Distributed Machine Learning

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PART ONE

Large-scale Learning to Rank using Boosted Decision Trees

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Abstract

The Web search ranking task has become increasingly important due to the rapid growth of the internet. With the growth of the Web and the number of Web search users, the amount of available training data for learning Web ranking models has also increased. We investigate the problem of learning to rank on a cluster using Web search data composed of 140,000 queries and approximately fourteen million URLs. For datasets much larger than this, distributed computing will become essential, due to both speed and memory constraints. We compare to a baseline algorithm that has been carefully engineered to allow training on the full dataset using a single machine, in order to evaluate the loss or gain incurred by the distributed algorithms we consider. The underlying algorithm we use is a boosted tree ranking algorithm called LambdaMART, where a split at a given vertex in each decision tree is determined by the split criterion for a particular feature. Our contributions are two-fold. First, we implement a method for improving the speed of training when the training data fits in main memory on a single machine by distributing the vertex split computations of the decision trees. The model produced is equivalent to the model produced from centralized training, but achieves faster training times. Second, we develop a training method for the case where the training data size exceeds the main memory of a single machine. Our second approach easily scales to far larger datasets, i.e., billions of examples, and is based on data distribution. Results of our methods on a real-world Web dataset indicate significant improvements in training speed.

1.1 Introduction

With the growth of the Web, large datasets are becoming increasingly common — a typical commercial search engine may gather several terabytes per day of queries and Web search interaction information. This opens a wide range of new opportunities, both because the best algorithm for a given problem may change dramatically as more data becomes available (Banko and Brill, 2001), and because such a wealth of data promises solutions to problems that could not be previously approached. In addition, powerful clusters of computers are becoming increasingly affordable. In light of these developments, the research area of understanding how to most effectively use both of these kinds of resources is rapidly developing. An example of a goal in this area might be to train a Web search ranker on billions of documents, using user-clicks as labels, in a few minutes. Here, we concentrate on training a Web search ranker on approximately fourteen million labeled URLs, and our methods can scale to billions of URLs.

In this chapter, we investigate two synchronous approaches for learning to rank on a distributed computer which target different computational scenarios. In both cases, the base algorithm we use is LambdaMART (Wu et al., 2009; Burges, 2010), which we describe in more detail below. LambdaMART is a linear combination of regression trees, and as such lends itself to parallelization in various ways. Our first method applies when the full training dataset fits in main memory on a single machine. In this case, our approach distributes the tree split computations, but not the data. Note that while this approach gives a speedup due to parallelizing the computation, it is limited in the amount of data that can be used since all of the training data must be stored in main memory on every node.

This limitation is removed in our second approach, which applies when the full training dataset is too large to fit in main memory on a single machine. In this case, our approach distributes the training data samples and corresponding training computations and is scalable to very large amounts of training data. We develop two methods of choosing the next regression tree in the ensemble for our second approach, and compare and contrast the resulting evaluation accuracy and training speed. In order to accurately investigate the benefits and challenges of our techniques, we compare to a standalone, centralized version that can train on the full training dataset on a single node. To this end, the standalone version has been carefully engineered (for example, memory usage is aggressively trimmed by using different numbers of bits to encode different features).

Our primary contributions are:

- A boosted decision tree ranking algorithm with the computations for determining the best feature and value to split on at a given vertex in the tree distributed across cluster nodes, designed to increase the speed of training when the full training dataset fits in main memory. The model produced is equivalent to the centralized counterpart, but the speed is dramatically faster.
- A ranking algorithm with the training data and training computations distributed, designed to exploit the full training dataset, and to yield accuracy gains over training on the subset of training data that can be stored in main memory on a single machine. The model produced is not equivalent to the centralized counterpart. We assume in this case that a single machine can only store a small subset of the entire training dataset, and correspondingly assume that the centralized model cannot be trained on all of the training data.
- An investigation of two techniques for selecting the next regression tree in the ensemble.
- An investigation of using disjoint versus overlapping training datasets.
- A comprehensive study of the tradeoffs in speed and accuracy of our distribution methods.

1.2 Related Work

There have been several approaches to distributed learning ranging from data sampling to software parallelization. A survey of approaches is given by Provost and Fayyad (1999). Many distributed learning techniques have been motivated by the increasing size of datasets and their inability to fit into main memory on a single machine. A distributed learning algorithm produces a model that is either equivalent to the model produced by training on the complete dataset on a single node, or comparable but not equivalent.

We first review previous work on algorithms where the output model is equivalent. Caragea et al. (2004) present a general strategy for transforming machine learning algorithms into distributed learning algorithms. They determine conditions for which a distributed approach is better than a centralized approach in training time and communication time. In (van Uyen and Chung, 2007), a synchronous, distributed version of AdaBoost is presented where subsets of the data are distributed to nodes. Exact equivalence is obtained by passing complete statistics about each sample to all other nodes. In (Panda et al., 2009), a scalable approach to learning tree ensembles is presented. The approach uses the MapReduce model (Dean and Ghemawat,

2004) and can run on commodity hardware. The split computations are distributed, rather than the data samples, and are converted into Map and Reduce jobs. A challenge with the approach is that the communication cost is linear in the number of training samples, which may lead to prohibitively expensive communication costs for extremely large datasets.

The following distributed algorithms produce a model that is not equivalent to the model produced from training on a centralized dataset. In (Domingos and Hulten, 2000, 2001), learning algorithms, in particular Kmeans clustering, are scaled to arbitrarily large datasets by minimizing the number of data samples used at each step of the algorithm and by guaranteeing that the model is not significantly different from one obtained with infinite data. The training speed improvements come from sampling the training data; explicit distribution methods detailing communication costs are not presented. Fan et al. (1999) present a distributed version of AdaBoost, where each node contains a subset of the training data. During each iteration, a classifier is built on a selected sample of training data. Two sampling methods are examined: r-sampling, where a set of samples are randomly chosen from the weighted training set, and d-sampling, where the weighted training set is partitioned into disjoint subsets, and a given subset is taken as a d-sample. After each round of boosting, the weights of all training samples are updated according to a global weight vector. The speed improvements are obtained through data sampling, while the communication cost scales with the number of training samples. The results indicate that their approach is comparable to boosting over the complete data set in only some cases. An extension of the work was developed in (Lazarevic, 2001; Lazarevic and Obradovic, 2002). Rather than add a classifier into the ensemble built from a single disjoint d-sample or r-sample, classifiers built from all distributed sites are combined into the ensemble. Several combination methods, including weighted voting and confidence-based weighting, are considered. Experimental results indicate that accuracy is the same or slightly better than boosting on centralized data. However, the large number of classifiers combined to form the ensemble and the communication of the global weight vector may be prohibitively expensive for practical use.

