

From RankNet to LambdaRank to LambdaMART: An Overview

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Abstract

LambdaMART is the boosted tree version of LambdaRank, which is based on RankNet. RankNet, LambdaRank, and LambdaMART have proven to be very successful algorithms for solving real world ranking problems: for example an ensemble of LambdaMART rankers won Track 1 of the 2010 Yahoo! Learning To Rank Challenge. The details of these algorithms are spread across several papers and reports, and so here we give a self-contained, detailed and complete description of them.

1 Introduction

LambdaMART is the boosted tree version of LambdaRank, which is based on RankNet. RankNet, LambdaRank, and LambdaMART have proven to be very successful algorithms for solving real world ranking problems: for example an ensemble of LambdaMART rankers won the recent Yahoo! Learning To Rank Challenge (Track 1) [5]. Although here we will concentrate on ranking, it is straightforward to modify MART in general, and LambdaMART in particular, to solve a wide range of supervised learning problems (including maximizing information retrieval functions, like NDCG, which are not smooth functions of the model scores).

This document attempts to give a self-contained explanation of these algorithms. The only mathematical background needed is basic vector calculus; some familiarity with the problem of learning to rank is assumed. Our hope is that this overview is sufficiently self-contained that, for example, a reader who wishes to train a boosted tree model to optimize some information retrieval measure they have in mind, can understand how to use these methods to achieve this. Ranking for web search is used as a concrete example throughout. Material in gray sections is background material

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that is not necessary for understanding the main thread. These ideas were originated over several years and appeared in several papers; the purpose of this report is to collect all of the ideas into one, easily accessible place (and to add background and more details where needed). To keep the exposition brief, no experimental results are presented in this chapter, and we do not compare to any other methods for learning to rank (of which there are many); these topics are addressed extensively elsewhere.

2 RankNet

For RankNet [2], the underlying model can be any model for which the output of the model is a differentiable function of the model parameters (typically we have used neural nets, but we have also implemented RankNet using boosted trees, which we will describe below). RankNet training works as follows. The training data is partitioned by query. At a given point during training, RankNet maps an input feature vector $x \in \mathcal{R}^n$ to a number $f(x)$. For a given query, each pair of urls U_i and U_j with differing labels is chosen, and each such pair (with feature vectors x_i and x_j) is presented to the model, which computes the scores $s_i = f(x_i)$ and $s_j = f(x_j)$. Let $U_i \triangleright U_j$ denote the event that U_i should be ranked higher than U_j (for example, because U_i has been labeled 'excellent' while U_j has been labeled 'bad' for this query; note that the labels for the same urls may be different for different queries). The two outputs of the model are mapped to a learned probability that U_i should be ranked higher than U_j via a sigmoid function, thus:

$$P_{ij} \equiv P(U_i \triangleright U_j) \equiv \frac{1}{1 + e^{-\sigma(s_i - s_j)}}$$

where the choice of the parameter σ determines the shape of the sigmoid. The use of the sigmoid is a known device in neural network training that has been shown to lead to good probability estimates [1]. We then apply the cross entropy cost function, which penalizes the deviation of the model output probabilities from the desired probabilities: let \bar{P}_{ij} be the known probability that training url U_i should be ranked higher than training url U_j . Then the cost is

$$C = -\bar{P}_{ij} \log P_{ij} - (1 - \bar{P}_{ij}) \log(1 - P_{ij})$$

For a given query, let $S_{ij} \in \{0, \pm 1\}$ be defined to be 1 if document i has been labeled to be more relevant than document j , -1 if document i has been labeled to be less relevant than document j , and 0 if they have the same label. Throughout this paper we assume that the desired ranking is deterministically known, so that $\bar{P}_{ij} = \frac{1}{2}(1 + S_{ij})$. (Note that the model can handle the more general case of measured probabilities, where, for example, \bar{P}_{ij} could be estimated by showing the pair to several judges). Combining the above two equations gives

跟query没有关系？不同的url根据query不同提取不同的特征向量x？？

$$C = \frac{1}{2}(1 - S_{ij})\sigma(s_i - s_j) + \log(1 + e^{-\sigma(s_i - s_j)})$$

