

# Training Big Random Forests with Little Resources

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## ABSTRACT

Without access to large compute clusters, building random forests on large datasets is still a challenging problem. This is, in particular, the case if fully-grown trees are desired. We propose a simple yet effective framework that allows to efficiently construct ensembles of huge trees for hundreds of millions or even billions of training instances using a cheap desktop computer with commodity hardware. The basic idea is to consider a multi-level construction scheme, which builds top trees for small random subsets of the available data and which subsequently distributes all training instances to the top trees' leaves for further processing. While being conceptually simple, the overall efficiency crucially depends on the particular implementation of the different phases. The practical merits of our approach are demonstrated using dense datasets with hundreds of millions of training instances.

## KEYWORDS

Machine learning; large-scale data analytics; classification and regression trees; ensemble methods; random forests

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## 1 INTRODUCTION

While large amounts of training data offer the opportunity to improve the quality of machine learning models, they can also render both the generation and the application of such models very challenging. Ideally, one would like to take all available data into account during the training phase: Using more independent and identically distributed data can—in expectation—not decrease the generalization performance and improves theoretical generalization guarantees. Furthermore, when searching for very rare patterns, ignoring parts of the training data or using subsampling strategies can lead to suboptimal models (simply randomly discarding training instances from the “negative” class can make it difficult to define the decision boundary around the rare “positive” instances).

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Such learning scenarios often occur in practice, for example in astronomy or remote sensing.

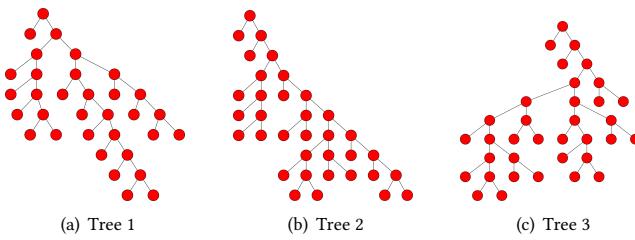
Ensemble methods are among the most successful models in data mining and machine learning [16, 23]. This is especially the case for random forests [3], which often yield very competitive accuracies while being, at the same time, conceptually simple and resilient against small changes of their hyperparameters [11]. Random forests have been extended and modified in various ways, e.g., to fit the requirements of special application domains or to build the involved trees in a parallel or distributed fashion in the context of large-scale learning scenarios. Ideally, one would like to build forests consisting of hundreds or even thousands of trees. However, depending on the data at hand, the construction of such forests can become extremely time- and memory-intensive.

For this reason, there has been a growing interest in developing frameworks and techniques that reduce the practical runtime for both the construction and the application of random forests. A popular line of research focuses on the construction of such tree ensembles in a parallel or distributed way making use of many individual compute nodes (e.g., by constructing one tree per compute node). While this can significantly reduce the practical runtime, such frameworks naturally require expensive distributed computing environments. Furthermore, the efficient construction of a single tree might cause problems in case the dataset or the tree becomes too large to fit into the main memory of a single system.

We propose a simple yet effective scheme for building random forests with fully-grown trees at large scale. The main idea is to construct each of the trees in three phases: Initially, a top tree is built from a small random subset of the data. In the second phase, all training instances are distributed to the leaves of that tree. Finally, one or more bottom tree(s) are built for each leaf. The intermediate leaf subsets can be stored on disk and, subsequently, handled individually. Hence, by using such top trees, one essentially obtains a partition of the data into much smaller and, hence, manageable subsets. The final trees correspond to standard random forest trees with slightly different splits conducted in their upper parts. Our experimental evaluation shows that our implementation can efficiently handle scenarios with hundreds of millions of training instances using systems with both limited computational and memory resources. To the best of our knowledge, no other publicly available implementation exists that can handle datasets of this size without resorting to compute clusters.

## 2 BACKGROUND

We start by providing the background related to the construction of large-scale random forests. Let  $T = \{(x_1, y_1), \dots, (x_n, y_n)\} \subset \mathbb{R}^d \times \mathcal{Y}$  be a set of training patterns with  $\mathcal{Y} = \mathbb{R}$  for regression and  $\mathcal{Y} = \{c_1, \dots, c_K\}$  for classification scenarios. A random forest is



**Figure 1: A random forest consisting of three trees.**

an ensemble of  $B$  trees whose prediction  $f(\mathbf{x})$  for a new pattern  $\mathbf{x} \in \mathbb{R}^d$  is based on a combination of the predictions  $f_b(\mathbf{x})$  made by the individual trees  $\mathcal{T}_1, \dots, \mathcal{T}_B$ , i.e.,

$$f(\mathbf{x}) = C(f_1(\mathbf{x}), \dots, f_B(\mathbf{x})), \quad (1)$$

where  $C : \mathbb{R}^B \rightarrow \mathbb{R}$  depends on the learning scenario. For regression tasks, a common choice is  $C(f_1(\mathbf{x}), \dots, f_B(\mathbf{x})) = \frac{1}{B} \sum_{b=1}^B f_b(\mathbf{x})$ , whereas  $C(f_1(\mathbf{x}), \dots, f_B(\mathbf{x})) = \operatorname{argmax}_{c \in \mathcal{Y}} |\{i \mid f_i(\mathbf{x}) = c\}|$  is the standard choice for classification tasks [3, 16, 23].

A tree is built recursively starting from the root and a subset  $T' \subseteq T$  of the training data. Each node splits the available data into two subsets, which are used to build two subtrees becoming the children of the node. A node becomes a leaf when the associated training data subset is *pure* (i.e., only instances with the same label are left) or some other stopping criterion is fulfilled (e.g., a maximum tree depth is reached). A simple example is given in Figure 1. For an internal node corresponding to a subset  $S \subseteq T'$  of training instances, one searches for a splitting dimension  $i$  and a threshold  $\theta$  that maximize the *information gain*

$$G_{i,\theta}(S) = Q(S) - \frac{|L_{i,\theta}|}{|S|} Q(L_{i,\theta}) - \frac{|R_{i,\theta}|}{|S|} Q(R_{i,\theta}) \quad (2)$$

with  $L_{i,\theta} = \{(\mathbf{x}, y) \in S \mid x_i \leq \theta\}$ ,  $R_{i,\theta} = \{(\mathbf{x}, y) \in S \mid x_i > \theta\}$ . This corresponds to minimizing the weighted *impurities* of the subsets as measured by an *impurity measure*  $Q$  [3, 16, 23]. For regression scenarios, one usually chooses

$$Q(S) = \sum_{(\mathbf{x}, y) \in S} (y - \bar{y})^2 \quad (3)$$

with  $\bar{y} = \frac{1}{|S|} \sum_{(\mathbf{x}, y) \in S} y$ . The *Gini index*

$$Q(S) = \sum_{k=1}^K p_S^k (1 - p_S^k) \quad (4)$$

is a common choice for classification problems, where  $p_S^k$  is the fraction of points belonging to class  $k$  in  $S$ .

