique forest system, but the implementation suffered because of high latency and low throughput inferences, Ref. 4. This poor inference speed, particularly latency, is endemic to decision forests and thus makes the systems unusable for many real-time applications such as computer vision and spam detection. Poor inference speeds are caused by the combination of large model sizes combined with random memory access patterns. As an ensemble classifier, decision forests are composed of many weak classifiers, each of which may have a size on order with the training set, leading to a large overall memory footprint. When the model size is larger than a system's cache, typically KBytes for fast cache and low MBytes for slow cache, the inference operation relies on the order of magnitude slower main memory. The paths through a decision forest are purposefully uncorrelated, which leads to random accesses throughout the model for each inference task, making common acceleration tools—such as GPUs—unusable for general forest inference.

Decision forest research typically focuses on model training systems without mention of run time operation. Application of these powerful tools is hindered by this oversight, which has lead to increased research into forest inference acceleration and development of several third-party post training optimizations [14, 15]. Current solutions either place structure limiting requirements on the forests, e.g. maximum node depth, or focus on increasing throughput at the cost of increased inference latency, e.g. batching. The method described here, Forest Packing, extends previous research on this topic by introducing several tree storage memory optimizations and a reordering of the tree traversal process to take advantage of modern CPU enhancements.

5.2 Methods and Technical Solutions

Attempts to increase the speed of decision forest inference falls into two categories: memory access optimizations and inference algorithm modifications. Our proposed improvement to forest based inference, Forest Packing, takes advantage of both improvement types. We use inference latency, specifically classification latency, to indicate model performance (training time is a popular complementary topic that we do not consider here). Other decision forest variants such as regression or distance learning forests are not specifically discussed here, but the techniques we describe should extend to these tools. The input to forest packing is a trained forest, F, that consists of decision trees, t. Each internal node of the trees describes a splitting condition on the data and has two children. Each leaf node contains a single class label; a criteria typical of random forests [10, 26], but not true for all variants. One of the novel optimizations that we present relies on the single class assumption.

Forest Packing, the system presented here, reorganizes the trees in a forest to minimize cache misses, allow for use of modern CPU capabilities, and improve parallel scalability. The system outputs $\lceil T/B \rceil$ bins, where T is the number of trees in the forest and B is the bin size—a user provided parameter defining the number of trees in a bin. A bin is a grouping of at most B trees into a contiguous memory structure. Most bins will contain B trees while one bin may contain between 1 and B-1 trees. Within each bin, we interleave low-level nodes of multiple trees to realize memory parallelism in each cache line access. We decrease cache misses by using split cardinality information to store popular paths contiguously in memory. During inference, each bin is assigned to an OpenMP thread (for shared memory). Forest packing includes a runtime system that prefetches data and evaluates tree nodes out-of-order as data is ready, leveraging the memory layout to maximize performance.

5.2.1 Memory Layout Optimization

We describe our memory layout as a progression of improvements over the breadth-first layout, BF, typically used in random forests, with each improvement reducing cache misses or encoding parallelism. Fig. 5.1 describes this evolution with each panel displaying a tree in which the nodes are numbered breadth-first and the resulting layout in memory is shown as an array at the bottom of the panel. Breadth-first layouts are typical in decision forests because they provide the sequential traversal through all nodes used by batched inference processing. The depth-first (DF) layout is preferred for single observation inference because it allows for the possible reuse of a memory load. We will use aspects of both breadth- and depth-first layouts in our ultimate design.

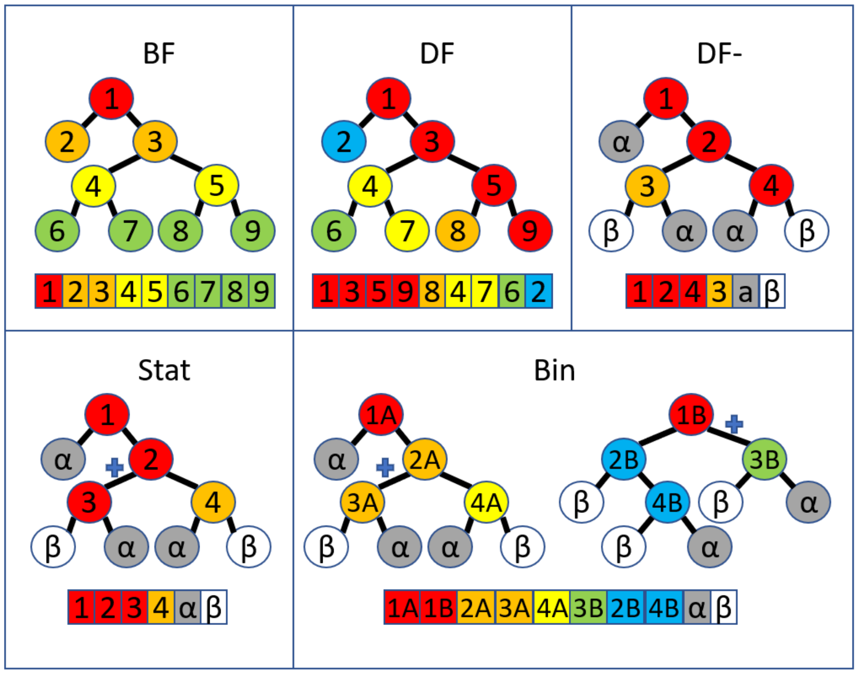


Figure 5.1: The representation of trees as arrays of nodes in memory for breadth-first (BF), depth-first (DF), depth-first with class nodes (DF-), statistically ordered depth-first with leaf nodes replaced by class nodes (Stat), and root nodes interleaved among multiple trees (Bin). Colors denote order of processing, where like colors are placed contiguously in memory.

Our first optimization reduces the duplication of information contained in leaf nodes thereby reducing the number of nodes in the forest almost in half. In many classification forest variants, each leaf node provides both a signal that the tree traversal is complete and a class label determined during training by the plurality observation class in a leaf node. Rather than pointing parent nodes to their own unique children, parent nodes instead point to communal leaf nodes which provide the functionality of a typical leaf node without the duplication. We call this encoding DF-. We are unaware of other literature recommending this encoding, which reduces the size of a tree from n nodes to $n/2 + C$ nodes, where C is the number of classes present in a dataset.

In most datasets, the number of distinct classes are many orders of magnitude smaller than the number of nodes in the tree and so we expect the DF- trees to be nearly half the size of DF trees. Removing these nodes has the dual benefit of allowing more useful nodes to be loaded by each memory fetch (a fact we exploit in the Stat layout) and also greatly reduces cache pollution. The class nodes that replace leaf nodes are placed at the end of each tree's block of contiguous memory. The DF- panel of Fig. 5.1 shows the resulting layout when building a decision tree for a two-class (α, β) problem. DF- indicates depth-first with leaf nodes removed.

The next improvement encodes paths through trees sequentially in memory based on the number of observations used to create the nodes during training. This statistical redefinition of the BF- layout is called Stat. We use the leaf cardinalities collected during training to determine the likelihood that any given data point routes to a specific leaf. If cardinality information is unavailable, these statistics can be inferred after training using a suitably large set of observations. We then enumerate depth first paths based on their probability of access. The Stat panel of Fig. 5.1 illustrates this process with "+" indicating a more likely path, leading to the decision to enumerate the path to node 3 prior to node 4. The statistical ordering applies to nodes from the root to the leaf parents, because class nodes that replace leaf nodes are at the end of the block of memory and so are not considered for statistical ordering.

In more detail, Stat considers each parent node and its two children. The child that is accessed most often is placed adjacent to the parent node in memory while the less accessed child is placed later in the block of memory. If a parent node has a leaf node child and an internal node child, the internal child node is always placed adjacent to the parent while the leaf node is shared among all leaf nodes of the same class at the end of the memory block. Similar optimizations have been recommended in one form or another by other researchers [27].

Our final memory optimization, Bin, interleaves the nodes of multiple trees into a single block of memory, called a bin, to both reduce memory latency and to allow for the encoding of parallel memory accesses. This layout takes advantage of the fact that a parent node is accessed about twice as often as each of it's children and so nodes at lower levels of a tree are accessed far more often then nodes at higher levels. This is similar to the hot (often used nodes) and cold (rarely used nodes) memory model recommended by Chilimbi et al. [28]. By interleaving the lower level nodes from multiple trees in a bin, we are increasing the density of "likely to be used" nodes which allows a single cache line fetch to be more useful while also reducing cache pollution. The Bin panel of Fig. 5.1 shows the root (level 0) nodes interleaved in the layout and all higher level nodes are stored one tree at a time using the Stat method. A similar recommendation was proposed by Ren et al. where trees are interleaved by level for the entirety of the tree [29]. In our testing, interleaving trees past a certain depth results in an increase of inference latency, Fig. 5.2.