We present two methods of distributing LambdaMART. Our feature-distributed method is similar to the approach in (Panda et al., 2009), except that our method has a communication cost that is constant in the number of training samples. Our data-distributed method differs from the previous methods in that (1) we aim to produce a comparable, but not equivalent, model, (2) we engineer our methods for a ranking task with billions of training samples, and (3) we use minimal communication cost that is constant

in the number of training samples. Previous methods have required communication of global statistics to achieve both exact and approximate models, and in each case the communication requirements scale with the number of training samples. Since our second approach distributes by data sample, the amount of training data (rather than the number of features) can scale with cluster size, which is usually more desirable than scaling with the number of features since the number of training samples tends to far exceed the number of features. Each tree in the ensemble is trained using a small subset of the data, and the best tree at a given iteration is chosen using the complement of its training data as a validation set, so the model is well-regularized. In the remainder of this chapter, we describe our experiences with developing a distributed version of LambdaMART. We detail the benefits and challenges of our two approaches, including the communication costs, training times, and scalability to terabyte-size datasets.

1.3 LambdaMART

We use the LambdaMART algorithm for our boosted tree ranker (Wu et al., 2009; Burges, 2010). LambdaMART combines MART (Friedman, 2001) and LambdaRank (Burges et al., 2006; Burges, 2010). LambdaMART and LambdaRank were the primary components of the winning ranking system in the recent Yahoo! Learning to Rank Challenge for Web search (Yahoo! Learning to Rank Challenge, 2010; Burges et al., 2011). We briefly describe these algorithms here.

LambdaRank is a general method for learning to rank given an arbitrary cost function, and it circumvents the problem that most information retrieval measures have ill-posed gradients. It has been shown empirically that LambdaRank can optimize general IR measures (Donmez et al., 2009). A key idea in LambdaRank is to define the derivatives (of the cost with respect to the model scores) after the documents have been sorted by the current model scores, which circumvents the problem of defining a derivative of a measure whose value depends on the sorted order of a set of documents. These derivatives are called λ -gradients. A second key observation in LambdaRank is to note that many training algorithms (for example, neural network training and MART) do not need to know the cost directly; they only need the derivatives of the cost with respect to the model scores.

For example, the λ -gradient for NDCG (Jarvelin and Kekalainen, 2000) for a pair of documents D_i and D_j , where D_i is more relevant to query q than D_j , can be defined as the product of the derivative of a convex cost

 C_{ij} and the NDCG gained by swapping the two documents:

$$\lambda_{ij} \equiv \left| \Delta \text{NDCG} \frac{\delta C_{ij}}{\delta o_{ij}} \right| \tag{1.1}$$

where o_{ij} is the difference in the model scores of the two documents. The λ -gradient for a single document is computed by marginalizing over the pairwise λ -gradients: $\lambda_i = \sum_{j \in P} \lambda_{ij}$, where the sum is over all pairs P for query q which contain document i.

MART is a class of boosting algorithms that may be viewed as performing gradient descent in function space, using regression trees. The final model maps an input feature vector $\mathbf{x} \in \mathbb{R}^d$ to a score $f(\mathbf{x}) \in \mathbb{R}$. MART is a class of algorithms, rather than a single algorithm, because it can be trained to minimize general costs (to solve, for example, classification, regression or ranking problems). The final score f can be written as

$$f(\mathbf{x}, N) = \sum_{n=1}^{N} \alpha_n f_n(\mathbf{x}) ,$$

where each $f_n(\mathbf{x}) \in \mathbb{R}$ is a function modeled by a single regression tree and the $\alpha_n \in \mathbb{R}$ are weights. Both the f_n and the α_n are learned during training. We refer to $\alpha_n f_n$ as the weak hypothesis h_n . A given f_n maps a given \mathbf{x} to a real value by passing \mathbf{x} down the tree, where the path (left or right) at a given node in the tree is determined by the value of a particular feature $x_j, j = 1, \ldots, d$ and where the output of the tree is taken to be a fixed value associated with each leaf, $v_{\ell n}$, $\ell = 1, \ldots, L$, $n = 1, \ldots, N$, where L is the number of leaves and N is the number of trees. For a given task (in our case, ranking), given training and validation sets, the user-chosen parameters of the training algorithm are the number of trees N, a fixed learning rate η (that multiplies every $v_{\ell n}$ for every tree), and the number of leaves L. The binary decision functions at each node of each tree and the $v_{\ell n}$ are learned during training; the decision functions are chosen to minimize a least-squares loss.

Clearly, since MART models derivatives, and LambdaRank works by specifying the derivatives at any point during training, the two algorithms are well suited to each other. LambdaMART is the marriage of the two, and we refer the reader to (Burges et al., 2006; Burges, 2010) for details. The set of M scores (one for each training sample) is computed, and the λ -gradient λ_m , m=1,...,M, of the cost function with respect to each model score is computed. Thus a single number is associated to each training sample,

One can also allow the number of leaves to vary at each iteration, but we do not consider such models here.

namely, the gradient of the cost with respect to the score which the model assigns to that sample. Tree f_n is then just a least-squares regression tree that models this set of gradients (so each leaf models a single value of the gradient). The overall cost is then reduced by taking a step along the gradient. This is often done by computing a Newton step $v_{\ell n}$ for each leaf, where the $v_{\ell n}$ can be computed exactly for some costs. Every leaf value is then multiplied by a learning rate η . Taking a step that is smaller than the optimal step size (i.e., the step size that is estimated to maximally reduce the cost) acts as a form of regularization for the model that can significantly improve test accuracy. The LambdaMART algorithm is outlined in Algorithm 1, where we have added the notion that the first model trained can be any previously trained model (Step 3), which is useful for model adaptation tasks.

Algorithm 1 LambdaMART.

```
1: Input: Training Data: \{\mathbf{x}_m, y_m\}, m = 1, \dots, M;
     Number of Trees: N;
    Number of Leaves: L;
     Learning Rate: \eta;
 2: Output: Model: f(\mathbf{x}, N);
 3: f(\mathbf{x}, 0) = BaseModel(\mathbf{x}) \{BaseModel \text{ may be empty.}\}
 4: for n = 1 to N do
        for m = 1 to M do
 5:
           \lambda_m = G(q, \mathbf{x}, y, m) {Calculate \lambda-gradient for sample m as a function
 6:
           of the query q and the documents and labels \mathbf{x}, y associated with
           w_m = \frac{\partial \lambda_m}{\partial f(\mathbf{x}_m)} {Calculate derivative of \lambda-gradient for sample m.}
 7:
        \{R_{\ell n}\}_{\ell=1}^L {Create L-leaf regression tree on \{\mathbf{x}_m, \lambda_m\}_{m=1}^M.}
 9:
       for \ell = 1 to L do
v_{\ell n} = \frac{\sum_{\mathbf{x}_m \in R_{\ell n}} \lambda_m}{\sum_{x_m \in R_{\ell n}} w_m} {Find the leaf values based on approximate New-
10:
11:
           ton step.
        end for
12:
        f(\mathbf{x}_m, n) = f(\mathbf{x}_m, n-1) + \eta \sum_{\ell} v_{\ell n} 1(\mathbf{x}_m \in R_{\ell n}) {Update model based
        on approximate Newton step and learning rate.
14: end for
```