The overall construction of a random forest is sketched in Algorithm 1. An ensemble model exploits the diversity of its members. For standard random forests, one usually considers  $B$  subsets of the training patterns. These *bootstrap samples* are drawn uniformly at random (with replacement) from  $T$  to obtain slightly different training datasets and, hence, trees. Another strategy to introduce randomness is to vary the splitting mechanism at the internal nodes during the construction by, e.g., considering different subsets  $\{i_1, \dots, i_F\}$  of features for each node split among which

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**Algorithm 1** BUILDRANDOMFOREST( $T, B, F$ )

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**Require:**  $T = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\} \subset \mathbb{R}^d \times \mathcal{Y}$ ,  $B \in \mathbb{N}$ , and  $F \in \{1, \dots, d\}$ .  
**Ensure:** Trees  $\mathcal{T}_1, \dots, \mathcal{T}_B$  for  $T$ .

- 1: **for**  $b = 1, \dots, B$  **do**
- 2:     Draw bootstrap sample  $T'$  from  $T$
- 3:      $\mathcal{T}_b = \text{BUILDTREE}(T', F)$
- 4: **end for**
- 5: **return**  $\mathcal{T}_1, \dots, \mathcal{T}_B$

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**Algorithm 2** BUILDTREE( $S, F$ )

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**Require:** Set  $S \subseteq T$  and  $F \in \{1, \dots, d\}$ .  
**Ensure:** Tree  $\mathcal{T}$  built for  $S$

- 1: **if**  $S$  is pure (or some other criterion fulfilled) **then**
- 2:     **return** leaf node
- 3: **end if**
- 4:  $(i^*, \theta^*) = \operatorname{argmax}_{i \in \{i_1, \dots, i_F\} \subseteq \{1, \dots, d\}, \theta} G_{i,\theta}(S)$
- 5:  $\mathcal{T}_l = \text{BUILDTREE}(L_{i^*,\theta^*})$
- 6:  $\mathcal{T}_r = \text{BUILDTREE}(R_{i^*,\theta^*})$
- 7: Generate node storing the pair  $(i^*, \theta^*)$  and pointers to its subtrees  $\mathcal{T}_l$  and  $\mathcal{T}_r$ . Let  $\mathcal{T}$  denote the resulting tree.
- 8: **return**  $\mathcal{T}$

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the feature with the best splitting quality is selected (or by considering random splitting thresholds). The leaves of a single tree store the label information. For regression problems, one usually computes the mean of all labels associated with the leaf, whereas the most frequent label is stored for classification scenarios (or the distribution over the labels). The prediction  $f_b(\mathbf{x})$  for a single tree is obtained by traversing the tree from top to bottom based on the splitting thresholds stored in the internal nodes until a leaf node is reached. The associated label then determines the prediction of the tree.

## 2.1 Large-Scale Construction

The construction discussed so far corresponds to standard random forests [3]. Various alternatives have been suggested over the past years and the efficiency of the recursive construction of the individual trees via BUILDTREE heavily depends on the particular random forest variant that is considered and on the heuristics being used to accelerate the process. A popular alternative to the standard construction scheme is the concept of *extremely randomized trees* [13], which is based on random thresholds for each feature  $i$  in Line 4 of Algorithm 2 (more precisely, a random value between the minimum and the maximum is considered). In practice, resorting to potentially “suboptimal” splits often yields competitive and sometimes even superior tree ensembles. Furthermore, training such variants might also be faster. Another variant is proposed by Louppe and Geurts [22], who consider small subsets of the data, called *patches*. Each patch is based on a different subset of features and the overall ensemble consists of trees built independently on the patches.

Today’s state-of-the-art software makes use of various other implementation tricks to reduce the practical runtime. For instance, one can keep track of locally constant features (i.e., a dimension  $i$  does not need to be checked anymore for  $S$  and all the descendant

nodes in case all patterns in  $S$  exhibit the same value w.r.t. dimension  $i$ ). Furthermore, it is beneficial to represent a bootstrap sample  $T'$  via weights instead of duplicating training instances [21]. A popular well-engineered implementation based on highly-tuned C code is provided by the *Scikit-Learn* [26] package.

Random forests are known to be “embarrassingly parallelizable” since one can construct the involved trees separately from each other. A recent trend in machine learning is to make use of massively-parallel devices such as graphics processing units (GPUs) to accelerate the generation and application of random forests and other machine learning models [4, 6, 10, 14, 15, 18, 27, 29]. However, aiming at full, unpruned trees, such approaches do not seem to improve over a standard multi-core execution.

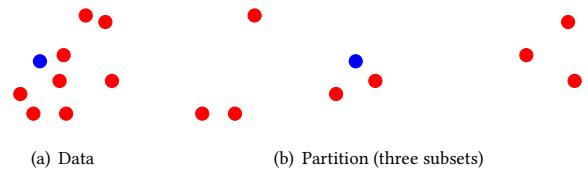
Another line of research is distributed computing: Given huge datasets, a single compute node might not be sufficient due to both the increased memory consumption and compute requirements. For such cases, the work needs to be distributed over multiple workstations. Distributed construction schemes have been proposed that are based on, e.g., *MapReduce* [7]. Several strategies to implement random forests via the MapReduce framework are described by del Río *et al.* [8]. A natural one (which is also implemented by the Apache Mahout™ library) is to consider subsets of the data and to build individual trees/forests for each of these subsets; the overall ensemble is then composed of all individual trees. The PLANET implementation [25] also resorts to MapReduce. Similarly to our work, it also stops the recursive construction as soon as the subsets become small enough to be handled by a single machine. However, the overall implementation aims at distributed computing environments and the construction of the upper parts of the trees are handled in a conceptually very different way. Furthermore, the trees are built independently from each other.

Finally, efficient implementations exist for the related task of computing ensembles of boosted trees [5]. These ensembles, however, rely on many shallow trees that are built in an iterative fashion. Accordingly, such implementations do not usually perform well when building deep, fully-grown trees.

## 2.2 Deep Trees

The original random forest implementation proposed by Breiman [3] grows full trees. A simple variant is to build trees up to a certain depth only. While the validation and test accuracies might still be good, the induced forest might lose its capability to deal with rare classes. The so-called  $m$ -out-of- $n$  subset strategy partitions the dataset into subsets and builds individual trees/forests for these subsets. While one makes use of all the data, this strategy might yield non-optimal results as well. As discussed by Genuer *et al.* [12] and del Río *et al.* [8], such subset strategies usually cause a shift towards the dominant classes and instances (in a certain region of the feature space). For example, assume that one is given a single rare instance (i.e.,  $P(y = c)$  very small for a class  $c$ ) and assume that one considers a partition of the data into three equal-sized subsets. The rare object would only be contained in one of the subsets and, hence, would never be predicted via the overall ensemble.