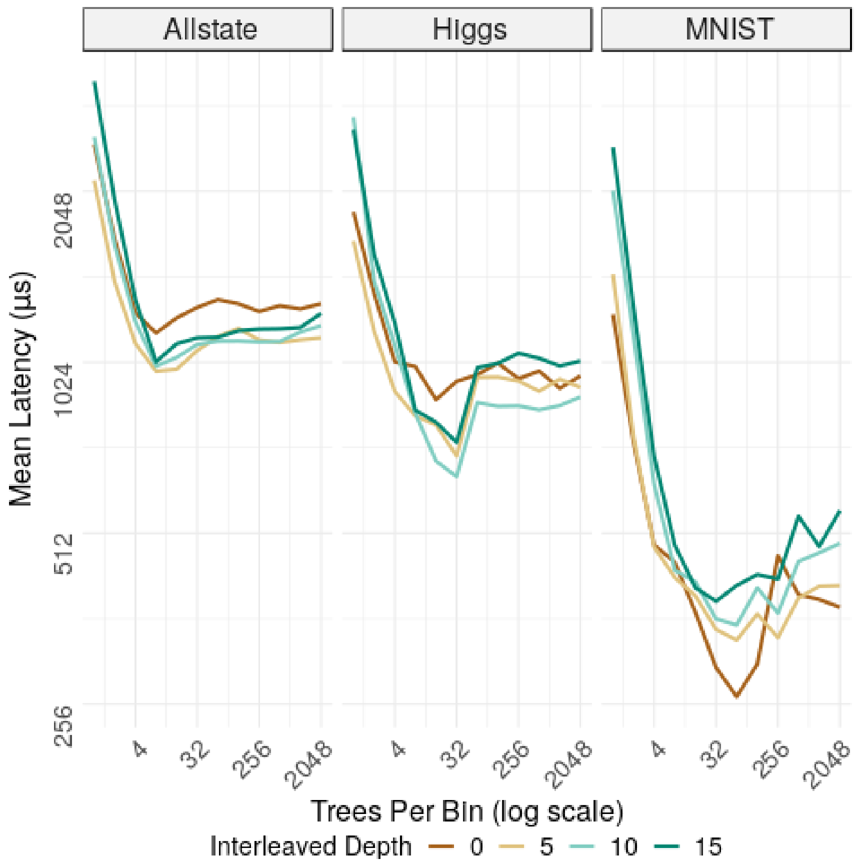
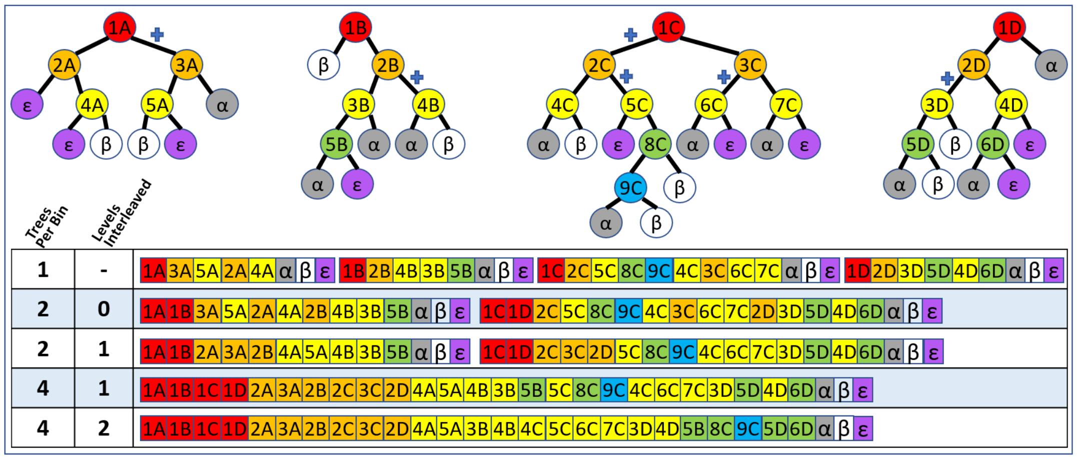


Figure 5.2: Prediction time as a function of the number of trees in each bin and their interleaved depths. Ideal bin parameters are forest dependent. Interleaving trees beyond a certain depth becomes detrimental to performance.

There are two parameters used when interleaving nodes. (1) The bin size determines the number of trees interleaved in a bin. Larger bin sizes encode more parallelism for each memory fetch at low levels in the tree. Each bin is an independent array of trees that can be distributed for parallel evaluation across threads or a cluster, so at least one bin is required per thread in order to occupy parallel resources. In other words, the number of bins will ideally be a multiple of the number of threads used to perform inference. (2) Interleaved depth determines how many lower levels of the trees in a bin are interleaved;

the remaining levels of each tree are stored according to the Stat encoding. Interleaving too many levels results in breadth-first like behavior resulting in degraded performance.

The Bin layout combines binned interleaving for the top levels of a tree and statistical depth-first layout, Stat, for the bottom levels in a tree. A more in depth example of this layout can be found in Fig. 5.3, which demonstrates the layout for a forest of 4 trees and 3 classes with varying bin sizes and depths interleaved. A design experiment helps choose the bin size that makes sense in light of the properties of the processor memory hierarchy and forest characteristics. Fig. 5.2 explores the effects bin size and interleaved depth has on a trained forest. The figure displays average prediction time (lower is better) for an observation given varying values of bin size. The characteristics of the datasets and their resulting forests can be seen in Table 5.1.



Trees Per Bin	Levels Interleaved	
1	-	1A 3A 5A 2A 4A α β ε 1B 2B 4B 3B 5B α β ε 1C 2C 5C 8C 9C 4C 3C 6C 7C α β ε 1D 2D 3D 5D 4D 6D α β ε
2	0	1A 1B 3A 5A 2A 4A 2B 4B 3B 5B α β ε 1C 1D 2C 5C 8C 9C 4C 3C 6C 7C 2D 3D 5D 4D 6D α β ε
2	1	1A 1B 2A 3A 2B 4A 5A 4B 3B 5B α β ε 1C 1D 2C 3C 2D 5C 8C 9C 4C 6C 7C 3D 5D 4D 6D α β ε
4	1	1A 1B 1C 1D 2A 3A 2B 2C 3C 2D 4A 5A 4B 3B 5B 5C 8C 9C 4C 6C 7C 3D 5D 4D 6D α β ε
4	2	1A 1B 1C 1D 2A 3A 2B 2C 3C 2D 4A 5A 3B 4B 4C 5C 6C 7C 3D 4D 5B 8C 9C 5D 6D α β ε

Figure 5.3: Forest packing with the Bin memory layout given four trees and varying setting. We show different parameterizations of number of trees per bin and depth of interleaving. Colors of internal nodes denote node level in the tree. Levels Interleaved denotes the highest level of each tree interleaved.

Table 5.1: Dataset and Resulting Forest Information

	Allstate	**Higgs**	**MNIST**
Observations	500000	250000	60000
Test Observations	50000	25000	10000
Features in Dataset	33	30	784
Trees in Forest	2048	2048	2048
Internal Nodes (avg)	90020	23964	5008
Avg Leaf Depth	25	21	17
Deepest Leaf Depth	74	65	50

Fig. 5.4 shows performance comparisons between the memory optimizations described above. The first three performance improvements (DF, DF-, and Stat) are purely reorganizations of nodes within memory. In addition to reorganizing nodes, Bin groups trees into bins and interleaves the nodes of trees within a bin.

5.2.2 Tree Traversal Modification

The inference algorithm includes the traversal of trees from root to leaf using a path determined by a simple comparison of data stored in each node to the test observation, Algorithm 2. The most common modification of this traversal processes multiple test observations through a tree simultaneously in batches. This optimization results in much higher throughput of classification inference [15, 13]. Although groups of observations are processed faster, the latency of each inference task is increased. Other methods have been used to accelerate forest based inference using GPUs, SIMD operations, traversal unrolling, and branch prediction [14, 15, 29]. Many of these optimizations place restrictions on forest structure such as a maximum depth or require a full tree [30].

The binned forest memory optimization, Bin, described in 5.2.1 allows us to efficiently modify the processing order of trees (Algorithm 3) to simultaneously traverse multiple trees in a manner that takes advantage of modern CPU enhancements while also allowing us to use intra-observation threaded parallelism. Forest Packing, our acceleration technique, is the use of the culmination of memory improvements, Bin, with this efficient tree traversal method described below. For brevity, we will refer to Forest Packing, the combination of memory improvements and efficient tree traversal, as Bin+.

Our binning strategy adds an additional layer of hierarchy within the forest (i.e. the bins) which provides for multiple levels of parallelism. The first level of parallelism, inter-bin parallelism, takes advantage of the embarrassingly parallel nature of trees, allowing each bin to be processed by a thread independent of work done in other bins. This form of parallelism was always available within forests using individual trees rather than bins.

Intra-bin parallelism realizes performance improvements through fine-grained, low-level prefetching and scheduling provided inherently in modern CPUs. Bin+ takes advantage of this capability by evaluating all trees in a bin using a round-robin order, thereby giving a single thread additional non-blocking avenues of work. This has the dual benefit of using more of each thread's processing capability and gives us an opportunity to explicitly prefetch the upcoming node prior to it being required (line 17, Algorithm 3).