1.4 Approaches to Distributing LambdaMART

As previously noted, we focus on the task of ranking, in particular Web search ranking, by learning boosted tree ensembles produced using LambdaMART. This means that the final model f is an ensemble defined as the sum $f(\mathbf{x}, N) = \sum_{n=1}^{N} h_n(\mathbf{x})$, where each h_n is a weak hypothesis. Moreover, f is constructed incrementally as weak hypotheses are added one by one. In this section, we present two approaches for distributed learning using LambdaMART:

- 1. Our first approach attempts to decrease training time by distributing the vertex split computations across the nodes and results in a solution which is equivalent to the solution resulting from training on all of the data on a single node (called the *centralized* model). We call this approach feature-distributed LambdaMART.
- 2. Our second approach distributes the training data across the nodes and does not produce a model equivalent to the centralized model. Rather, it attempts to dramatically reduce communication requirements without sacrificing accuracy and yields the possibility of training on billions of samples. We call this approach *data-distributed* LambdaMART. Within our second approach, we consider two weak hypothesis selection methods:
 - the master picks the weak hypothesis that maximizes the evaluation score (referred to as *full* selection)
 - the master picks a weak hypothesis at random, in order to decrease communication costs (referred to as *sample* selection)

Throughout the chapter, we assume that our distributed computer (cluster) has K+1 nodes, one of which may be designated as master, while the others are workers. We denote the workers by W_1, \ldots, W_K and use [K] to denote the set $\{1, \ldots, K\}$.

1.4.1 A Synchronous Approach based on Feature Distribution

In this section, we present feature-distributed LambdaMART, a synchronous distributed algorithm similar to the approach in (Panda et al., 2009) that distributes the vertex split computations in the boosted decision trees. Our method differs from that in (Panda et al., 2009) since the communication cost of our method is constant in the number of training samples (as opposed to linear). In addition, our method is based on MPI communication and does not use the Map-Reduce framework.

Recall that this approach targets the scenario where each node can store

the full training dataset in main memory. Due to extensive engineering and optimization, we have been able to store a dataset with several thousand features and over fourteen million samples in main memory on a single machine. Our goal is to train on such a large dataset on a cluster more quickly than on a single machine, while outputting the same model as the centralized counterpart.

Our algorithm, detailed in Algorithm 2, proceeds as follows. Let there be K workers and no master. We are given a training set S of M instance-label pairs. Each node stores the full training set S in memory. Let A be the set of features. The features are partitioned into K subsets, A_1, \ldots, A_K , such that each subset is assigned to one of the K workers. Every worker maintains a copy of the ensemble $f(\mathbf{x}, n)$ and updates it after each boosting iteration n. During each boosting iteration, a regression tree $\{R_{\ell n}\}_{\ell=1}^L$ is constructed. Each vertex in the tree is described by an optimal feature, corresponding split threshold, and change in loss, collectively denoted by φ . Each worker k computes the optimal feature and corresponding split threshold among its set of features A_k and sends the optimal feature, threshold, and change in loss, denoted by φ_k , to all other workers.

Every worker, after it has received all of the φ_k 's, determines the φ_k with the smallest loss, denoted by φ_* , creates the two new children for the model, and then computes which samples go left and which go right. Note that φ_* is the same for all workers, resulting in equivalent ensembles $f(\mathbf{x}, n)$ across all workers. The algorithm is synchronized as follows: each worker must wait until it receives all φ_k , $k = 1, \ldots, K$, before determining φ_* . Some workers will be idle while others are still computing their φ_k 's.

The challenge of this approach is that it requires that every worker contain a copy of the full training dataset. A benefit is the corresponding reduction in communication: each worker only sends a limited amount of information about a single feature for each vertex split computation. The total communication cost depends on the number of leaves L in a tree and the number of workers K in the cluster, but does not depend on the number of training samples or on the number of features.

1.4.2 A Synchronous Approach based on Data Distribution

Previous techniques of distributed boosted tree learning have focused on producing an ensemble that is equivalent to the ensemble produced by centralized training (Caragea et al., 2004; van Uyen and Chung, 2007; Panda et al., 2009). These approaches require that sufficient global statistics of the data be communicated among the master and the workers. Let there be

Algorithm 2 Feature-distributed LambdaMART.

```
1: Input: Training Data: \{x_m, y_m\}, m = 1, \dots, M;
    Number of Trees: N;
    Number of Leaves: L;
    Learning Rate: \eta;
    Number of Workers: K;
 2: Output: Model: f(\mathbf{x}, N);
    for k = 1 to K do
        f(\mathbf{x}, 0) = BaseModel(\mathbf{x}) \{BaseModel \text{ may be empty.}\}\
 4:
        for n = 1 to N do
 5:
           for m = 1 to M do
 6:
              \lambda_m = G(q, \mathbf{x}, y, m) {Calculate \lambda-gradient for sample m as a func-
 7:
              tion of the query q and the documents and labels \mathbf{x}, y associated
              w_m = \frac{\partial \lambda_m}{\partial f(\mathbf{x}_m)} {Calculate derivative of \lambda-gradient for sample m.}
 8:
           end for
 9:
           for \ell = 1 to L - 1 do
10:
              \varphi_k (Compute the optimal feature and split, \varphi_k, over features A_k
11:
              on worker k.
              Broadcast(\varphi_k) {Broadcast \varphi_k to all other workers.}
12:
              \varphi_* = \{\arg\max_k(\varphi_k)\}_{k=1}^K \{\text{Find optimal } \varphi_* \text{ across all } \varphi_k\text{'s.}\}
13:
              R_{\ell n} {Create regression tree on \varphi_* and \{\mathbf{x}_m, \lambda_m\}_{m=1}^M.}
14:
           end for
15:
          for \ell=1 to L do v_{\ell n}=\frac{\sum_{x_m\in R_{\ell n}}\lambda_m}{\sum_{x_m\in R_{\ell n}}w_\ell} {Find the leaf values based on approximate
16:
17:
              Newton step.
18:
           f(\mathbf{x}_m, n) = f(\mathbf{x}_m, n-1) + \eta \sum_{\ell} v_{\ell n} 1(\mathbf{x}_m \in R_{\ell n}) {Update model
19:
           based on approximate Newton step and learning rate.
        end for
20:
21: end for
```

a single master and K workers. The training set S is partitioned into K subsets, S_1, \ldots, S_K , and each subset resides on one of the workers of our distributed computer. For simplicity, assume that the subsets are equal in size, although this is not required in our derivation. However, we make no assumptions on how S is split, and specifically we do not require the subsets to be statistically equivalent.