Reweighting strategies applied in a post-processing phase aim at reducing these negative side-effects, see, e.g., del Río *et al.* [8] for several adaptions. However, finding appropriate weights is a



**Figure 2: An ensemble built via the three subsets cannot identify the blue object anymore since two of the three models do not contain this instance. Such an effect can also be observed in case  $P(y|x)$  is unbalanced for a subregion  $x$ .**

challenging task as well and such methods generally focus on shifts in  $P(y)$  introduced by subsampling. Such a bias towards a dominant class/label can also occur in any *region of the feature space*, as sketched in Figure 2. Hence, even in case a reasonable amount of labeled instances is given for a rare class, subsampling strategies might lead the model to completely ignore this class, see Genuer *et al.* [12] for a detailed discussion.

## 3 ALGORITHMIC FRAMEWORK

We propose a wrapper-based approach that can handle massive datasets on a single compute node.

### 3.1 Wrapper-Based Construction

We start by outlining the construction of a single tree; the overall implementation simultaneously constructs all trees, which is described in the next section. The basic idea is to build a “top tree” based on a small *random* subset of the training data and to use this tree to obtain a partition of *all* the training instances into (ideally) almost equal-sized subsets.

The overall workflow is shown in Algorithm 3: In the first phase, a top tree  $\mathcal{T}$  is built for a small subset  $S$  of  $T$  drawn uniformly at random (without replacement). Afterwards, all available training instances  $T$  are distributed to the leaves of the top tree. That is, one determines for each training instance  $(x_i, y_i)$  the index of the leaf within the top tree the pattern  $x_i$  would be assigned to. Finally, in the third phase, one computes for each of the induced subsets  $T_1, \dots, T_M$  an associated bottom tree, which is then attached to the corresponding leaf of the top tree. This yields the final tree  $\mathcal{T}$ . Thus, the overall tree  $\mathcal{T}$  basically corresponds to a standard tree built via `BUILDTREE` with potentially slightly different splits conducted due to the random subset used for the top tree. A direct implementation of this approach, however, does not necessarily yield an efficient implementation due to, e.g., potentially very unbalanced top trees. The modifications needed to render this approach efficient are described next.

**3.1.1 Construction of Top Trees.** Since the top tree is only built on a small subset, different and potentially “suboptimal” splits might be considered compared to a direct construction via `BUILDTREE`. Note, however, that the notion of “optimality” is anyway vague in this context. For instance, extremely randomized trees, which resort to simple random splitting thresholds, often even yield competitive

**Algorithm 3** BUILDBIGTREE

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**Require:**  $T = \{(x_1, y_1), \dots, (x_n, y_n)\} \subset \mathbb{R}^d \times \mathcal{Y}$ ,  $F \in \{1, \dots, d\}$ , subset size  $R$ , and leaf bucket size  $M$ .

**Ensure:** Tree  $\mathcal{T}$  built for  $T$

- 1: Retrieve random subset  $S \subset T$  with  $|S| = R$
- 2:  $\mathcal{T}_{\text{top}} = \text{BUILDTOPTREE}(S, M)$
- 3:  $T_1, \dots, T_N = \text{DISTRIBUTE}(\mathcal{T}_{\text{top}}, T)$
- 4:  $\mathcal{T} = \emptyset$
- 5: **for**  $j = 1, \dots, N$  **do**
- 6:    $\mathcal{T} = \mathcal{T} \cup \text{BUILDTREE}(T_j)$
- 7: **end for**
- 8: **return**  $\mathcal{T}$

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**Algorithm 4** BUILDTOPTREE

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**Require:** Set  $T' = \{(x_{i_1}, y_{i_1}), \dots, (x_{i_R}, y_{i_R})\} \subset \mathbb{R}^d \times \mathcal{Y}$  leaf desired bucket size  $M$ .

**Ensure:** Root node of a binary tree  $\mathcal{T}_{\text{top}}$ .

- 1: Create empty stack  $\mathcal{P}$ ; create root node  $N_0$
- 2:  $i_{\text{node}} = -1$
- 3:  $\mathcal{P}.\text{push}(T', N_0)$
- 4: **while**  $\mathcal{P}$  is not empty **do**
- 5:    $i_{\text{node}} = i_{\text{node}} + 1$
- 6:    $(\bar{T}, \bar{N}) = \mathcal{P}.\text{pop}()$
- 7:   **if**  $|\bar{T}| < \max(2, M \cdot \frac{R}{n})$  **then**
- 8:      $\bar{N}.\text{value} = i_{\text{node}}$
- 9:     **return**  $\bar{N}$
- 10:   **end if**
- 11:    $(j^*, \theta^*) = \text{argmax}_{(j, \theta)} \bar{G}_{i, \theta}(S)$
- 12:   Split  $T'$  into  $T'_l$  and  $T'_r$  according to  $(j^*, \theta^*)$
- 13:   Create left node  $N_l$  of  $\bar{N}$  and  $\mathcal{P}.\text{push}((T'_l, N_l))$
- 14:   Create right node  $N_r$  of  $\bar{N}$  and  $\mathcal{P}.\text{push}((T'_r, N_r))$
- 15: **end while**
- 16: **return**  $N_0$

---

or even superior overall ensembles compared to their counterparts that rely on “optimal” splitting thresholds.

In practice, simply resorting to a standard BUILDTREE construction scheme might not yield a feasible approach. This is due to the fact that, for some datasets, the top trees might become very unbalanced, leading to many small leaves that do not contain many training instances after the distribution phase. In addition, the standard splitting scheme might yield very big leaves after the distribution phase; while these leaves might be pure after the construction phase of the top tree, they might become unpure again after the distribution phase. This actually is a problem since the induced big leaves still have to be processed in the third phase—and this might not be possible given the restricted resources (e.g., such a big leaf might contain hundreds of millions of patterns).

For this reason, we adapt the construction of the top tree, see Algorithm 4: The workflow is essentially the same except for the following two minor yet crucial modifications:

- (1) *Stopping condition:* Firstly, the recursive construction *only* stops as soon as the minimal leaf size is reached. By doing so, we ensure that the resulting leaf buckets are small enough for the further processing (otherwise, almost pure leaves might yield very big leaf buckets). The parameter  $M$  specifies the desired maximum size of a leaf bucket *after* the distribution

**Algorithm 5** DISTRIBUTE

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**Require:** A set  $T = \{(x_1, y_1), \dots, (x_n, y_n)\} \subset \mathbb{R}^d \times \mathcal{Y}$  of training patterns and a top tree  $\mathcal{T}_{\text{top}}$ .