We use simple policies to encode execution overlap because more complex policies incur scheduling overheads that exceed gains. Overlap happens

Algorithm 2 Single Tree Traversal

```
1: procedure TREEPREDICTION($t, o[]$)
2:     ▷ Tree, $t$, an array of nodes
3:     $cn \leftarrow 0$                                    ▷ start at tree root
4:     while $t[cn]$ is internal node do
5:         ▷ get split feature of node cn
6:         $sf \leftarrow t[cn].splitFeature$
7:         ▷ compare observation's feature to split value
8:         if $o[sf] < t[cn].splitValue$ then
9:             $cn \leftarrow t[cn].leftChild$
10:        else
11:            $cn \leftarrow t[cn].rightChild$
12:        end if
13:    end while
14:    return $t[cn].classNumber$
15: end procedure
```

among tens of memory accesses and hundreds to thousands of instructions. Trying to control this fine-grained process in software is not practical. Instead, we assign a single thread to each interleaved bin which evaluates the bin's trees in round-robin order. For each node that we evaluate, we issue a prefetch instruction for the memory address of the resulting child node, with the idea that useful work from other trees can be performed while the resulting child node is being loaded into cache. We proceed navigating through the levels of the tree in the same order that we processed the root nodes. This round-robin scheduling submits independent instructions for each tree. In practice, the processor executes these independent instructions out-of-order as data becomes available.

5.3 Empirical Evaluation

We evaluate Forest Packing in order to quantify the benefits from memory layout and scheduling optimizations. We start with a breakdown of the contributions of each optimization, applying them incrementally. An overview experiment using CPU performance counters demonstrates the improvement of Forest Packing versus other layouts. We explore the scalability of each of the optimizations across a shared-memory multithread system to minimize inference latency. We finish our evaluation by comparing the inference latency of Forest Packing to two commonly used forest systems.

5.3.1 Experimental Setup

We implement all of the optimizations described in Section 5.2 and apply them successively. We start with BF as our baseline implementation because it performs similarly to a popular decision forest implementation, XGBoost. Thus, comparative evaluations are against our re-implementation, BF. We focus on standard decision forests that create deep trees with a single class per leaf node. We infer the class of each test observation sequentially, only starting the inference of an observation at the completion of the previous observation in order to measure test latency.

All experiments were run on a 64-bit Ubuntu 16.04 platform with four Intel Xeon E7-4860V2 2.6 GHz processors, with 1TB RAM. gcc 5.4.1 compiled the project using -fopenmp, -O3, and -ffast-math compiler flags.

We perform all experiments against three common machine-learning datasets that are widely used in competitions and benchmarks. Training

Algorithm 3 Binned Tree Traversal

```
procedure BinPrediction($b, o[]$)
    ▷ Bin, $b$, composed of intertwined trees
    ▷ $binSize \leftarrow$ number of trees in a bin
    ▷ int $np[binSize]$                                   ▷ node pointers
    ▷ int $predictions[numClasses] \leftarrow 0$
    $np[] \leftarrow 0 : binSize - 1$                     ▷ set np to root nodes
    do
        $notInLeaf \leftarrow 0$
        for all $p$ in $np$ do
            if $b[p]$ is an internal node then
                $sf \leftarrow b[p].splitFeature$
                if $o[sf] < b[p].splitValue$ then
                    $p \leftarrow b[p].leftChild$
                else
                    $p \leftarrow b[p].rightChild$
                end if
                prefetch(b[p])
                $++notInLeaf$
            end if
        end for
    while $notInLeaf \neq 0$
    for all $p$ in $np$ do
        $++predictions[b[p].classNumber]$
    end for
    return $predictions[]$
end procedure
```

size is reported here as this determines the size and structure of the resulting forests. Categorical data is one-hot encoded so that all datasets contain numeric data represented as doubles in our data structures. MNIST is a popular numeric dataset of 60,000 handwritten digit images. The Higgs dataset was used in a popular Kaggle competition and contains 250,000 observations of numeric features [31]. We use a subset of the Kaggle competition Allstate dataset which consists of categorical and numeric features [32]. Categorical features are converted to numeric features by the forest growing system (RerF or XGBoost). The principles shown are independent of the system used to grow the forest, but for benchmarking purposes RerF is used to create our forests which are then post-processed into packed forests. Further information about these datasets and resulting trained forests can be found in Table 5.1.

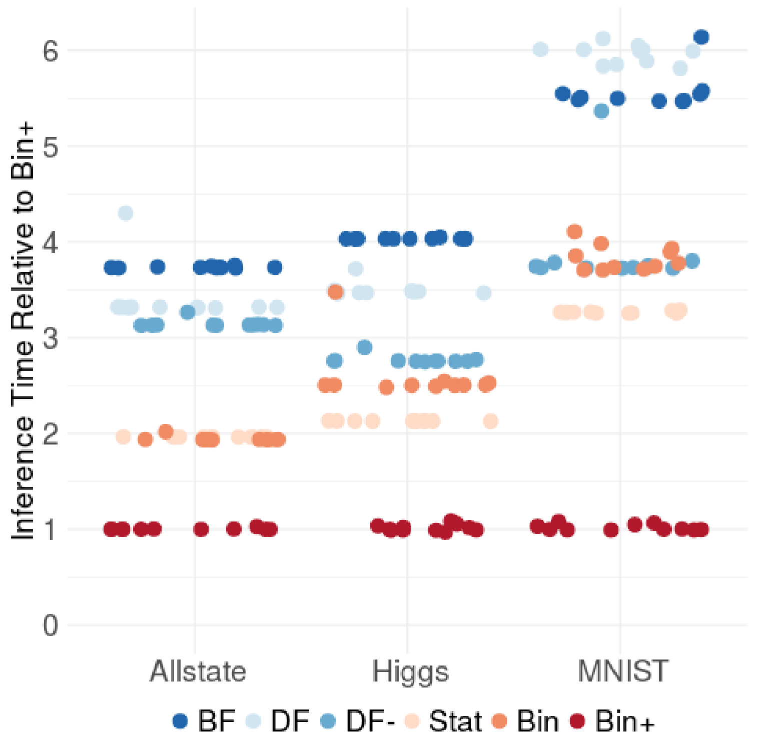


Figure 5.4: Encoding contributions to runtime reduction. Optimized breadth first (BF) layout serves as a baseline for all performance gains. Bin shows performance gains based on all memory layout optimizations. Bin+ is the combination of Bin with efficient tree traversal methods. This experiment uses a single thread.

Each of the datasets contain both training and testing observations. The training observations were used to train the forests and provide node traversal statistics. The testing observations were only used for measuring prediction speeds and were not used to determine traversal statistics.

5.3.2 Layout Contributions

We now turn to a detailed study of the effects of layout optimizations on runtime performance. Tab. 5.2 shows the incremental improvement of runtime statistics for the optimizations. The high ratio of wasted cycles of each of the encodings shows that runtimes are dominated by CPU stalls which are typically caused by slow memory accesses or high numbers of branch mispredictions. Because the runtime is nearly cut in half between the BF and Bin with little change in the numbers of instructions executed, branches, and branch mispredictions, we conclude that stalls occur mainly because of slow memory accesses. This is corroborated by greater than one Cycles Per Instruction (CPI), which indicates an application is memory bound.

We attribute the improvement of run times for DF, DF-, and Stat to reductions in the level at which cache misses are resolved. Average stall duration is reduced by finding required memory lower in the cache hierarchy, which is shown in "Avg Stall (cycles)" column of Tab. 5.2. The Bin optimization sees a slight increase in stall duration which we attribute to interleaving trees. This happens because "likely to be used" nodes, those near the roots, of several trees are stored together. This makes the access of a needed node in one tree likely to also load a soon to be useful node from another tree. Whereas other encodings quickly recover from stalls due to cache misses for often used nodes, the Bin encoding avoids these stalls altogether. In other words, the Bin optimization avoids quickly resolved stalls which increases the overall average stall duration.

Table 5.2: Execution Statistics for 25,000 Higgs Observations, Single Thread

	CPI	Instructions	Total Cycles	Wasted Cycles	Avg Stall Cycles	Branch	Branch Misses
BF	7.78	2.53e10	1.97e11	80.48%	12.67	4.24e9	6.33e8
DF	6.30	2.53e10	1.59e11	77.47%	11.74	4.24e9	6.33e8
DF-	5.70	2.53e10	1.44e11	75.05%	10.58	4.24e9	6.32e8
Stat	5.09	2.53e10	1.28e11	73.38%	10.05	4.24e9	6.32e8
Bin	4.33	2.68e10	1.17e11	73.30%	10.43	4.66e9	6.35e8
Bin+	1.28	5.13e10	6.69e10	37.45%	4.64	7.91e9	7.76e8

5.3.3 Algorithm Contributions

Fig. 5.4 shows the inference time of the encodings relative to Bin+, the combination of memory and algorithm improvements. Bin+, improves single thread performance by a factor of five on the MNIST forest and by a factor of three on the Allstate forest. The Bin and Bin+ layouts use a bin size of 32 trees per bin and interleaved level of 3.

Forest Packing, Bin+ reduces the affects of being memory bound by reordering tree traversals (Algorithm 3). Our improvement paradoxically doubles the number of CPU instructions and branches required during runtime—leading to an increase in branch mispredictions. Despite these negative changes, Forest Packing halves the ratio of wasted cycles and stall duration, leading to the demonstrated performance improvements.