The cost is comfortably symmetric (swapping i and j and changing the sign of S_{ij} should leave the cost invariant): for $S_{ij} = 1$,

$$C = \log(1 + e^{-\sigma(s_i - s_j)})$$

while for $S_{ij} = -1$,

$$C = \log(1 + e^{-\sigma(s_j - s_i)})$$

Note that when $s_i = s_j$, the cost is $\log 2$, so the model incorporates a **margin** (that is, documents with different labels, but to which the model assigns the same scores, are still pushed away from each other in the ranking). Also, asymptotically, the cost becomes linear (if the scores give the wrong ranking), or zero (if they give the correct ranking). This gives

$$\frac{\partial C}{\partial s_i} = \sigma \left(\frac{1}{2}(1 - S_{ij}) - \frac{1}{1 + e^{\sigma(s_i - s_j)}} \right) = -\frac{\partial C}{\partial s_j} \quad (1)$$

This gradient is used to update the weights $w_k \in \mathcal{R}$ (i.e. the model parameters) so as to reduce the cost via stochastic gradient descent¹:

$$w_k \rightarrow w_k - \eta \frac{\partial C}{\partial w_k} = w_k - \eta \left(\frac{\partial C}{\partial s_i} \frac{\partial s_i}{\partial w_k} + \frac{\partial C}{\partial s_j} \frac{\partial s_j}{\partial w_k} \right) \quad (2)$$

where η is a positive learning rate (a parameter chosen using a validation set; typically, in our experiments, $1e-3$ to $1e-5$). Explicitly:

$$\delta C = \sum_k \frac{\partial C}{\partial w_k} \delta w_k = \sum_k \frac{\partial C}{\partial w_k} \left(-\eta \frac{\partial C}{\partial w_k} \right) = -\eta \sum_k \left(\frac{\partial C}{\partial w_k} \right)^2 < 0$$

The idea of learning via gradient descent is a key idea that appears throughout this paper (even when the desired cost doesn't have well-posed gradients, and even when the model (such as an ensemble of boosted trees) doesn't have differentiable parameters): **to update the model, we must specify the gradient of the cost with respect to the model parameters w_k , and in order to do that, we need the gradient of the cost with respect to the model scores s_i .** The gradient descent formulation of boosted trees (such as MART [8]) bypasses the need to compute $\partial C / \partial w_k$ by directly modeling $\partial C / \partial s_i$.

为求 (2)，我们必须得到 (1)

¹ We use the convention that if two quantities appear as a product and they share an index, then that index is summed over.

2.1 Factoring RankNet: Speeding Up Ranknet Training

The above leads to a factorization that is the key observation that led to LambdaRank [4]: for a given pair of urls U_i, U_j (again, summations over repeated indices are assumed):

$$\begin{aligned}\frac{\partial C}{\partial w_k} &= \frac{\partial C}{\partial s_i} \frac{\partial s_i}{\partial w_k} + \frac{\partial C}{\partial s_j} \frac{\partial s_j}{\partial w_k} = \sigma \left(\frac{1}{2}(1 - S_{ij}) - \frac{1}{1 + e^{\sigma(s_i - s_j)}} \right) \left(\frac{\partial s_i}{\partial w_k} - \frac{\partial s_j}{\partial w_k} \right) \\ &= \lambda_{ij} \left(\frac{\partial s_i}{\partial w_k} - \frac{\partial s_j}{\partial w_k} \right)\end{aligned}$$

where we have defined

$$\lambda_{ij} \equiv \frac{\partial C(s_i - s_j)}{\partial s_i} = \sigma \left(\frac{1}{2}(1 - S_{ij}) - \frac{1}{1 + e^{\sigma(s_i - s_j)}} \right) \quad (3)$$

为啥是不同label的pairs?