**Ensure:** A partition  $T_1, \dots, T_N$  of  $T$ .

- 1:  $LI = \text{GETLEAVESINDICES}(T)$
- 2:  $T_1, \dots, T_N = \text{PARTITION}(LI, T)$
- 3: **return**  $T_1, \dots, T_N$

---

phase. Since the actual number of assigned instances is only known after the distribution of all instances, we resort to an estimate  $\tilde{M} = \max(2, M \cdot \frac{R}{n})$  for  $M$ .

- (2) *Balanced splits:* Secondly, to handle degenerated cases, we consider the following modified information gain criterion  $\bar{G}_{i, \theta}(S)$  that favors balanced partitions in the top tree:

$$\bar{G}_{j, \theta}(S) = (1 - \lambda)G_{j, \theta}(S) - \lambda \frac{\|L_{j, \theta}\| - \|R_{j, \theta}\|}{|S|} \quad (5)$$

Here, the right part of the above objective favors balanced partitions, which are similar to those conducted for standard  $k$ -d trees [2].<sup>1</sup> The parameter  $\lambda \in [0, 1]$  determines the tradeoff between the standard information gain and favoring balanced partitions.

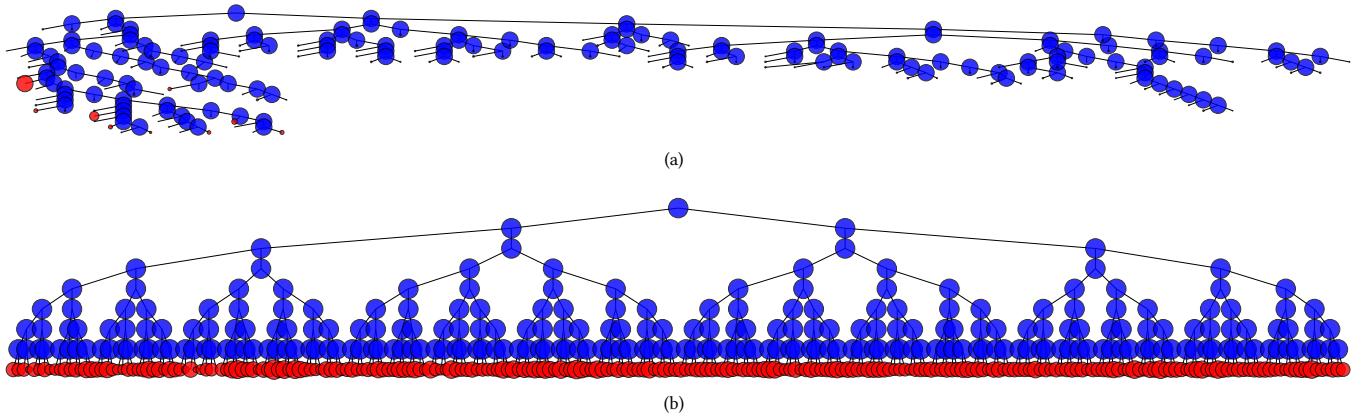
Finally, no bootstrap samples are drawn for the construction of top trees as well as optimal splits w.r.t. (5) are considered. Note that the adapted information gain is especially important for splits of almost pure nodes. Here, the first part of (5) will yield similar gains for various thresholds. However, the second part will enforce the splits to be balanced.

An example for a very unbalanced tree with a single leaf containing most of the patterns is given in Figure 3 (which is based on the landsat-osm dataset, see Appendix B). The few very big leaves depict a problem since they might become unpure again after the distribution phase and, hence, still have to be considered and processed in the third phase. The adapted construction scheme outlined above with  $\lambda = 1$  yields almost equal-sized partitions, all being sufficiently small such that the leaves will contain about  $M$  patterns *after* the distribution phase.

Note that the adapted splitting scheme actually continues splitting up pure nodes until a leaf size of  $\tilde{M}$  is reached. While this seems like an unnecessary operation, it is crucial to obtain manageable partitions for the third phase, the construction of the bottom trees. A potential drawback of this approach is that more splits than needed are actually conducted. Since one only knows about the properties of the final leaves after the distribution phase, this cannot be avoided. Furthermore, favoring balanced partitions using, e.g.,  $\lambda = 1$ , might yield to similar top trees and, hence, less randomness in the upper parts of the final trees. Also, the splits conducted might be “suboptimal” w.r.t. the original information gain criterion  $G_{j, \theta}(S)$ , which might lead to suboptimal top parts of the trees (e.g., no feature selection is conducted).<sup>2</sup>

<sup>1</sup>Note that using the median does not necessarily yield almost equal-sized partitions.

<sup>2</sup>For large-scale scenarios with millions or even billions of training patterns, these potential drawbacks do not seem to have a significant influence (basically, only a few suboptimal splits are conducted in the upper parts of the generally very deep trees). Note that the adapted node splitting (in case  $\lambda = 1$  is used) is related to Mondarian Forests [20], which only resort to label-independent node splits.



**Figure 3:** Two top trees built via `BUILDTOPTREE` using  $\bar{G}_{j,\theta}(S)$  with (a)  $\lambda = 0$  and (b)  $\lambda = 1$ , respectively. The size of a leaf (red) is proportional to the number of points assigned to it. The standard construction scheme that stops as soon as a node is pure and which resorts to the normal information gain ( $\lambda = 0$ ) might yield very unbalanced leaves (a few leaves contain almost all instances!). The adapted construction scheme with  $\lambda = 1$  yields very balanced partitions. In expectation, all these leaves will contain about  $M$  leaves after the distribution phase and are, hence, small enough for the construction of bottom trees.

**3.1.2 Distribution & Construction of Bottom Trees.** Given the top tree, all training instances are distributed to the top tree’s leaves, see Algorithm 5. The top tree is modified in such a way that the leaf index is returned for a query instead of a (label-based) prediction. The resulting indices can then be used to partition all the training data  $T$  to the different leaf buckets.

Finally, one or more bottom trees are built for each of the leaf buckets  $T_1, \dots, T_N$ . The number  $n_b \geq 1$  of bottom trees built per bucket can be defined by the user. For large-scale scenarios, sharing top trees among the different overall trees can be computationally very advantageous since less calls to `DISTRIBUTE` (Algorithm 5)—and, hence, passes over the data—are needed and since the construction of all bottom trees can effectively be parallelized (using the same chunk of data fitting in the system’s memory). However, sharing top trees this way generally leads to less randomness in the overall ensemble, which might reduce the model’s quality. Thus, there is a trade-off between runtime and tree diversity.

## 3.2 Implementation

The wrapper-based construction outlined above yields much smaller partitions associated with the leaves of the top tree, which can be handled more efficiently. Its efficiency, however, depends on a careful implementation of the involved steps.