The Bin+ optimization is less likely to stall because of the overlapped, out-of-order, execution allowed by our traversal modification. When using Algorithm 2 a thread recovers from a stall when the sole execution buffer slot in use becomes ready to execute its instructions. The updated traversal method allows the thread to use all execution buffers. The loading of any of the multiple execution buffers in use allows the thread to continue execution, thereby reducing both the liklihood a stall occurs and the duration of a stall when it does occur.

The benefits of Bin+ can only be realized with many concurrent tree traversals. As the inference process progresses through a bin, the trees arrive at their leaf nodes at different depths. The overlap of memory requests is reduced for each tree in a bin that reaches it's leaf node. This potential for skew is shown in Table 5.1, where the average leaf depth and deepest leaf depth of each of the test forests is shown, the latter being triple the former. As an example, when all but one tree finishes processing, the remaining tree will no longer benefit from out-of-order execution because there are no other trees with which to overlap memory accesses. When this occurs the remainder of the tree traversal reverts back to the Stat traversal pattern.

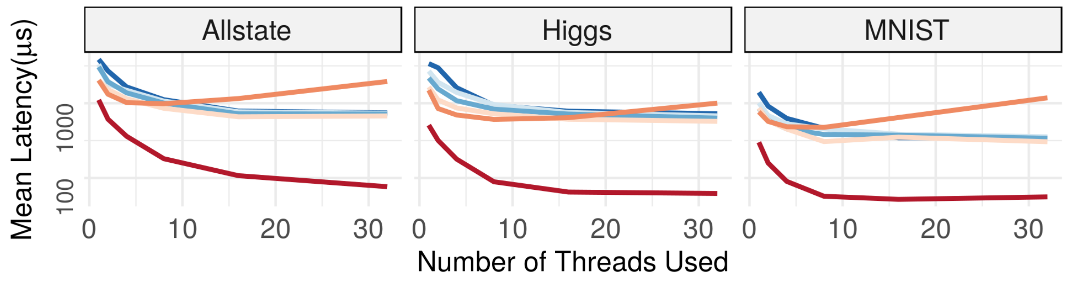
5.3.4 Parallel Evaluation to Reduce Latency

We study the effect on latency of parallelizing classification in a shared memory multithreaded system. This is a strong scaling experiment that runs a single classification on one to 32 threads. For the Bin and Bin+ encodings, the number of trees per bin is set to 16 and nodes are interleaved to depth of 3. To focus on reducing latency, we only begin processing an observation at the completion of the previous observation.

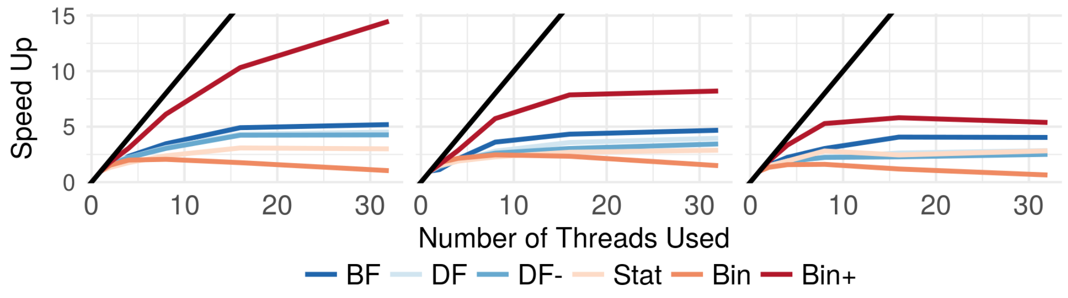
The bin data structure and improved algorithm allows Bin+ to scale more efficiently than the other encodings. Binning allows us to statically pin an execution thread to a subset of bins which allows a thread to process a subset of trees using out-of-order execution, maintain usefulness of all levels of cache, and reduce skew. Without the optimizations provided by binning, we can pin trees to threads and experience degraded parallelism due to skewed execution, or, we can allow threads to dynamically process trees and experience degraded parallelism due to poor use of cache. In neither case can we take advantage of out-of-order processing.

Shared-memory parallelism reduces latency effectively for each of the encodings (except Bin), but, despite being embarrassingly parallel, scaling is sublinear, Fig. 5.5. We expected this suboptimal scaling due to both increased contention in the memory subsystem and the skewed nature of observation traversal depths (Table 5.1). Multithread Bin performs poorly because threads receive extraneous nodes with each memory request because of the interleaved trees. This adds cache pollution, reduces cache locality, and requires multiple requests for cache lines with interleaved nodes.

To realize the full benefit of both threaded parallelism and the intra-thread parallelism provided by out-of-order execution, it is necessary that the number of trees in the forest be at least 16 to 32 times the number of threads used. This limitation can be seen in Fig. 5.6 where intra-thread parallelism is shown to work well with at least 16 to 32 trees per bin. In addition, the number of bins in a forest should be a multiple of the intended number of threads used for parallelism in order to ensure equal workloads are provided to each thread. In general, larger bin sizes perform better during multithread



(a) Per observations prediction time. The Y axis is log10 scale.



(b) Speed-up with additional threads.

Figure 5.5: Multithread characteristics of inference techniques. Bin+ performance with one thread is superior to the other encodings and scales better with additional resources.

operation, but increasing bin sizes reduces the number of bins available for threaded parallelism.

5.3.5 Comparison to Popular Tools

We found no forests implementations that specifically target the reduction of inference latency, so instead comparisons will be made to two popular decision tree systems: XGBoost and RerF. Because both of these systems typically process observations in batches, we chose to use throughput as a measurement of comparison despite our system being optimized to reduce latency. We vary the size of forests in both the number of trees and size of

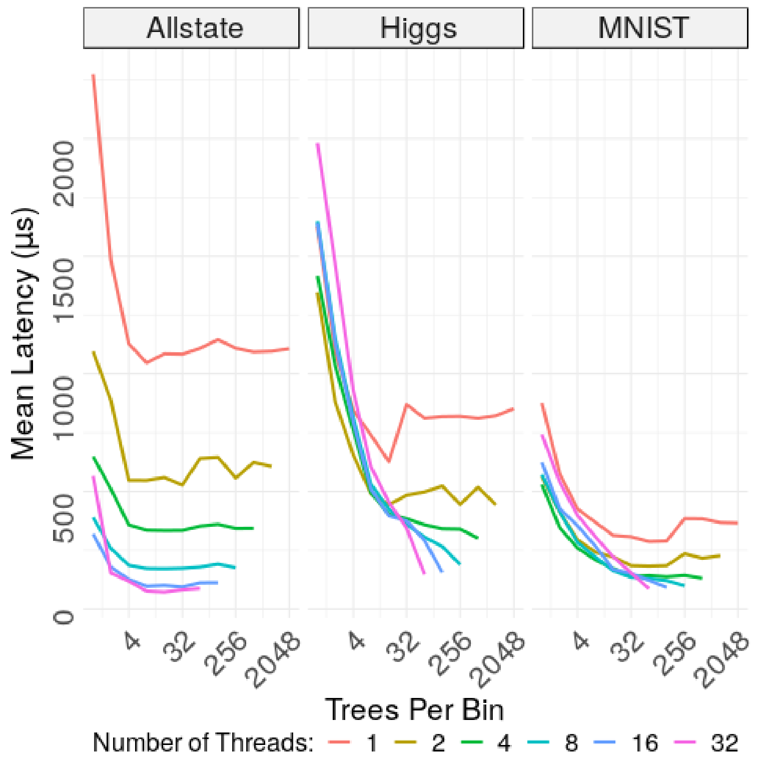


Figure 5.6: Effects of bin size on multithread performance for a 2048 tree forest. Increasing bin size allows for more intra-thread parallelism but limits thread level parallelism.

trees (using max depth) to show the efficacy of Forest Packing for a variety of forest sizes, Fig. 5.7. We set the batch size to 5000 for XGBoost and RerF. All systems except Forest Packing use all 96 threads of our machine—XGBoost uses forest characteristics to dynamically choose how many of the 96 threads to use. We limit Forest Packing to use only 16 threads in order to maximize intra-thread parallelism, a limitation described in Sec. 5.3.4. The use of 16 threads requires the use of at least 16 bins, which, for 2048 trees, limits the bin size to 128 trees. For a forest of 128 trees, the use of 16 threads limits the bin size to 8 trees. Despite the limitation on thread use, Forest Packing continues to outperform all other systems.