Let I denote the set of pairs of indices $\{i, j\}$, for which we desire U_i to be ranked differently from U_j (for a given query). I must include each pair just once, so it is convenient to adopt the convention that I contains pairs of indices $\{i, j\}$ for which $U_i \triangleright U_j$, so that $S_{ij} = 1$ (which simplifies the notation considerably, and we will assume this from now on). Note that since RankNet learns from probabilities and outputs probabilities, it does not require that the urls be labeled; it just needs the set I , which could also be determined by gathering pairwise preferences (which is much more general, since it can be inconsistent: for example a confused judge may have decided that for a given query, $U_1 \triangleright U_2$, $U_2 \triangleright U_3$, and $U_3 \triangleright U_1$). Now summing all the contributions to the update of weight w_k gives

RankNet分两步, output probabilities和probabilities

$$\delta w_k = -\eta \sum_{\{i,j\} \in I} \left(\lambda_{ij} \frac{\partial s_i}{\partial w_k} - \lambda_{ij} \frac{\partial s_j}{\partial w_k} \right) \equiv -\eta \sum_i \lambda_i \frac{\partial s_i}{\partial w_k}$$

where we have introduced the λ_i (one λ_i for each url: note that the λ 's with one subscript are sums of the λ 's with two). To compute λ_i (for url U_i), we find all j for which $\{i, j\} \in I$ and all k for which $\{k, i\} \in I$. For the former, we increment λ_i by λ_{ij} , and for the latter, we decrement λ_i by λ_{ki} . For example, if there were just one pair with $U_1 \triangleright U_2$, then $I = \{\{1, 2\}\}$, and $\lambda_1 = \lambda_{12} = -\lambda_2$. In general, we have:

$$\lambda_i = \sum_{j: \{i,j\} \in I} \lambda_{ij} - \sum_{j: \{j,i\} \in I} \lambda_{ij} \quad (4)$$

As we will see below, you can think of the λ 's as little arrows (or forces), one attached to each (sorted) url, the direction of which indicates the direction we'd like the url to move (to increase relevance), the length of which indicates by how much, and where the λ for a given url is computed from all the pairs in which that url is a member. When we first implemented RankNet, we used true stochastic gradient descent: the weights were updated after each pair of urls (with different labels) were examined. The above shows that instead, we can accumulate the λ 's for each url,

summing its contributions from all pairs of urls (where a pair consists of two urls with different labels), and then do the update. This is mini-batch learning, where all the weight updates are first computed for a given query, and then applied, but the speedup results from the way the problem factorizes, not from using mini-batch alone. This led to a very significant speedup in RankNet training (since a weight update is expensive, since e.g. for a neural net model, it requires a backprop). In fact training time dropped from close to quadratic in the number of urls per query, to close to linear. It also laid the groundwork for LambdaRank, but before we discuss that, let's review the information retrieval measures we wish to learn.

3 Information Retrieval Measures

Information retrieval researchers use ranking quality measures such as Mean Reciprocal Rank (MRR), Mean Average Precision (MAP), Expected Reciprocal Rank (ERR), and **Normalized Discounted Cumulative Gain (NDCG)**. NDCG [9] and ERR [6] have the advantage that they handle multiple levels of relevance (whereas MRR and MAP are designed for binary relevance levels), and that the measure includes a position dependence for results shown to the user (that gives higher ranked results more weight), which is particularly appropriate for web search. All of these measures, however, have the unfortunate property that viewed as functions of the model scores, they are everywhere either discontinuous or flat, so gradient descent appears to be problematic, since the gradient is everywhere either zero or not defined. For example, NDCG is defined as follows. The DCG (Discounted Cumulative Gain) for a given set of search results (for a given query) is

处理多级相关性

$$DCG@T \equiv \sum_{i=1}^T \frac{2^{l_i} - 1}{\log(1 + i)} \quad (5)$$

where T is the truncation level (for example, if we only care about the first page of returned results, we might take $T = 10$), and l_i is the label of the i th listed URL. We typically use five levels of relevance: $l_i \in \{0, 1, 2, 3, 4\}$. The NDCG is the normalized version of this:

$$NDCG@T \equiv \frac{DCG@T}{\max DCG@T}$$

where the denominator is the maximum $DCG@T$ attainable for that query, so that $NDCG@T \in [0, 1]$.