Some of the steps are conducted simultaneously for the different trees to be built. More precisely, the construction of the  $n_t$  top trees as well as the distribution of the patterns are done via two single passes over the training instances. Each pass is conducted by processing all the data in chunks using a certain chunk size  $C$  (e.g.,  $C = 1,000,000$ ). In the first pass over the data, random subsets are extracted for the top trees. Given the subsets, the top trees are built, which are then used to distribute all instances to the top trees’ leaves. Note that considering random subsets based on a full pass over the data might be crucial for the top trees’ leaves having appropriate sizes, i.e., that stopping the construction as soon as  $|\bar{T}| < \max(2, M \cdot \frac{R}{n})$  yields leaf buckets having size of about  $M$  after

the distribution phase. During the distribution phase, a new subset of training instances is created for each leaf bucket, which is either stored in memory or on disk (using HDF5 [28]).

The construction of all  $n_t$  top trees can be done using  $O(R + C)$  additional memory, where  $R$  is the size of a single random subset and  $C$  the chunk size. Furthermore, the distribution of the instances can be done spending  $O(R + C)$  additional memory as well. Finally, for the third phase, one needs  $O(\bar{M})$  additional memory with  $\bar{M}$  being the maximal size of a leaf bucket after the distribution phase.

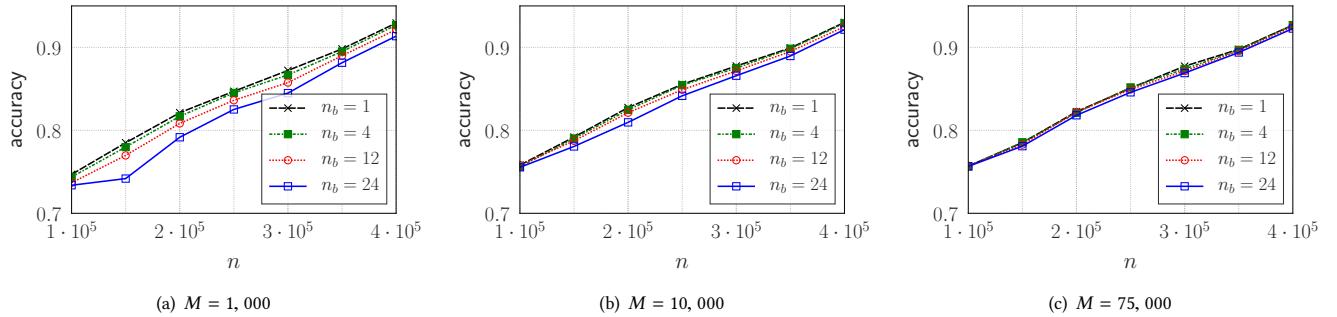
The general wrapper-based framework is implemented in Python (version 2.7.11), where the `Numpy` package (version 1.11.2) [19] is used for all matrix/vector-based operations. For the computation of both the top and the bottom trees, we resort to a pure C implementation that follows the construction scheme implemented by the `Scikit-Learn` package (version 0.18.1) [26]; `Swig` [1] is used to generate a Python extension. The overall implementation is made publicly available on <https://github.com/gieseke/woody> under the *GNU General Public License v3.0*. The standard random forest implementation has also been integrated into the open-source software library `Shark` [17].

## 4 EXPERIMENTS

We considered a standard multi-core machine for all experiments and compared our approach with three state-of-the-art competitors. The experiments can be reproduced using the code made available on <https://github.com/gieseke/woody>.

### 4.1 Experimental Setup

All experiments were conducted on a standard desktop computer with an Intel(R) Core(TM) i7-3770 CPU at 3.40GHz (4 cores, 8 hardware threads), 16GB RAM, and 16GB swap space. The operating system was Ubuntu 16.04 (64 Bit). We focused on runtimes for the construction phases as well as on the accuracies obtained on the test set. All results reported are averages over four runs. Our



**Figure 4: Influence of the number  $n_b$  of bottom trees per top tree on the accuracy given the covtype dataset and an increasing number  $n$  of training patterns. For each result (line), 24 trees were built in total. Three different woody instances induced by different assignments for  $M$  were considered.**

**Table 1: Datasets**

Name	$n_{\text{train}}$	$n_{\text{test}}$	$d$
covtype	464,809	116,203	54
susy	5,000,000	500,000	18
higgs	11,000,000	1,000,000	28
landsat-osm	1,000,000,000	2,964,607	81

approach can, in principle, be applied to any kind of random forest variant (e.g., extremely randomized trees). For the sake of simplicity, we resorted to standard random forests as described in Section 2. For the experimental evaluation, we considered the following four implementations:

- (1) The first one was the wrapper-based construction scheme proposed in this work, referred to as *woody*.
- (2) The second one was *subsets*, a simple scheme that resorts to subsets drawn uniformly at random from *all* the available training instances. For each such subset, a single classification tree is built. The overall implementation resembles the wrapper-based implementation outlined above, i.e., random subsets are extracted via a pass over all instances. However, instead of top trees, standard trees are built for these subsets. The remaining points are *not* distributed/considered. Intermediate results are stored on disk, as it is done for *woody*.
- (3) The third one, *sklearn*, was the *RandomForestClassifier* implementation provided by the *Scikit-Learn* [26] package.
- (4) The fourth one, *h2o*, was the implementation provided by the *H2O* package (*H2ORandomForestEstimator*).<sup>3</sup>

Most parameters were set to their default values. Some of the parameters were automatically adapted to the specific dataset at hand, see Appendix A for details. We focused on classification scenarios to assess the classification performances. In all cases, we considered a separate test set for evaluating the classification accuracy. For the different experiments,  $n_{\text{train}}$  training instances,  $n_{\text{test}}$  test instances, and  $d$  features were considered, see Table 1. Despite the three medium-sized datasets *covtype*, *susy*, and *higgs* [9], we also

<sup>3</sup><http://docs.h2o.ai>

considered *landsat-osm*, a large-scale dataset from the field of remote sensing containing up to one billion training instances, see Appendix B for details.

## 4.2 Model Parameters

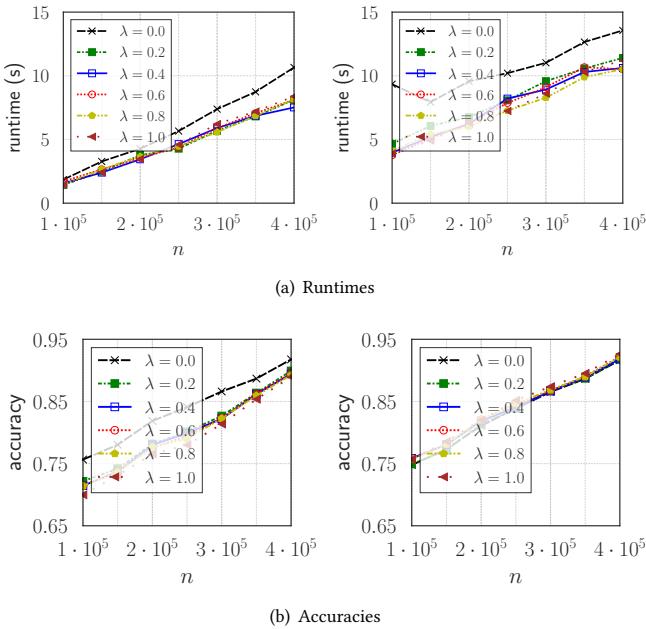
We started by analyzing the influence of two of the main model parameters introduced by the wrapper-based scheme.