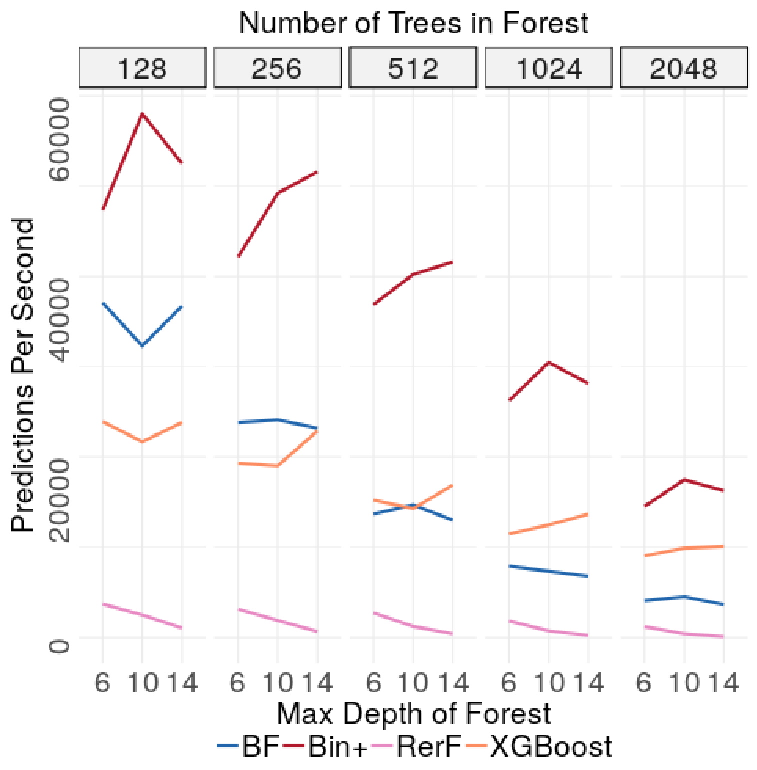


Figure 5.7: Inference throughput when varying number of trees in forest (defined above the chart) and tree depth. Forests were created using the MNIST dataset. Experiment uses multiple threads and batch size of 5000 where applicable.

5.4 Conclusions

The two major contributions provided by Forest Packing are the reduced memory footprint of a forest model and the novel tree traversal process made possible by tree binning. The removal of redundant leaf nodes halves decision forest memory requirements, which is a critical improvement for machine learning applications on memory limited devices such as mobile devices or stand-alone sensors. The tree traversal modification provides a faster, more scalable, system with multithread performance more than an order of magnitude faster than the naive solution. This reduced latency can make decision forests a more competitive option for real-time vision, recommender, and anomaly detection systems. Using Forest Packing to process trained decision forests such as those created by R-RerF allows for state of the art inference speeds.

Chapter 6

Dynamic Forest Packing

In Chapter 4 we described R-RerF which produced state of the art accuracy when used on many popular datasets. This system suffered from poor inference speed performance, which we addressed in Chapter 5 with the post processing step we called Forest Packing. This chapter outlines fastRerF, a system that fixes the final deficiency of R-RerF — slower than state-of-the-art training speeds — while also performing forest packing simultaneously with training.

We describe several training optimization alternatives to typical decision forest implementations, introduce a node level subsampling, and dynamically pack forests to reduce inference time. The benefits of these improvements are shown using several widely used datasets to compare our memory efficient systems, fastRF and fastRerF, against other popular forest implementations. The resulting system provides state-of-the-art accuracy, training speeds, and inference speeds.

6.1 fastRerF Optimizations

The most popular training time optimization used in decision forest systems entails presorting each feature, which is not a feasible enhancement for RerF. Presorting features in RerF would entail materializing all possible features, sorting them, and storing pointer data to required observation properties such as class label and weight. This is not feasible because there are on the order of $d!$ possible linear combinations that would each form a new feature, where d is the number of features in a dataset. This would grow the memory requirements of the algorithm beyond a system's available resources for all but the smallest datasets. With the presorting optimization unavailable for our system, we instead focused on memory reduction techniques, node level subsampling, and efficient parallelism.

6.1.1 Memory Reduction

Randomer Forest, like typical decision forests, is a memory bound algorithm that suffers from the high load latencies experienced when performing random reads from memory. Criminisi et al recommends storing a tree's mapping from observation indices to node in a single vector rather than node specific index vectors [8]. Indices are rearranged within this data structure as observations are split into children nodes. The importance of this technique increases when performing functions such as determining observation distances, which require maintaining index locations for the duration of the tree growing process, rather than just indices in the frontier nodes. This method only requires storing a vector iterator for the first and last location of each node's indices, which defines a subregion of the vector which also encompasses all descendant node indices.

The fastRF system processes nodes in a memory efficient order. Most decision forest systems process nodes at a per level processing order, allowing them to quickly process an entire level of a tree by streaming over each feature in a single pass. As the number of nodes doubles at each level, so too does the memory required to store the unprocessed node data. For this reason fastRF uses a depth first traversal order which requires storing at most L unprocessed nodes vs the 2^L nodes stored when processing in a breadth first order, where L is the maximum depth of a tree.

Another memory reducing method is a suggestion from Criminisi to maintain a tree wide vector to map observation indices to nodes [8]. A naive decision forest implementation will maintain a per node vector of resident observations, thereby duplicating data at each level of a tree. Rather than duplicating data, the use of a single N length vector can be used, where observation indices are moved within the vector according to node residency. This in-place tracking of observations reduces the allocation of node tracking vectors. Movement of indices within the vector is an efficient operation commonly employed in the quicksort algorithm.

The final memory optimization employed by fastRF is the use of C index vectors, where C is the number of classes in a dataset, to store the location of observations in a tree. This serves two purposes, first, it reduces memory by tying an observation's class label to the entire vector rather than storing a class label for each observation. The second benefit is an increase in cache load efficiency due to processing observations in class order, which increases the likelihood a cache load is used multiple times prior to eviction. This secondary benefit is only realized when a training set is ordered by class label.

6.1.2 Node Level Stratified Subsampling

There are several approximation techniques used to reduce the amount of work required at each node. For instance, XGBoost reduces the number of potential splitting points to explore at each node when $\tilde{N}$ is above a user defined cutoff value. When $\tilde{N}$ is large all observation values are binned and only splits between these bins are considered. Louppe detailed a subsampling method that subsamples both observations and features from the training data for each tree and uses this reduced subset of observations and features for training [24]. This method reduces the number of features explored at each node and reduces the number of observations resident in each node, thereby reducing training time but also reducing the efficacy of a tree. Our subsampling method is inspired by these two techniques.

FastRerF employs a stratified subsampling of observations at each node when $\tilde{N}$ surpasses a user defined threshold. Whereas XGBoost's method loads all observations into a histogram, FastRerF only loads the subsampled observations, which reduces gathering, sorting, and searching time. In addition, Louppe's subsampling may select poor features and thus have a poorly performing tree, FastRerF chooses a subset at each node and so a bad sampling of uninformative features only affects a single node rather than an entire tree.

6.1.3 Parallelism

FastRerf uses tree level parallelism, the most coarse grained form of parallelism available in forests. This choice almost completely removes both false sharing between threads and all thread synchronization, but duplicates tree growing structures in each thread. We tolerate this small memory duplication because the structures are duplicated in independent caches and so the increased memory use is tempered by a high cache coherency.

6.1.4 Dynamic Forest Packing

Forest Packing showed the node representation in memory and traversal method through trees could result in an order of magnitude difference in inference times as compared to non optimized methods, Chapter 5. As a post processing step forest packing is an inconvenience to data scientists and so would, in all likelihood, be relegated to use only in forest deployment scenarios, such as in embedded sensors. But, by modifying both the processing order of nodes and rearranging the forest data structure, it is possible to closely replicate the implementation of Packed Forests during forest growing. An enhancement we call Dynamic Forest Packing.

fastRF uses a depth first traversal order, sect. 6.1.1, in order to minimize memory use. This is implemented via a stack of unprocessed nodes, where nodes are popped after processing, which results in either two children nodes being pushed onto the stack or nodes becoming leaf nodes within the forest structure. Placing the right child on the stack followed by the left child results in the traditional depth first creation of a forest. Forest Packing requires nodes to reside in the forest adjacent to the child which is most likely to be traversed, the child node whose set of observations has the higher cardinality. To achieve this order within the resulting forest structure, the nodes must be processed in order of cardinality, where the sibling with higher cardinality must be processed first, which results from the lower cardinality node being placed on the processing stack first.

The trees within the forest must also be binned in order to gain the full benefits of Forest Packing. The bin structure of Forest Packing consists of $\tilde{T}$ trees combined into a single data structure where roots are adjacent, the first several levels of each tree are intertwined, per-tree nodes are stored according to cardinality, and leaf nodes are stored at the end of the structure. fastRerF is unable to completely match this formatting because the final bin size in memory is unknown until the training process is complete. So instead, during fastRerF training, the number of trees per bin is calculated and the initial forest structure is created with leaf nodes stored at the beginning of the contiguous memory structure rather than at the end. Trees within the bin are grown sequentially with the nodes in the intertwined layers being placed in their predefined position and later nodes are placed sequentially at the end of the growing data structure.

Parallelism is also modified to be on a bin per thread basis rather than the previously used tree per thread basis. Each bin uses an independent number generator, seeded by a forest level number generator, to maintain reproducibility and reduce synchronization among threads. The number of bins used in a forest should be a multiple of the number of threads used to train the forest in order to maximize thread use.

6.2 System Evaluation

We evaluate FastRerF and FastRF against other popular and well performing decision forest systems. Ideally, FastRerF would be compared against other OSPFs but there are no implementations that scale beyond trivially large datasets. We explore the scalability of our system as it pertains to number of cores and training dataset characteristics. We also isolate dataset characteristics to demonstrate the effects these particular characteristics have on training time. Finally, we show the effects of stratified subsampling on training time and test accuracy.