Let data subset S_k reside on node k. To achieve a model equivalent to

the centralized model, we could, for each vertex in the tree, send from each worker k to the master the split information for each feature, which includes which samples in S_k go left or right when split on that feature. The master then determines the best feature and split values based on S. In this case, the communication cost per regression tree is dependent on the number of vertices in the tree, the range of split values considered, the number of features, and the number of data samples. The communication resources per vertex have a linear dependence on the number of training samples, precluding the use of the approach when the number of samples is in the billions. We would like to devise an algorithm that achieves comparable accuracy, but requires far less communication resources, namely, a communication cost that is independent of the number of training samples. We now describe our approach.

Assume that we have already performed N-1 iterations of our algorithm and therefore the master already has an ensemble $f(\mathbf{x}, N-1)$ composed of N-1 weak hypotheses. The task is now to choose a new weak hypothesis to add to the ensemble. Each worker has a copy of $f(\mathbf{x}, N-1)$ and uses its portion of the data to train a candidate weak hypothesis. Namely, worker k uses ensemble $f(\mathbf{x}, N-1)$ and dataset S_k to generate the weak hypothesis $h_{N,k}(\mathbf{x})$ and sends it to all other workers.

Each worker now evaluates all of the candidates constructed by the other workers. Namely, worker k evaluates the set $\{h_{N,k}(\mathbf{x})\}_{[K]\setminus\{k\}}$, where $f_k(\mathbf{x},N) = f(\mathbf{x},N-1) + h_{N,k}(\mathbf{x})$, and calculates the set of values $\{C_k(f_k(\mathbf{x},N))\}_{[K]\setminus\{k\}}$ and returns these values to the master, where C is the evaluation measure.

The master then chooses the candidate with the largest evaluation score C on the entire training set S. This step of cross-validation adds a further regularization component to the training. We call this method the full selection method. Letting V denote the set of indices of candidates, the master calculates

$$C(f_k(\mathbf{x}, N)) = \sum_{i \in V} C_i(f_k(\mathbf{x}, N))$$
,

for each candidate k. Finally, the master chooses the candidate with the largest average score, and sets

$$f(\mathbf{x}, N) = \underset{f_k(\mathbf{x}, N)}{\operatorname{argmax}} C(f_k(\mathbf{x}, N)) .$$

The master sends the index k of the selected weak hypothesis to all workers. Each worker then updates the model: $f(\mathbf{x}, N) = f(\mathbf{x}, N - 1) + h_{N,k}(\mathbf{x})$. On the next iteration, all of the workers attempt to add another weak learner to $f(\mathbf{x}, N)$.

The intuition behind our approach is that if the hypotheses are sufficiently diverse, then the hypotheses will exhibit dramatically different evaluation scores. The cross-validation ideally results in an ensemble of weak hypotheses that is highly regularized; we test this hypothesis through experiments in Section 1.5.

The communication cost of our approach is dependent on the size of the weak hypothesis and the number of workers, but is not dependent on the size of the training data. In addition, communication only occurs *once* per boosting iteration, removing the need to communicate once per vertex split computation. Each weak hypothesis must be communicated to all other workers, and the resulting evaluation scores must be communicated from each worker to the master. Essentially, the scores are an array of doubles, where the length of the array is the number of weak hypotheses evaluated. Once the master has determined the best weak hypothesis to add to the ensemble, the master need only communicate the index of the best model back to the workers. Each worker updates its model accordingly.

1.4.3 Adding Randomization

The straightforward data-distributed approach presented in Section 1.4.2 has the workers performing two different types of tasks: constructing candidate weak hypotheses and evaluating candidate ensembles that were constructed by others. If the training data size is fixed, and as the number of workers K increases, each worker trains on a smaller portion of the training data, namely $\frac{|S|}{K}$, then the task of constructing candidates can be completed faster. On the other hand, assuming that evaluation time is linear in the number of samples, the total time spent evaluating other candidates stays roughly constant. To see this, note that each worker has to evaluate K-1 candidates on $\frac{|S|}{K}$ samples, for a total evaluation time on the order of $|S| \frac{K-1}{K}$. To resolve this problem, we need to reduce the number of evaluations; we accomplish this using the power of sampling. We call this method the sample selection method.

The algorithm proceeds as before: all of the workers are given the same ensemble $f(\mathbf{x}, N-1)$ and use their datasets to construct candidates. Worker k constructs $f_k(\mathbf{x}, N)$. Rather than the master receiving K candidate weak hypotheses, it chooses a random worker k among the set and the chosen worker communicates $h_{N,k}(\mathbf{x})$ to all other workers (replacing Steps 15–17 in Algorithm 3 with random selection of a hypothesis). The randomized selection of a candidate removes the need for extensive evaluation and requires only communicating the chosen candidate weak hypothesis from the master

Algorithm 3 Data-distributed LambdaMART.

```
1: Input: Training Data: \{x_m, y_m\}, m = 1, \dots, M;
    Number of Trees: N;
    Number of Leaves: L;
    Learning Rate: \eta;
    Number of Workers: K;
 2: Output: Model: f(\mathbf{x}, N);
    for k = 1 to K do
       f(\mathbf{x}, 0) = BaseModel(\mathbf{x}) \{BaseModel \text{ may be empty.}\}\
 4:
       for n = 1 to N do
 5:
          for all m \in S_k do
 6:
              \lambda_m = G(q, \mathbf{x}, y, m) {Calculate \lambda-gradient for sample m as a func-
 7:
             tion of the query q and the documents and labels \mathbf{x}, y associated
              with q, where m is in the fraction of training data S_k on worker
             w_m = \frac{\partial \lambda_m}{\partial f(\mathbf{x}_m)} {Calculate derivative of \lambda-gradient for sample m.}
 8:
          end for
 9:
          \{R_{\ell n}\}_{\ell=1}^L
                                       L-leaf regression tree \{R_{\ell nk}\}_{\ell=1}^L
                         {Create
10:
           \{\mathbf{x}_m, \lambda_m\}, \ m \in S_k.\}
          for \ell = 1 to L do
v_{\ell n} = \frac{\sum_{\mathbf{x}_m \in R_{\ell n}} \lambda_m}{\sum_{\mathbf{x}_m \in R_{\ell n}} w_m}
11:
                                        {Find the leaf values based on approximate
12:
             Newton step.
13:
          end for
          f_k(\mathbf{x}_m, n) = f(\mathbf{x}_m, n-1) + \eta \sum_{\ell} v_{\ell n} 1(\mathbf{x}_m \in R_{\ell nk}) {Update model
14:
          based on approximate Newton step and learning rate.
          \{C_k(f_k(\mathbf{x},n))\}_{[K]\setminus\{k\}} {Compute candidate weak hypotheses cost
15:
          values.
          C(f_k(\mathbf{x}, n)) = \sum_{i \in V} C_i(f_k(\mathbf{x}, n)) {Evaluate candidate weak hy-
16:
          potheses from all other workers.
          f(\mathbf{x}, n) = \operatorname{argmax} C(f_k(\mathbf{x}, n)) {Choose best weak hypothesis and
17:
          update model.}
       end for
18:
19: end for
```

to the workers. This rough estimate may be enough to offer additional regularization over always choosing the same data sample to construct the weak hypothesis. It eliminates the expensive evaluation step previously required

for each candidate at each boosting iteration in the full selection method and will work well if the hypotheses in fact exhibit very little diversity.