**4.2.1 Influence of  $n_b$ .** The initial two phases can consume a significant part of the overall runtime. Especially the distribution phase involves extracting many large subsets that might have to be stored on disk. To reduce the overhead for these two phases, one can construct  $n_b > 1$  bottom trees per top tree. This essentially leads to final trees sharing upper parts, which, in turn, might lead to less randomness in the overall ensemble. To investigate the influence of this parameter, we considered the *covtype* dataset and three different instances of *woody* induced by different assignments for  $M$  (1,000, 20,000, and 75,000). If  $M$  is small, larger top trees are built. For large  $M$ , the top trees have small sizes. Hence, we expected a slightly worse performance for small  $M$  and a competitive performance for large  $M$ .

We considered 1, 4, 12 and 24 as values for  $n_b$ . In all cases, 24 trees were built in total (i.e.,  $n_b \cdot n_t = 24$ ). The results are shown in Figure 4. As expected, the accuracies were slightly worse for large  $n_b$ . However, the differences were generally very small, indicating that sharing upper parts did not significantly hurt the performance. Furthermore, the differences between the three instances of *woody* for varying  $M$  were very small as well, indicating that sharing larger parts did not lead to a significant drop w.r.t. the accuracy as long as sufficiently large bottom trees were built.

**4.2.2 Influence of  $\lambda$ .** We considered two models to investigate the influence of  $\lambda$ : A standard random forest implementation that resorted to the adapted information gain criterion as well as *woody*. In both cases, we considered the *covtype* dataset and different assignments for  $\lambda$  ( $\lambda = 0, 0.2, \dots, 1.0$ ). Both ensembles consisted of 24 trees, where  $n_t = 6$  and  $n_b = 4$  were used for *woody*.

The outcome is shown in Figure 5: As expected, smaller values for  $\lambda$  generally yielded slightly better accuracies. This was especially the case for the standard random forest implementation, which yielded the full trees using the adapted criterion. However, the



**Figure 5: Influence of  $\lambda$  given the covtype dataset and an increasing number  $n$  of training instances. Left: Standard random forest with adapted information gain  $\tilde{G}$ . Right: The wrapper-based approach woody with only the top tree being built via  $\tilde{G}$  (bottom trees were built via  $G$ ).**

results also indicate that the adapted information gain did not severely affect the accuracy. Also, the accuracies still improved in general the more data were taken into account.<sup>4</sup> Finally, the influence of  $\lambda$  was even less for woody, which is due to the fact that the wrapper-based approach only resorted to  $\tilde{G}$  for the construction of the top trees. To conclude, we observe that the accuracy was not severely affected, especially in case  $\tilde{G}$  was used for the construction of the top trees only.

Note that balanced splits are, however, in general important to quickly reduce the nodes' sizes for woody. This is in particular the case for almost pure nodes, which still have to be split to achieve the desired leaf sizes  $M$ .

### 4.3 Small Data

Next, we compared the training times and test accuracies induced by the covtype, susy, and higgs datasets. Again, we considered ensembles consisting of 24 classification trees ( $n_t = 6$  and  $n_b = 4$  for woody); all other parameters were set to the values described in Appendix A. The results are shown in Figure 6: Except for subsets, all implementations yielded similar results. The h2o implementation also exhibited a slightly worse classification accuracy on the covtype dataset (most likely due to the maximum tree depth of 20 not being sufficient for this dataset). The training runtimes were also similar for all implementations. Here, woody was slightly faster than sklearn on both the susy and the higgs dataset and slightly

<sup>4</sup>These results are in line with the ones reported for Mondrian Forests [20], which resort to a label-independent information gain.

slower on the covtype dataset. The subsets scheme performed worse on both the covtype and higgs dataset. In both cases, it can be seen that not taking all the available training instances into account led to a “stagnating” and slightly worse accuracy.<sup>5</sup>

To conclude, all implementations yielded very similar accuracies and the modifications for woody only had a negligible effect on the classification performance. The direct competitor, subsets, which only builds trees for subsets of instances, did not seem to benefit from more data, as indicated by the worse performance on both covtype and higgs. Note that the wrapper-based construction scheme can incorporate significantly larger datasets, which potentially yields much better ensembles (see below). Also, it is worth mentioning again that *fully-grown* trees are obtained via woody, which might be a crucial for dealing with rare instances.