6.2.1 Experimental Setup

We compare FastRerF and FastRF to Ranger, LightGBM, and XGBoost. Ranger is one of the fastest Random Forest implementations, particularly on datasets with few unique feature values. LightGBM and XGBoost are boosted systems which are popular due to their fast training speed and successes in Kaggle competitions. The algorithms employed by these forests are similar in that they are decision forests that split nodes based on some minimization criteria. Similar parameters are used when comparing forests and defaults are used for forest specific parameters not used by the other variants.

Four commonly used real world and simulated datasets are used to demonstrate performance: Higgs, MNIST, p53, and SVHN. The Higgs dataset was used in a popular Kaggle competition, is composed of simulated background and signal events from the Atlas experiment, and contains 250,000 observations and 28 features[31]. MNIST is a popular numeric dataset of 60,000 handwritten digit images, 0-9. p53 is a two class biophysical dataset of 16772 observations with 5408 features [33]. The SVHN dataset consists of house numbers, 0-9, taken from Google's Street View, consists of 531131 observations of 1024 pixels in three color channels for a total of 3072 features [34].

All experiments were run using R version 3.4.4 on a 64-bit Ubuntu 18.04.1 LTS platform with four Intel Xeon E7-4860V2 2.6 GHz processors, 48 cores (with hyperthreading there are 96 threads), with 1TB RAM. R wrappers were used for each system: Ranger and XGBoost were CRAN installable and the remaining systems were installed via their github site.

6.2.2 Training Time and Scalability

An important metric for machine learning algorithms is training time, which is influenced by processing hardware, dataset characteristics, and algorithm parameters. Our initial test shows how fast similar operations can be completed by the various test systems. Using the three representative datasets, forests containing 96 trees are grown by exploring $\sqrt{d}$ features at each node. Our results, Fig. 6.1, show that on two of the three datasets, fastRF and fastRerF train faster than Ranger when using a few cores and always performs better when using many threads. This demonstrates that the per tree parallelism scales better than the per feature parallelism implemented in Ranger. Of the boosted forests, LightGBM is able to quickly train the Higgs dataset due to the few number of classes and number of features, but otherwise, the training

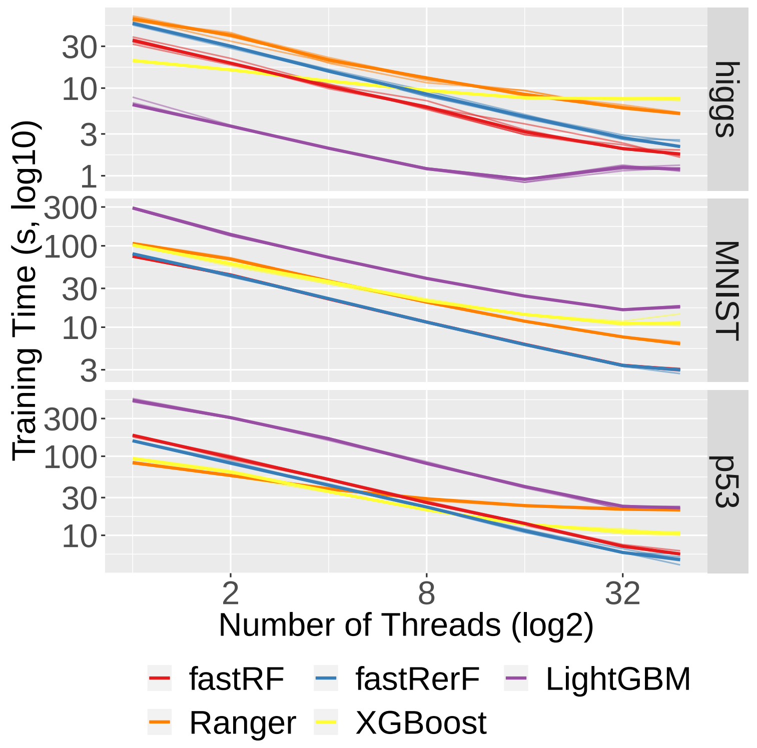


Figure 6.1: Multicore performance comparing fastRF and fastRerF training times to those of popular decision forest variants. Forests contain 96 trees

times of boosted forests are slower than those of fastRF and fastRerF.

The Speed-Up charts in Fig. 6.2 further demonstrate the superior scalability of our systems. Ideally, fastRF and fastRerF speed-ups would track closer to the ideal — the black line — because the per tree parallelism greatly reduces thread synchronization and cache line sharing as compared to other forms of parallelism. The bottleneck preventing a perfect speed-up is the contention over memory bandwidth.

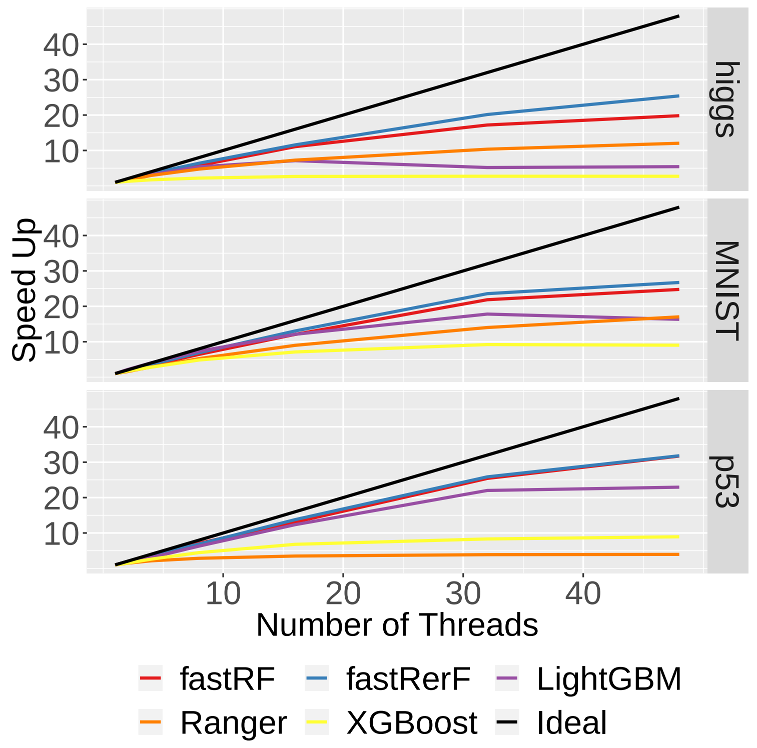


Figure 6.2: Multicore speed-up of fastRF and fastRerF compared with other popular decision forest variants. Forests contain 96 trees.

6.2.3 Dataset Characteristics Effects

The training time required by decision forests are dependent on many dataset specific characteristics. We use the SVHN dataset to explore the effects dataset characteristics have on training times by creating a subsampling of the SVHN dataset with the required characteristics. Our baseline dataset is composed of 5 classes, 60000 observations, and 1024 features. Each test is performed on a subsampling of the data using two of the three baseline settings, while the third setting is varied. This allows us to observe how training times vary based on these specific dataset characteristics.

Fig. 6.3 shows fastRF and fastRerF training times grow sublinearly with the number of classes. This is expected because only one third of node splitting, the exhaustive search, is effected by the number of classes, Sect. 4.3.1. Boosting algorithms scale linearly with the number of classes because boosting algorithms require a forest to be created for each class.

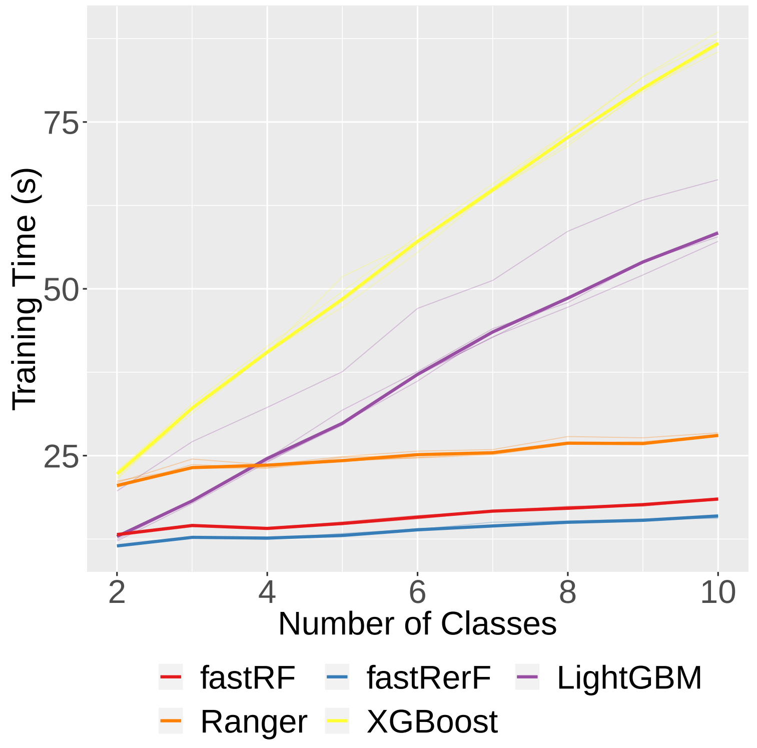


Figure 6.3: Affect of number of classes in dataset on fastRF and fastRerF training times. 60000 observations, 1024 features, and 16 threads, 128 trees.