1.5 Experiments

In this section, we evaluate our proposed methods on a real-world Web dataset. We ran all of our experiments on a 40-node MPI cluster, running Microsoft HPC Server 2008. One node serves as the cluster scheduler, and the remaining 39 are compute nodes. Each node has two 4-core Intel Xeon 5550 processors running at 2.67GHz and 48 GB of RAM. Each node is connected to two 1Gb Ethernet networks: a private network dedicated to MPI traffic and a public network. Each network is provided by a Cisco 3750e Ethernet switch. The communication layer between nodes on our cluster was written using MPI.NET.

Total train time was measured as the time in seconds between the completion of the loading of the data on the cluster nodes and the completion of the final round of boosting. The time does not include loading data or testing the final model. To mitigate effects of varying cluster conditions, we ran each experimental setting three times and plot all three values.

We swept a range of parameter values for each experiment: we varied the learning rate η from 0.05 to 0.5 and the number of leaves L from 20 to 220, and trained for N=1000 boosting iterations. We determined the best iteration and set of parameter values based on the evaluation accuracy of the model on a validation set.

1.5.1 Data

Our real-world Web data collection contains queries sampled from query log files of a commercial search engine and corresponding URLs. All queries are English queries and contain up to 10 query terms. We perform some stemming on queries. Each query is associated with on average 150–200 documents (URLs), each with a vector of several thousand feature values extracted for the query-URL pair and a human-generated relevance label $l \in \{0,1,2,3,4\}$, with 0 meaning document d is not relevant to query q and 4 meaning d is highly relevant to q. The dataset contains 140,000 queries and corresponding URLs (14,533,212 query-URL pairs). We refer to the dataset size in terms of the number queries, where an n-query dataset means a dataset consisting of all query-URL pairs for those n queries.

We divide the dataset into train, valid, and test sets by selecting a random 80% of samples for training, a random 10% for validation, and a random 10%

for test. We require that for a given query, all corresponding URLs (samples) reside in the same data split. In some experiments, we reduce the amount of training data by $\frac{1}{k}$, $k = \{2, 4, 8, 16, 32\}$. The resulting change in accuracy will indicate the sensitivity of the algorithms to the training data size.

1.5.2 Evaluation Measure

We evaluate using NDCG, Normalized Discounted Cumulative Gain (NDCG) (Jarvelin and Kekalainen, 2000), a widely used measure for search metrics. It operates on multilevel relevance labels; in our work, relevance is measured on a 5-level scale. NDCG for a given query q is defined as follows:

NDCG@
$$T(q) = \frac{100}{Z} \sum_{r=1}^{T} \frac{2^{l(r)} - 1}{\log(1+r)}$$
 (1.2)

where $l(r) \in \{0,\dots,4\}$ is the relevance label of the document at rank position r and T is the truncation level to which NDCG is computed. Z is chosen such that the perfect ranking would result in NDCG@T(q) = 100. Mean NDCG@T is the normalized sum over all queries: $\frac{1}{Q}\sum_{q=1}^{Q} \text{NDCG}@T(q)$. NDCG is particularly well-suited for Web search applications since it accounts for multilevel relevance labels and the truncation level can be set to model user behavior. In our studies, we evaluate our results using mean NDCG@1,3,10. For brevity, we write NDCG@1,3,10. We also perform a significance t-test with a significance level of 0.05. A significant difference should be read as significant at the 95% confidence level. All accuracy results are reported on the same 14K-query test set.

1.5.3 Time Complexity Comparison

We first examine the speed improvements and communication requirements of our distributed LambdaMART algorithms compared to the centralized LambdaMART algorithm. A major advantage of training a distributed learning algorithm over a centralized learning algorithm, in addition to being able to take advantage of more data, is the decrease in training time.

The total training time complexities of centralized LambdaMART, feature-distributed LambdaMART, and data-distributed LambdaMART are O(|S||A|), $O(|S||A_k|)$, and $O(|S_k||A|)$, respectively, where |S| is the size of the training data, |A| is the number of features, and k indexes the node. Sample data-distributed LambdaMART requires only a constant additional communication cost and no evaluation cost. When the number of features is

large, the feature-distributed algorithm is significantly more efficient than the centralized algorithm. When $|A| \ll |S|$, which is commonly the case, the sample data-distributed algorithm is significantly more efficient than both the centralized and feature-distributed algorithms.

Figures 1.1(a)–(d) show the difference in total training time between centralized LambdaMART and feature-distributed LambdaMART. We vary the number of workers K from 1–32, and the number of features |A| from 500–4000. For feature-distributed LambdaMART, $\frac{|A|}{K}$ features are assigned to each node. We employ the same set of parameters for each algorithm to provide fair training time comparisons; the parameters are set to $\eta = 0.1$, N = 500, and L = 200. We evaluated the total train time of feature-distributed LambdaMART on two types of clusters. The first cluster is as previously described, and we denote it as Type I. Each node in the second cluster, denoted as Type II, has 32.0 GB RAM and two quad-core Intel Xeon 5430 processors running at 2.67 GHz.

As shown in Figure 1.1, feature-distributed LambdaMART (solid lines) achieves significantly faster training times than centralized LambdaMART (dotted lines) on both clusters. When trained on Type II with 500 features, feature-distributed LambdaMART with 8 workers achieves almost a two-fold speed-up over centralized LambdaMART (Fig. 1.1(a)). When the number of features is small, as the number of workers increases, the cost of communication among the workers outweighs the speed-ups due to feature distribution, as seen by the increase in time when $K \geq 8$ for Type II (Fig. 1.1(a)–(b)). However, as the number of features increases, communication occupies a smaller percentage of the training time, resulting in decreasing training times. For example, feature-distributed LambdaMART on Type II with 4000 features (Fig. 1.1(d)) exhibits decreasing training times as the number of workers increases and achieves a factor of 6 speed-up over centralized LambdaMART when trained on 32 workers. When trained on Type I, feature-distributed LambdaMART exhibits decreasing training times as the number of workers grows; with 32 workers training on 4000 features, roughly a 3-fold speed-up is obtained.