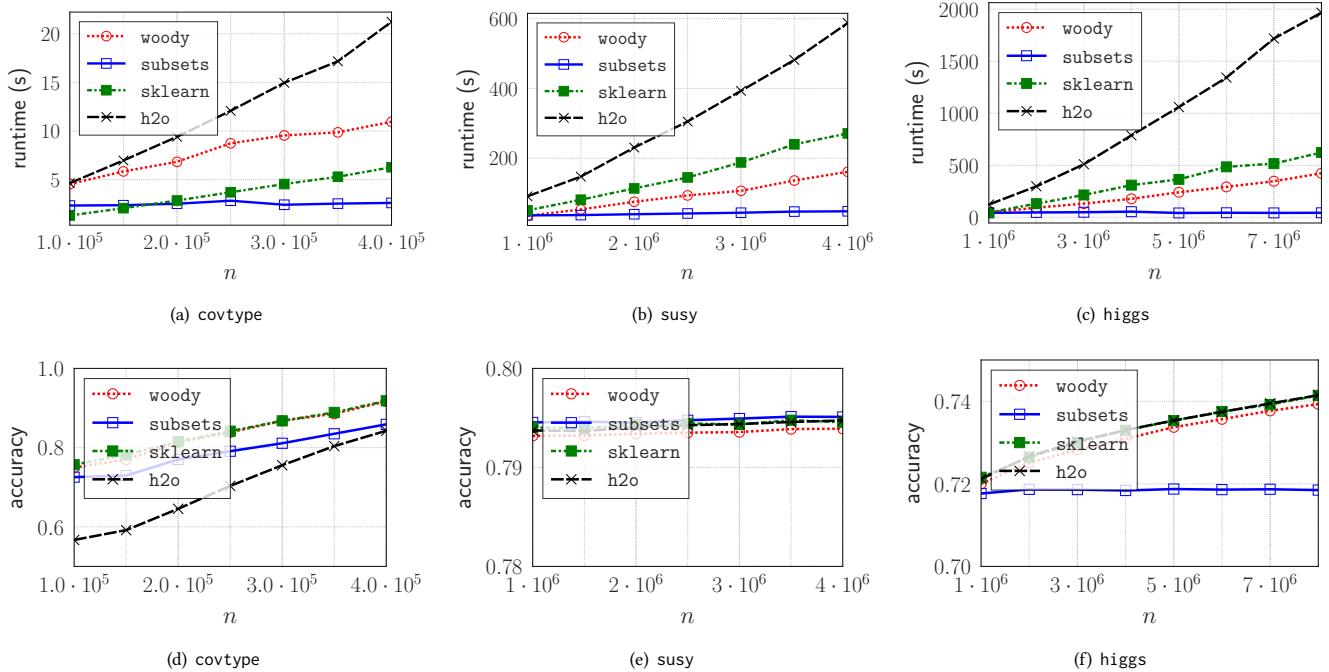
### 4.4 Big Data

Next, we made use of the landsat-osm dataset described in Appendix B and considered up to 50 million training instances; the classification accuracies were evaluated on about three million test instances. We used the same parameters for the different implementations as before and considered twelve estimators ( $n_t = 3$  and  $n_b = 4$  as well as  $\lambda = 1.0$  for woody). Intermediate results were now stored on disk instead in main memory for woody and subsets.

The results are shown in Figure 7. It can be seen that both woody and subsets were able to successfully process all training instances. Furthermore, taking more training instances into account led to better accuracies. The average accuracy of subsets was also slightly worse than the one of woody. The other two implementations could not handle these large-scale scenarios well: The sklearn implementation was only able to deal with ten million training instances without running into memory problems. For this single dataset instance, it yielded an average test accuracy of 0.72, which was about the same as the one achieved by woody in this case. While the h2o implementation could process dataset instances with up to 30 million instances, the average test accuracy was below 0.24 in all cases (not shown). To conclude, woody was capable of taking all the available training instances into account. While the improvement over subsets w.r.t. the accuracy was moderate for the dataset at hand, we would like to stress woody's capability to build fully-grown trees while taking all the training instances into account—this can be crucial for correctly classifying rare instances.

Finally, we made use of all one billion training instances given in the landsat-osm dataset and evaluated the runtime behavior of the woody implementation ( $n_t = 1$  and  $n_b = 4$ ). This dataset contains very dominant classes (e.g., the ‘water’ class) and, thus, can lead to very unbalanced top trees in case the standard information gain criterion  $G$  is used. In our experiments, using the modified information gain  $\tilde{G}$  with  $\lambda = 1$  yielded balanced top trees with only few leaves (about 1,000). Hence, the top trees successfully partitioned the huge dataset into much smaller chunks. The runtimes of the different phases (single run) are shown in Figure 8. It can be seen that woody was capable of efficiently handling the one billion training instances, where the distribution and bottom tree construction phases dominated the practical runtime.

<sup>5</sup>While subsets performed slightly better on susy, we do not consider the differences to be relevant (less than 0.2% differences w.r.t. the classification accuracy).



**Figure 6: Training runtimes and test accuracies for the three medium-sized datasets given an increasing number  $n$  of training instances (mean runtimes/accuracies based on four runs with different seeds). The runtimes and accuracies were very similar to each other, indicating that the changes made for woody did not significantly affect the outcome.**

## 5 CONCLUSION

We propose woody, a wrapper-based construction framework for building large random forests for hundreds of millions of training instances. The key idea is to use top trees to partition all the available training data into smaller subsets associated with the top trees' leaves and to build bottom trees for these subsets. While being conceptually simple, the framework allows the construction of ensembles with fully-grown trees for very large datasets. The practical benefits of our approach were empirically demonstrated on three medium-sized datasets and a large-scale application from the field of remote sensing with up to one billion data points.

We expect these results to carry over to other learning tasks making woody a powerful tool for mining big datasets—without requiring expensive compute resources. To the best of our knowledge, woody is the first implementation that renders the construction of random forests possible for datasets containing hundreds of millions of instances using a standard desktop computer. We think that the woody implementation—made publicly available on <https://github.com/gieseke/woody>—will be of significant practical importance for many real-world tasks in future.

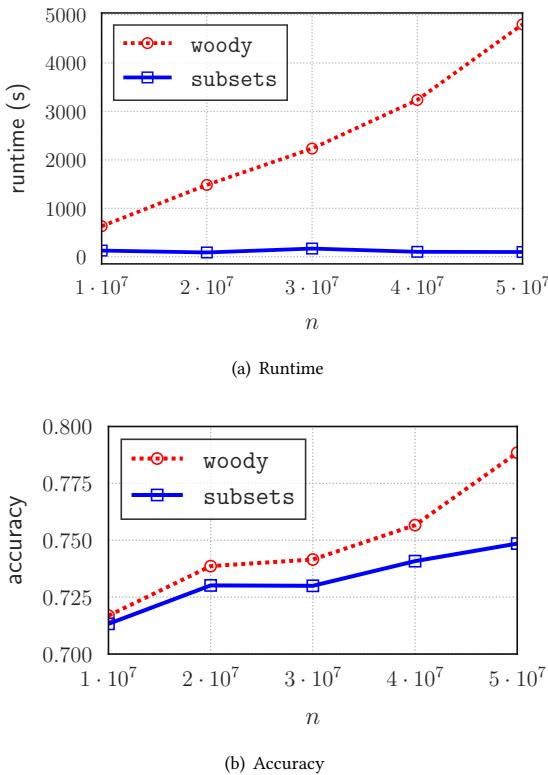
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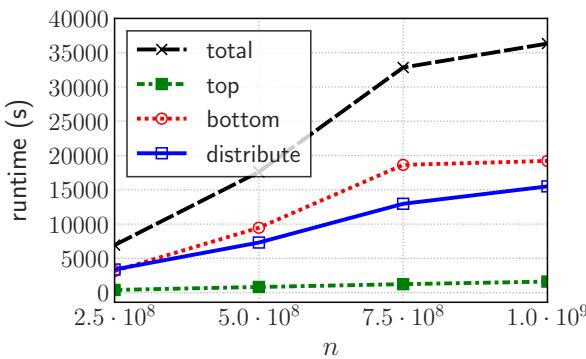
from the Innovation Fund Denmark through the *Danish Center for Big Data Analytics Driven Innovation* (DABAI).