Fig. 6.4 shows fastRF and fastRerF training times grow sublinearly with the number of features. All systems were set to search $\sqrt{d}$ features at each node. Training time as a function of d is an important metric as forest variants differ in recommended values for $mtry$: $\sqrt{d}$ for Random Forests, d for boosted forests, and between $2d$ and d^2 for OSPFs.

Fig. 6.5 shows fastRF and fastRerF training times grow linearly with the

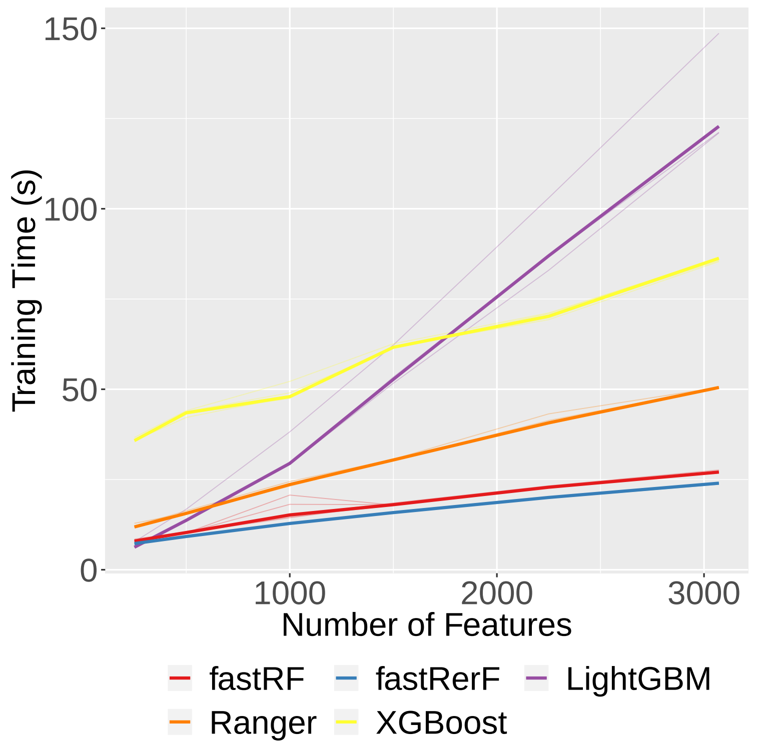


Figure 6.4: Affect of number of features in dataset on fastRF and fastRerF training times. 60000 observations, 5 Classes, and 16 threads, 128 trees. All systems set to use $\sqrt{d}$ features at each node.

number of observations, whereas the other systems grow superlinearly. All systems use N observations to populate root nodes, although some observations are duplicated in the non-boosted systems. Louppe suggests a much smaller sample may be sufficient for many training sets, a notion which we exploit in our per node stratified subsampling [24].

6.2.4 Effects of Node Level Subsampling

We test two aspects of our node level subsampling method: training time and test accuracy. Using the Higgs dataset we train forests using 128 trees and default parameters. We vary the the number of observations from one to

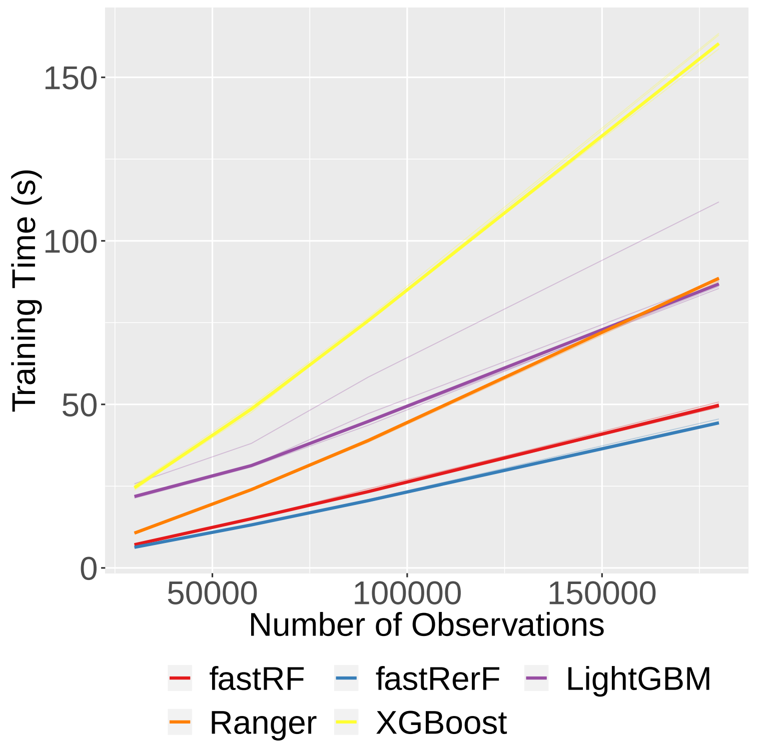


Figure 6.5: Affect of number of observations in dataset fastRF and fastRerF training times. 60000 observations, 1024 features, and 16 threads, 128 trees.

four million. The node level subsampling size (i.e. the maximum number of observations used to determine a cut value) varies from 100 to 1600 samples and we also use the full sample (i.e. no subsampling was used) as a baseline, Fig. 6.6. This shows that subsampling can reduce training times to 50% of unsubsampled nodes. The reduction in training times comes at the cost of slightly reduced model efficacy when subsampling is too small, Fig. 6.7.

6.2.5 Effects of Dynamic Forest Packing

Forest Packing is an enhancement designed for use in Random Forests, so we compare our Dynamic Forest Packing to our implementation of an unpacked

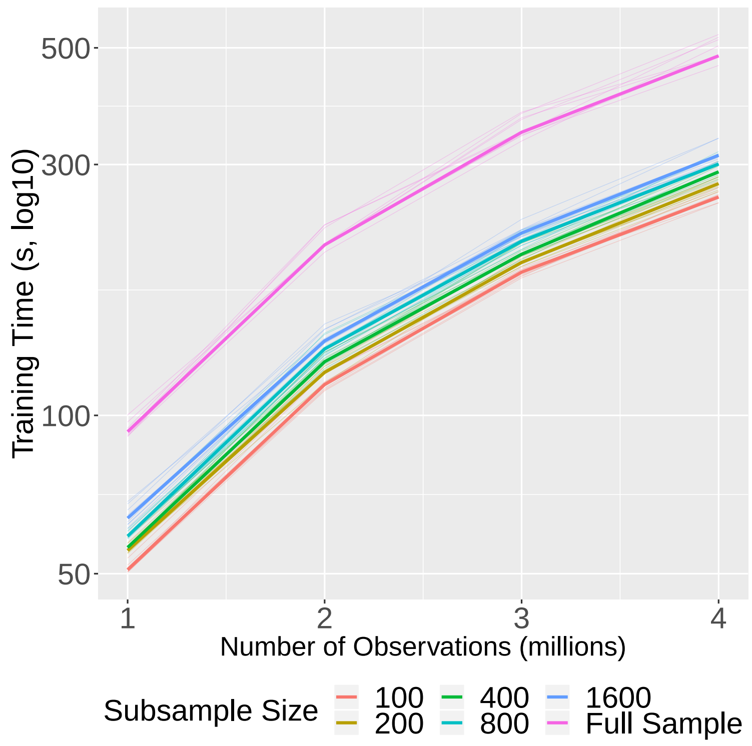


Figure 6.6: Effects of subsampling size on training time. MNIST dataset, 128 trees.

forest; Ranger is also included in the comparisons as a baseline. We first show the effects of Dynamic Forest Packing on forest training times, Fig. 6.8, using the MNIST dataset with its accompanying 10000 observation test set. The difference between our nonpacked and dynamically packed forest is small, with changes only in node placement because our nonpacked version uses the cardinality based processing order. Our Dynamically Packed Forest is slightly faster due to the reduction in tree size caused by sharing leaf nodes.