Our full data-distributed algorithm incurs an additional cost for the evaluation of weak hypotheses and the communication of the evaluation results and the chosen weak hypothesis. The evaluation cost is linear in the number of training samples |S|, but unlike previous methods, the communication cost is independent of the number of training samples, therefore network communication is not a bottleneck as |S| increases to billions of samples. The communication cost scales linearly with the number of nodes and is de-

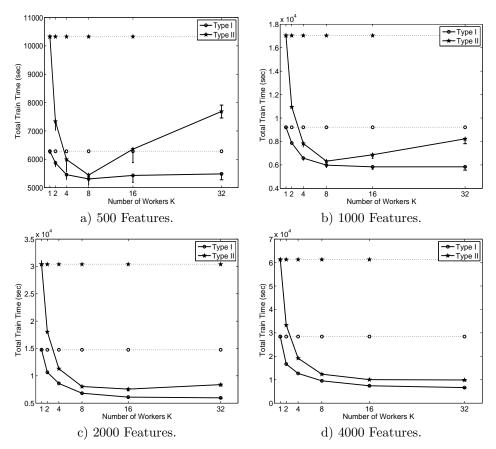


Figure 1.1 Number of Workers K versus Total Training Time in seconds for centralized (dotted) and feature-distributed (solid) LambdaMART, for 500–4000 features and two cluster types. Centralized was trained on the full dataset for all K. Each experimental setting was run three times; times are shown by the bars around each point. Invisible bars indicate times are roughly equivalent.

pendent on the size of the weak learner being broadcast, which is dependent on the number of leaves and the precision of the split thresholds (and is relatively small in practice). Previous approaches consider passing the weight vectors or passing data samples; these approaches are much more expensive in communication time.

The bottleneck of our full data-distributed approach is the cost of evaluation. Our *sample* data-distributed approach has only the additional cost of communicating the randomly chosen weak hypothesis to all nodes, and does not require evaluation. Both data-distributed algorithms result in shorter

training times than the centralized algorithm since the training data per worker k is smaller, $\frac{|S|}{k}$.

Figure 1.2 shows the number of workers versus the total training time in seconds, for weak hypotheses with varying numbers of leaves, for centralized, and full and sample data-distributed LambdaMART. The same parameter settings are used for the three approaches: $L=20,\,N=1000,\,$ and $\eta=0.1.$ The x-axis indicates the number of workers K, where each worker trains on $\frac{|S|}{32}\approx 3500$ queries; with respect to centralized LambdaMART, the x-axis indicates the number of training queries residing on the single worker, $\frac{|S|}{32}K$. The point at K=1 represents training centralized LambdaMART

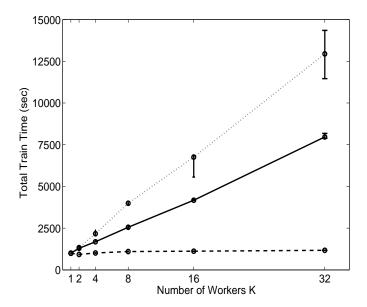


Figure 1.2 Number of Workers K: total data used = 3500K queries versus Training Time in seconds for centralized (dotted), full data-distributed (solid), and sample data-distributed (dashed) LambdaMART with L=20 leaves. Each experimental setting was run three times; times are shown by the bars around each point. Invisible bars indicate times are roughly equivalent.

on $\frac{|S|}{32} \approx 3500$ queries. As K increases, the total train time increases since the communication costs grow with the number of workers K. Since the evaluation and communication costs are almost negligible in sample data-distributed LambdaMART, the total train time is roughly equivalent to training on a single node, even though the amount of training data across the cluster increases with K.

We next evaluate the time required to train on |S| queries, where the

queries are split among K workers. For the centralized algorithm, a single worker trains on |S| queries. We set $\eta=0.1,\,L=\{100,200\}$, and N=1000. Figure 1.3 plots the number of workers K versus the total train time in seconds; every point represents a model trained on all |S| queries. For the data-distributed algorithms, the training data S is split among K workers: as K increases, the number of queries on a single worker $(\frac{|S|}{K})$ decreases, but the total number of queries across all nodes remains constant (|S|). The two

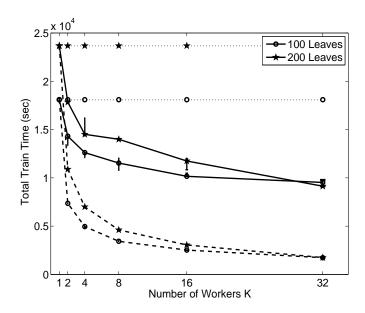


Figure 1.3 Number of Workers K versus Training Time in seconds for centralized (dotted), full data-distributed (solid), and sample data-distributed (dashed) LambdaMART on fourteen million samples (query-URL pairs). Each experimental setting was run three times; times are shown by the bars around each point.

points at K=1 represent the training times of centralized LambdaMART trained on fourteen million URLs. The central model at K=1 is plotted at all K values for reference (shown by the dotted lines). When K>1, the train times of full and sample data-distributed LambdaMART are significantly less than the centralized algorithm. Particularly notable is the reduction in train time obtained by the sample data-distributed LambdaMART algorithm.

1.5.4 Accuracy Comparison

In this section, we evaluate the prediction accuracy of our data-distributed algorithm using the full and sample selection strategies². We consider the case where the training data S cannot fit in the main memory of a single machine. We compare the accuracy of our data-distributed algorithms and the accuracy of the centralized algorithm on a separate test set consisting of 14K queries, while varying the number of nodes K and the amount of training data. Table 1.1 lists for each experimental setting the model parameters that produced the best validation accuracy.

The first experiment evaluates the change in accuracy of our data-distributed algorithms as the number of workers increases. We simulate memory constraints by assuming one worker can store at most 3500 queries — in order to exploit more training data, the data must reside on separate workers. As the number of workers increases, it simulates the case where more and more training data is available, but the memory capacity of a single worker remains the same. The training set S is randomly partitioned into 32 disjoint subsets and each subset resides on one of the 32 nodes in our cluster. Each partition contains roughly 3500 queries and corresponding URLs. When K=1, a single worker trains on 3500 queries, when K=2, two workers train on 3500 queries each, and so on.

Figure 1.4 plots the number of workers K versus NDCG for full and sample data-distributed LambdaMART³. The training data distributed among the workers in the cluster acts as additional validation data since it is used for the evaluation and selection of the weak hypothesis. Full and sample selection strategies result, for each K, in similar NDCG scores, and exhibit NDCG accuracy increases as K increases. Having 3500K queries in the cluster, for $K = \{8, 16, 32\}$, yields significant gains in NDCG@3 and 10 over training on 3500 queries (K = 1). Thus, additional data, although mostly used for validation, significantly increases NDCG accuracy.