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**Figure 7: Training runtimes and test accuracies for the landsat-osm dataset with up to 50 million instances. The sklearn implementation could not handle more than 10 million training instances due to memory errors. For 10 million training instances, it yielded an average accuracy of about 0.72. While the h2o implementation could process the dataset instances, the accuracy on the test set was below 0.24 in all cases (not shown in the plots).**



**Figure 8: Runtimes for the different phases of woody for the landsat-osm dataset using up to one billion instances.**

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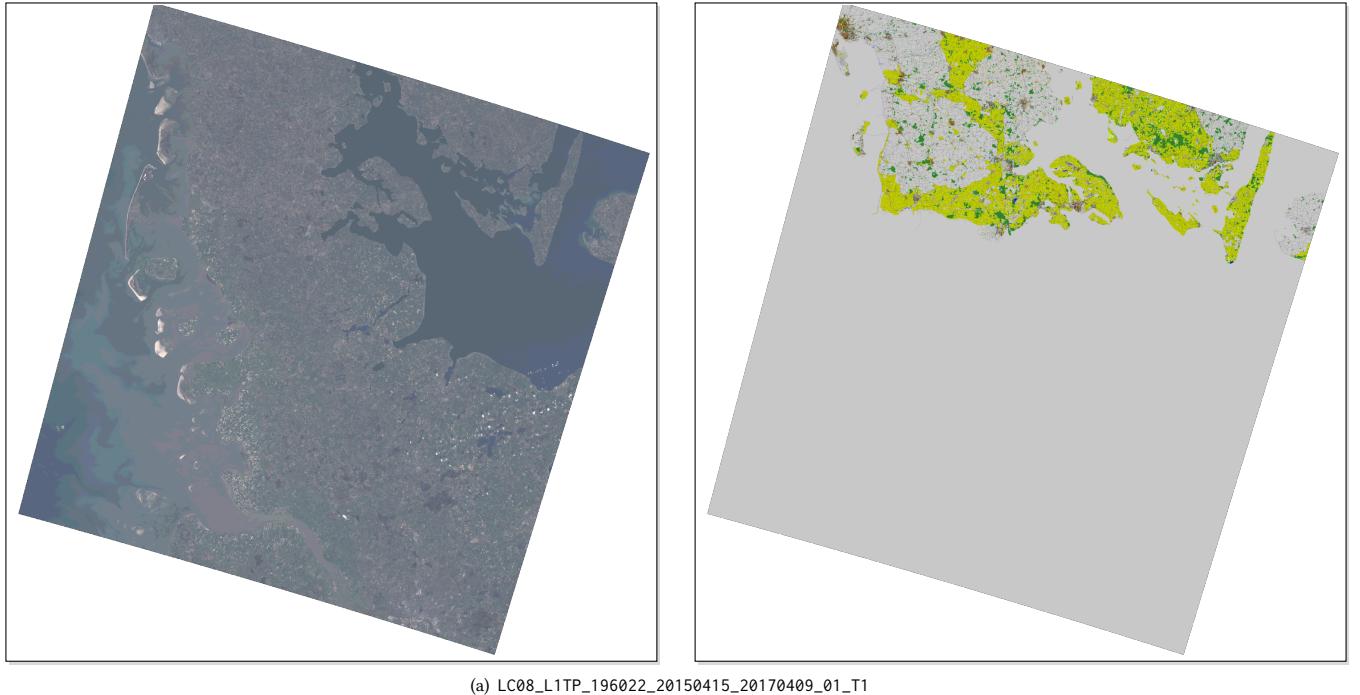
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## A PARAMETERS

If not stated otherwise, the parameters were fixed to the following values (same notation as for sklearn): `max_features="sqrt"`, `bootstrap=True`, `criterion="gini"`, `n_jobs=4`, `max_depth=None`, `min_samples_leaf=1`, and `min_samples_split=2`. Note that woody is based on C code for the construction of bottom trees, which follows the way random forests are built by sklearn. The parameters for h2o were adapted accordingly. In contrast to the other two implementations, the maximum tree depths was set to 20 for h2o (default value); larger tree depths led to memory errors.

For woody, the bottom trees were built in the same way as via the sklearn implementation (using the same parameters), except for the bootstrap parameter (bootstrap samples were extracted during the distribution phase). Both, the number of samples for the top trees as well as the desired leaf sizes for the bottom trees were defined via  $\min(500000, n, \max(100\sqrt{n}, 100000))$ . For the experiments, either a MemoryStore or a DiskStore was considered.



**Figure 9: Illustration of the first part of the `landsat-osm` dataset containing more than 50 million training instances (used for the results shown in Figure 7). The gray pixels correspond to unlabeled instances; the other ones to the labeled instances.**

The former one was used for the runtime comparison shown in Figure 6, where both the training data as well as the intermediate results were stored in memory (to obtain a fair comparison with `sklearn`). For the other large-scale experiments, `DiskStore` was used that loads the data from disk (in chunks) and also stores the intermediate results on disk. For the `covtype` dataset, the chunk size was fixed to  $C = 100,000$ , whereas for all other datasets, a chunk size of  $C = 1,000,000$  was used. For subsets, we considered subsets of size 50,000 for `covtype` and of size 500,000 for all other datasets. We refer to <https://github.com/gieseke/woody> for the code and the experimental setup.

## B LANDSAT-OSM

The features for the `landsat-osm` dataset were based on satellite data from the *Landsat 8* [30] project, see Figure 9. The associated labels stemmed from the *OpenStreetMap* (OSM) [24] project. More precisely, we considered 9 bands (grayscale images) and  $3 \times 3$  image patches, resulting in 81 features. We extracted such patches from the following Landsat scenes:<sup>6</sup>

- LC08\_L1TP\_193022\_20170501\_20170515\_01\_T1
- LC08\_L1TP\_194022\_20160606\_20170324\_01\_T1
- LC08\_L1TP\_195021\_20160512\_20170324\_01\_T1
- LC08\_L1TP\_195022\_20160512\_20170324\_01\_T1
- LC08\_L1TP\_196021\_20150821\_20170406\_01\_T1
- LC08\_L1TP\_196022\_20150415\_20170409\_01\_T1
- LC08\_L1TP\_197020\_20150422\_20170409\_01\_T1

<sup>6</sup>These scenes can be downloaded via the EarthExplorer framework, see <https://earthexplorer.usgs.gov/>.

- LC08\_L1TP\_197021\_20150422\_20170409\_01\_T1
- The LC08\_L1TP\_196022\_20150415\_20170409\_01\_T1 scene was split into two parts, where 5% were used as test set (random subset) and the remaining 95% as training set. The other scenes were attached to the training set for the runtime evaluation provided in Figure 8, which yielded one billion training instances. Prior to extracting the patches, we pansharpened all images [30].

Finally, the label for each such image patch was based on an OSM label extracted for the pixel at the center of the patch. The following OSM labels were extracted for all patches [24]:

- (1) landuse:forest,
- (2) landuse:meadow,
- (3) waterway:riverbank,
- (4) highway:all,
- (5) building:all,
- (6) landuse:reservoir,
- (7) natural:grassland,
- (8) railway:light\_rail, and
- (9) landuse:farmland.

The overall dataset consisted of more than one billion labeled patches and provided a realistic benchmark problem for supervised classification scenarios.