We then compare inference times using MNIST's test set, Fig. 6.9. Inference times grow as expected with the addition of trees to the forest. The use of binning can be seen when comparing the fastRF and fastRF(binned) results. Overall, binning reduces inference times an order of magnitude as compared

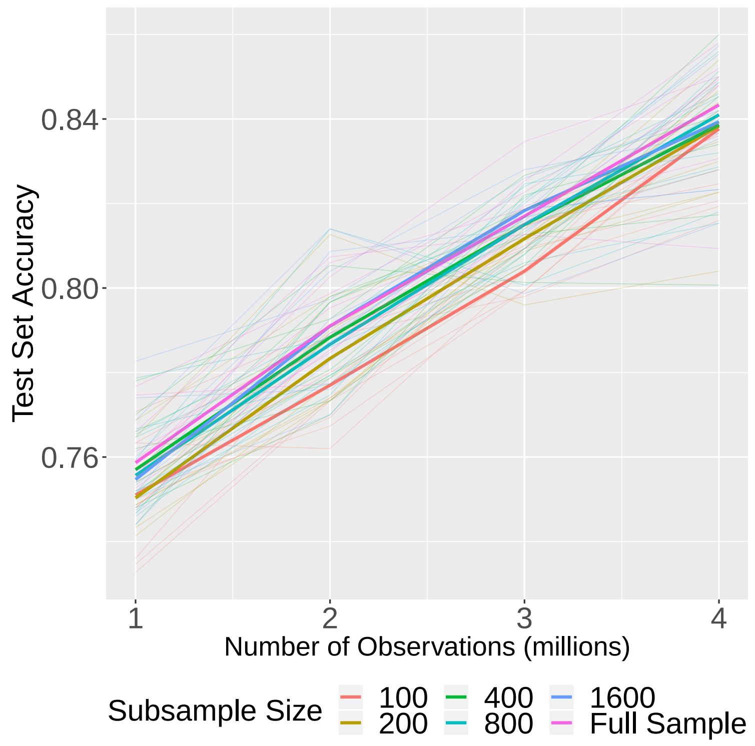


Figure 6.7: Effects of subsampling size on test set accuracy. MNIST dataset, 128 trees.

to the other systems.

6.3 Conclusion

OSPFs provide greater discernability between classes as compared to other forest variants, but had no scalable implementation. This chapter outlines several design choices used to reduce memory accesses with the aim of creating a highly scalable system. We create both fastRF and fastRerF and show that their efficient use of memory can outperform the widely used decision forest optimizations that trade memory efficiency for a reduction in computation. The use of stratified subsampling allows us to reduce the gathering, sorting,

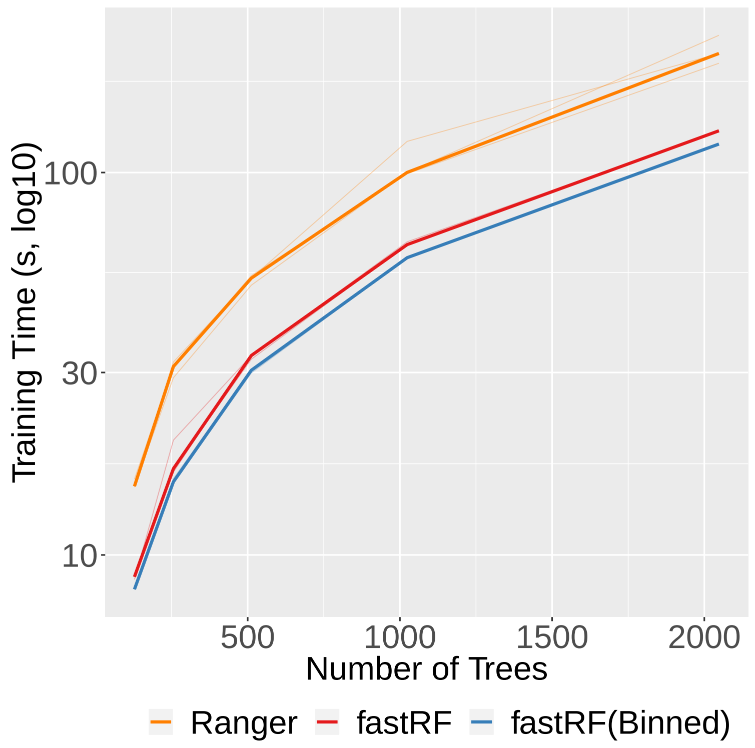


Figure 6.8: Affects on training time of dynamically binning fastRF. MNIST dataset.

and cut value searching required at each node by reducing the number of considered observations. Testing shows that this subsampling can reduce training time in half with minimal effects to model efficacy. fastRF and fastRerF scale more efficiently with increased resources and can train forests faster than popular forest variants over a large range of dataset characteristics. The resulting system, fastRerF, provides the high accuracy of OSPFs, training times lower than popular decision forest systems, and state-of-the-art inference times.

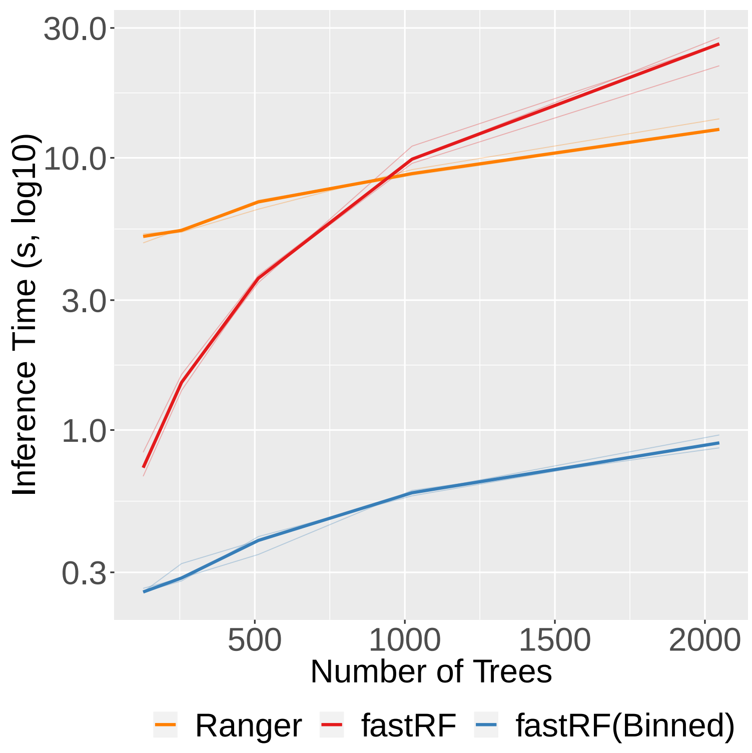


Figure 6.9: Effects of dynamic binning on inference time. MNIST dataset.

Chapter 7

Discussion and Conclusion

The purpose of this dissertation was to explore the feasibility of designing and implementing a scalable Oblique Sparse Projection Forest (OSPF). The benefits of these forests have been known since the conception of decision forests over two decades ago, but no scalable implementation has ever been developed, despite computational complexities similar to that of other popular forest variants. The reason for this oversight is not definitively known, but this researcher contends, after delving into many decision forest implementations, that typical forest acceleration techniques cannot extend to sparse projection forests and thus, without the use of the typical optimizations, oblique forests were computationally untenable.

This exploration started with the development of R-RerF, a mostly R version of Tyler Tomita's sparse projection forest, Randomer Forest (RerF). The implementation was highly optimized, scaled similarly to state of the art forest implementations, and provided an easily extensible framework that allowed for easy implementation of other sparse projection forests. We showed R-RerF's training speeds were similar to the speeds found in other forest variants and R-RerF's ability to scale with increased resources surpassed other implementations. In addition we provided a CRAN package that implements RerF, Random Forest, Random-Rotation Random Forest and S-RerF, a patch processing OSPF used for image classification. Although this implementation scaled well, it suffered from excessive memory use and slow inference speeds.

The slow inference speeds of decision forest algorithms was an interesting problem that others had explored before. Prior to our investigation though, solutions focused on data representations of trees in memory and batched processing of test observations. We were able to improve upon the state-of-the-art inference speeds by intertwining trees in a bin structure, removing duplicate leaf nodes, relocating leaf nodes to the end of bins so that multiple trees would share nodes, and changing the traversal order of trees in the forest to take advantage of modern CPU architectures. Our overall product, Forest Packing, reduced tree memory requirements in half, provided single core inference faster than a many threaded naive implementation, scaled better with additional resources, and increased throughput while reducing per inference latencies as compared to other popular forest implementations. The realization of these benefits required data scientists to perform an offline, multistep process to save the forest to disk, analyze the forest, rewrite the forest in an optimized format, and reload the forest into memory.

The final contribution of this dissertation was to create an optimized version of RerF that would dynamically pack a forest's nodes for fast inference. Prior to implementing our system we analyzed several fast decision forests with the aim of finding optimizations for our new system, but instead we found the typical forest optimizations were not extendable to OSPFs. We instead focused on several memory reduction design choices and introduced a per node subsampling method inspired by similar well performing methods. Our final product is more memory efficient than other state of the art decision forests, trains faster on many datasets, scales better with additional resources, and provides state-of-the-art inference speeds.

The culmination of our efforts is available with front end interfaces for both R and Python, with packages available via CRAN and pip. There are plans to extend fastRerF beyond the RerF and Random Forest algorithms currently provided to include unsupervised methods such as U-RerF and other OSPFs such as S-RerF. In addition to added algorithms, we also plan to make the current implementations feature rich with support for common Random Forest features such as observation proximity and feature importance.

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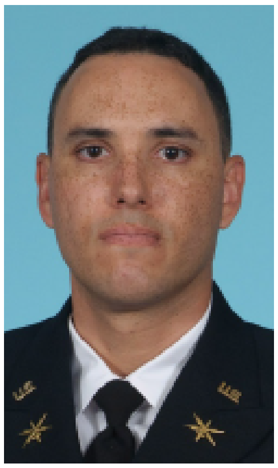
Vita



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