In Figure 1.4(d), we analyze the effect of lifting the memory constraint and plot the centralized algorithm accuracy trained on 3500K queries (dotted line) on a single worker, for increasing values of K. For $K = \{4, 8, 16, 32\}$, the resulting model is significantly better than the corresponding data-distributed models trained on 3500K queries, indicating that when able to use additional data directly for training, it is preferable to using it for cross-validation.

Somewhat surprisingly, as the amount of data increases, even though the

² Recall that the feature-distributed algorithm outputs the same model as the centralized algorithm and thus has the same prediction accuracy.

³ The corresponding training time plots were given in Figure 1.2.

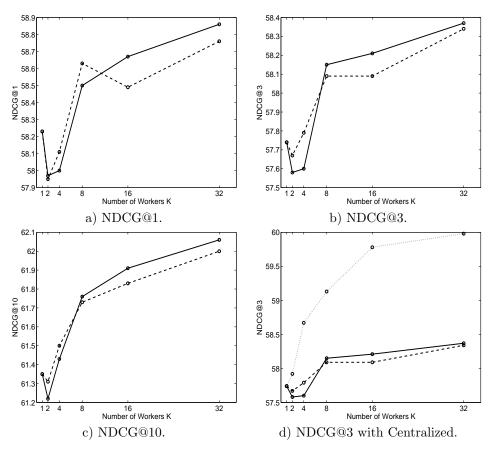


Figure 1.4 Number of Workers K versus NDCG@1, 3, 10 for full (solid) and sample (dashed) data-distributed LambdaMART. Each worker trains on 3500 queries. Figure (d) includes centralized LambdaMART (dotted) trained on 3500K queries at each x-axis point. Signficant differences are stated in the text.

data is highly distributed, the optimal values of the learning rate η and number of leaves L change dramatically for data-distributed LambdaMART (see Table 1.1). Even though it is only the amount of validation data that increases as K increases, the parameters behave similarly to increasing the amount of centralized training data.

For our second experiment, we investigate how training on overlapping sets of data affects NDCG accuracy. Assume that a single worker can store at most 7000 queries and let the amount of training data available be 3500K queries. We construct our overlapping sets as follows: the training data S is divided into K sets, S_1, \ldots, S_K . Worker k stores set S_k and set S_{k+1} , resulting in 7000 queries. For example, when K = 4, $S_1 + S_2$, $S_2 + S_3$, $S_3 + S_4 + S_5 +$

 S_4 , $S_4 + S_1$ reside on workers 1, 2, 3, 4, respectively. The total number of unique queries in the cluster remains 3500K. This approach can easily scale to larger datasets.

Figure 1.5 plots the number of workers K versus NDCG, where each worker contains an overlapping set of 7000 queries, compared to 3500 queries. The accuracy gains from training on 7000 queries per worker instead of 3500 are significant for all K at NDCG@3 and 10, further indicating that training on more data is better than validating over more data, and also indicating that the samples need not be unique across the workers. In particular, training K=8 workers on overlapping 7000-query sets results in similar accuracy to training K=32 workers on 3500-query sets. In all cases, full and sample selection strategies result in similar accuracies.

In Figure 1.5(d), we again lift the memory constraint, and plot the NDCG@3 accuracy of the central model on 3500K queries (dotted line). The results highlight the benefit of increasing the amount of training data per worker over using additional validation data, as seen by the significant gap between the central and data-distributed models.

Even though the central model is superior in accuracy to our data-distributed models (assuming memory of a single worker is not constrained), our data-distributed algorithms exhibit significant gains when the memory of a single worker is exhausted. In this scenario, a benefit of our data-distributed algorithm is not only parallelized training, but also that the amount of information communicated between the master and the workers is independent of the amount of training data; it is dependent on the number of workers and the size of a weak hypothesis. Our full data-distributed algorithm relies on the diversity of each weak hypothesis, yet upon examination of the NDCG scores of the weak hypotheses, we found that during early rounds of boosting the weak hypotheses exhibited diversity, but after only a few rounds of boosting, the weak hypotheses achieved almost identical NDCG scores on the large validation data, indicating that we may be able to eliminate the evaluation step entirely and select a worker at random to produce the weak hypothesis at each iteration.

By eliminating the evaluation step at each iteration, the training time decreases dramatically, as previously shown in Figure 1.2, since the cost of evaluation is linear in the size of the largest split S_k , and the accuracies are equivalent to choosing the best weak hypothesis based on NDCG evaluation. Thus, our sample selection algorithm can be efficiently applied to billions of samples and achieve comparable accuracy to the full selection strategy. The sample selection algorithm also points to the advantages that an asynchronous distributed approach may have over a synchronous one.

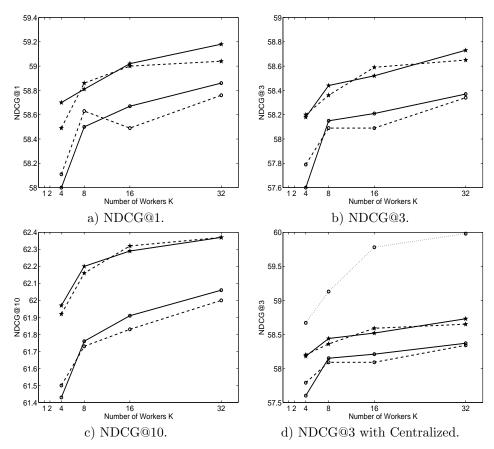


Figure 1.5 Number of Workers K versus NDCG@1, 3, 10 for full (solid) and sample (dashed) data-distributed LambdaMART. Each worker trains on 7000 overlapping queries (stars). Results from training on 3500 queries per worker (circles) are plotted for comparison. Figure (d) includes centralized LambdaMART (dotted) trained on 3500K queries at each x-axis point. Signficant differences are stated in the text.

Since each worker k trains on a random subset S_k of the training data, then an asynchronous algorithm could assign idle workers different tasks, such as evaluating or training a regression tree for a future iteration. Such an approach could possibly yield improvements in speed or accuracy by taking advantage of the large number of workers available at any given time.

Our sample approach can also be applied to centralized training: at each round of boosting, sample the training data and train a weak hypothesis on that sample. If the complete training dataset fits in memory on a single machine, then the training time will decrease by training on a sample of the data during each boosting iteration. However, if the training data must

reside on separate machines, then to train on a single machine, at each round of boosting, the sample must be sent to the machine and then loaded into memory on the machine. The sample must be sampled across all of the machines. The process of communicating the data samples from the many nodes that store the data will be costly and prohibit the use of the algorithm on very large datasets.

1.5.5 Additional Remarks on Data-distributed LambdaMART

We have shown that our data-distributed approach is a viable method for exploiting additional training data when the main memory of a single machine is exceeded. In this section, we consider the case where the main memory of the workers is not exhausted and we have a fixed amount of training data. One goal of a distributed learning algorithm is to achieve comparable or better accuracy compared to the centralized algorithm, but with much shorter training times. We conduct a series of experiments to determine if our data-distributed approach achieves comparable accuracy with shorter training times compared to the centralized algorithm.