ERR was introduced more recently [6] and is inspired by **cascade models**, where a user is assumed to read down the list of returned urls until they find one they like. ERR is defined as

$$\sum_{r=1}^n \frac{1}{r} R_r \prod_{i=1}^{r-1} (1 - R_i)$$

where, if l_m is the maximum label value,

$$R_i = \frac{2^{l_i} - 1}{2^{l_m}}$$

R_i models the probability that the user finds the document at rank position i relevant. Naively one might expect that the cost of computing Δ_{ERR} (the change in ERR resulting from swapping two document's ranks while leaving all other ranks unchanged) would be cubic in the number of documents for a given query, since the documents whose ranks lie between the two ranks considered contribute to Δ_{ERR} , and since this contribution must be computed for every pair of documents. However the computation has quadratic cost (where the quadratic cost arises from the need to compute Δ_{ERR} for every pair of documents with different labels), since it can be ordered as follows. Let Δ denote Δ_{ERR} . Letting $T_i \equiv 1 - R_i$, create an array A whose i th component is the ERR computed only to level i . (Computing A has linear complexity). Then:

1. Compute $\pi_i \equiv \prod_{n=1}^i T_n$ for $i > 0$, and set $\pi_0 = 1$.
2. Set $\Delta = \pi_{i-1}(R_i - R_j)/r_i$.
3. Increment Δ by

$$\begin{aligned} & (T_i - T_j) \left(\frac{R_{i+1}}{r_{i+1}} + \frac{T_{i+1}R_{i+2}}{r_{i+2}} + \dots + \frac{T_{i+1} \dots T_{j-2}R_{j-1}}{r_{j-1}} \right) \pi_{i-1} \\ & \equiv (T_i - T_j) \left(\frac{A_{j-1} - A_i}{T_i} \right) \end{aligned}$$

4. Further increment Δ by

$$\frac{\pi_{i-1}}{r_j} T_{i+1} T_{i+2} \dots T_{j-1} (T_i R_j - T_j R_i) = \frac{\pi_{j-1}}{r_j} \left(R_j - \frac{T_j R_i}{T_i} \right).$$

Note that unlike NDCG, the change in ERR induced by swapping two urls U_i and U_j , keeping all other urls fixed (with the same rank), depends on the labels and ranks of the urls with ranks between those of U_i and U_j . As a result, the curious reader might wonder if ERR is consistent: if $U_i \triangleright U_j$, and the two rank positions are swapped, does ERR necessarily decrease? It's easy to see that it must by showing that the above Δ is nonnegative when $R_i > R_j$. Collecting terms, we have that

$$\Delta = \frac{\pi_i(R_i - R_j)}{T_i} \left(\frac{1}{r_i} - \frac{R_{i+1}}{r_{i+1}} - \frac{T_{i+1}R_{i+2}}{r_{i+2}} - \dots - \frac{T_{i+1} \dots T_{j-2}R_{j-1}}{r_{j-1}} - \frac{T_{i+1} \dots T_{j-1}}{r_j} \right)$$

Since $r_{i+1} > r_i$, this is certainly nonnegative if

$$R_{i+1} + T_{i+1}R_{i+2} + \dots + T_{i+1} \dots T_{j-2}R_{j-1} + T_{i+1} \dots T_{j-1} \leq 1.$$

But since $R_i + T_i = 1$, the left hand side just collapses to 1.

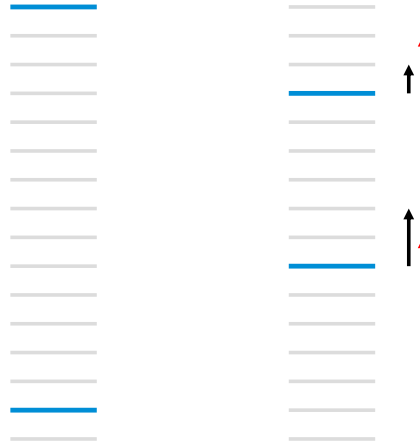


Fig. 1 A set of urls ordered for a given query using a binary relevance measure. The light gray bars represent urls that are not relevant to the query, while the dark blue bars represent urls that are relevant to the query. Left: the total number of pairwise errors is thirteen. Right: by moving the top url down three rank levels, and the bottom relevant url up five, the total number of pairwise errors has been reduced to eleven. However for IR measures like NDCG and ERR that emphasize the top few results, this is not what we want. The (black) arrows on the left denote the RankNet gradients (which increase with the number of pairwise errors), whereas what we'd really like are the (red) arrows on the right.