We first determine the effect of decreasing the training data size on the centralized algorithm's accuracy. Let the size of the training set residing on the central machine decrease as $\frac{|S|}{K}$, with increasing values of K. Figure 1.6 plots the training set size versus NDCG for the centralized model (dotted line). When training on 50% of the training data, the NDCG@1, 3, 10 accuracy compared to training on 100% of the data is statistically similar. It is also noteworthy that as the training set size decreases, the optimal number of leaves decreases, while the optimal learning rate stays constant across the training data sizes (Table 1.1).

We next determine the accuracy of full and sample data-distributed LambdaMART, where the training data S is split across K workers and each worker contains $\frac{|S|}{K}$ queries⁴. Figure 1.6 contains the centralized and full and sample data-distributed accuracy results. In the central case, the x-axis indicates the size of the training set on the single node. In the data-distributed cases, the x-axis indicates the number of workers K and correspondingly the amount of training data $\frac{|S|}{K}$ on a given worker. The results indicate that choosing a weak hypothesis among the K nodes, either by full or sample selection, is better than choosing the same weak hypothesis from the same node at each iteration. This is seen by looking at a given value of K: the data-distributed NDCG scores are consistently higher than the centralized

⁴ The corresponding training time plot was given in Figure 1.3.

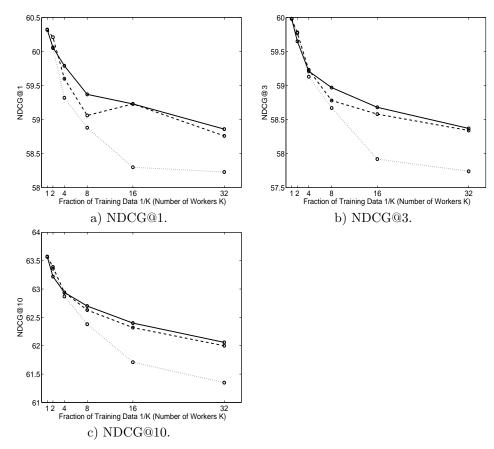


Figure 1.6 Number of Workers K vs. NDCG@1, 3, 10 for centralized (dotted) and full (solid) and sample (dashed) data-distributed LambdaMART. Each worker trains on $\frac{|S|}{K}$ queries. The central model was trained on $\frac{|S|}{K}$ queries on a single worker. Significant differences are stated in the text.

NDCG scores and statistically significantly higher for $K \geq 16$. However, there is not a single point on the data-distributed curves that outperforms training on the full data set using the centralized algorithm (the point at K=1). Splitting the data across an increasing number of workers K causes a gradual and continual drop in accuracy, with significant losses compared to the point at K=1 when $K\geq 4$.

The experiment additionally shows that choosing a single weak hypothesis from a worker at random (sample selection) performs similarly to choosing the best weak hypothesis among the K workers based on the evaluation step.

Finally, we determine if training on larger overlapping sets of data achieves

comparable accuracy to the central model, but with less training time. We consider K=4 workers and divide the training data S into 4 sets S_1, S_2, S_3, S_4 . Each set contains 25% of the full training set. Worker k is assigned sets $S_k + S_{k+1} + S_{k+2}$, and thus produces a weak hypothesis based on 75% of the full training set. At each iteration, we use sample selection to produce the next weak hypothesis in the ensemble. We find that training on 75% of the training queries per node yields equivalent NDCG scores to the central model trained on 100% of the training data, but trains in less than half of the time.

Table 1.1 The learning rate η and the number of leaves L for centralized LambdaMART, and full and sample data-distributed LambdaMART, respectively. The first set of columns are the parameters when training on 3500 queries per worker; in the central case, a single worker trains on 3500K queries. The second set of columns are the parameters when training on 7000 overlapping queries per worker; in the central case, a single worker trains on 7000K queries. The final columns contain the parameters when training on $\frac{|S|}{K}$ queries per worker; in the central case, a single worker trains on $\frac{|S|}{K}$ queries.

	350	00	70	00	Al	1
K	η	L	η	L	η	L
1	0.1, 0.1, 0.1	20, 20, 20	0.1, 0.1, 0.1	80, 80, 80	0.1, 0.1, 0.1	20, 20, 20
2	0.1, 0.05, 0.05	80, 80, 80	0.1, 0.1, 0.1	180, 180, 180	0.1, 0.1, 0.1	80, 190, 200
4	0.1, 0.1, 0.05	180, 80, 80	0.1, 0.05, 0.05	200, 200, 200	0.1, 0.05, 0.05	180, 170, 200
8	0.1, 0.05, 0.05	200, 120, 120	0.1, 0.05, 0.05	200, 200, 200	0.05, 0.05, 0.05	200, 180, 200
16	0.1, 0.05, 0.05	200, 140, 140	0.1, 0.05, 0.05	200, 200, 200	0.1, 0.05, 0.05	200, 170, 160
32	0.1, 0.05, 0.05	200, 140, 140	0.1, 0.05, 0.05	200, 140, 140	0.1, 0.05, 0.05	200, 100, 140

1.6 Conclusions and Future Work

In summary, we have presented two approaches for distributing LambdaMART. The first distributes by feature by distributing the vertex split computations and requires that the full training set fit in main memory on each node in the cluster. Our feature-distributed approach achieves up to 6-fold significant speed-ups over centralized LambdaMART while producing the same model and accuracy. Our second approach distributes the data across the nodes in the compute cluster and employs one of two strategies for selec-

tion of the next weak hypothesis: (1) select the next weak hypothesis based on evaluation scores on the training data residing on other nodes (full) (2) select the next weak hypothesis at random (sample). We have shown that both selection strategies offer significant training time speed-ups resulting in training up to 2–4 times faster than centralized LambdaMART. In particular, sample data-distributed LambdaMART demonstrates no significant accuracy loss compared to full data-distributed LambdaMART, and achieves even more significant training time speed-ups. Unlike the feature-distributed approach, our data-distributed approaches can scale to billions of training samples.

Our data-distributed algorithms, however, do not match the centralized algorithm in accuracy. The accuracy results were disappointing and indicate that using data for massive cross-validation results in significant accuracy loss. In the future, it is worth determining a distributed method that can scale to billions of examples, but with accuracy that is equivalent or superior to training on centralized data, and with a communication cost that does not scale with the number of samples. Future work needs to be done to determine the bottlenecks of our data-distributed approaches, and to determine how best to take advantage of distributed data without sacrificing the speed-ups obtained by our methods. We have developed a first step toward achieving this goal in that we have presented a method where the communication is independent of the number of samples.

1.7 Acknowledgements

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Notes

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