4 LambdaRank

Although RankNet can be made to work quite well with the above measures by simply using the measure as a stopping criterion on a validation set, we can do better. RankNet is optimizing for (a smooth, convex approximation to) the number of pairwise errors, which is fine if that is the desired cost, but it does not match well with some other information retrieval measures. Figure 1 is a schematic depicting the problem. The idea of writing down the desired gradients directly (shown as arrows in the Figure), rather than deriving them from a cost, is one of the ideas underlying LambdaRank [4]: it allows us to bypass the difficulties introduced by the sort in most IR measures. Note that this does not mean that the gradients are not gradients of a cost. In this section, for concreteness we assume that we are designing a model to learn NDCG.

4.1 From RankNet to LambdaRank

The key observation of LambdaRank is thus that in order to train a model, we don't need the costs themselves: we only need the gradients (of the costs with respect to the model scores). The arrows (λ 's) mentioned above are exactly those gradients. The λ 's for a given URL U_1 get contributions from all other URLs for the same query that have different labels. The λ 's can also be interpreted as forces (which are gradients of a potential function, when the forces are conservative): if U_2 is more relevant than U_1 , then U_1 will get a push downwards of size $|\lambda|$ (and U_2 , an equal and opposite push upwards); if U_2 is less relevant than U_1 , then U_1 will get a push upwards of size $|\lambda|$ (and U_2 , an equal and opposite push downwards).

Experiments have shown that modifying Eq. (3) by simply multiplying by the size of the change in NDCG ($|\Delta_{NDCG}|$) given by swapping the rank positions of U_1 and U_2 (while leaving the rank positions of all other urls unchanged) gives very good results [4]. Hence in LambdaRank we imagine that there is a utility C such that²

$$\lambda_{ij} = \frac{\partial C(s_i - s_j)}{\partial s_i} = \frac{-\sigma}{1 + e^{\sigma(s_i - s_j)}} |\Delta_{NDCG}| \quad (6)$$

Since here we want to maximize C , equation (2) (for the contribution to the k th weight) is replaced by

$$w_k \rightarrow w_k + \eta \frac{\partial C}{\partial w_k}$$

so that

$$\delta C = \frac{\partial C}{\partial w_k} \delta w_k = \eta \left(\frac{\partial C}{\partial w_k} \right)^2 > 0 \quad (7)$$

Thus although Information Retrieval measures, viewed as functions of the model scores, are either flat or discontinuous everywhere, the LambdaRank idea bypasses this problem by computing the gradients after the urls have been sorted by their scores. We have shown empirically that, intriguingly, such a model actually optimizes NDCG directly [12, 7]. In fact we have further shown that if you want to optimize some other information retrieval measure, such as MRR or MAP, then LambdaRank can be trivially modified to accomplish this: the only change is that $|\Delta_{NDCG}|$ above is replaced by the corresponding change in the chosen IR measure [7].

For a given pair, a λ is computed, and the λ 's for U_1 and U_2 are incremented by that λ , where the sign is chosen so that $s_2 - s_1$ becomes more negative, so that U_1 tends to move up the list of sorted urls while U_2 tends to move down. Again, given more than one pair of urls, if each url U_i has a score s_i , then for any particular pair $\{U_i, U_j\}$ (recall we assume that U_i is more relevant than U_j), we separate the

² We have switched from cost to utility here since NDCG is a measure of goodness (which we want to maximize). Recall also that $S_{ij} = 1$.

calculation:

$$\begin{aligned}\delta s_i &= \frac{\partial s_i}{\partial w_k} \delta w_k = \frac{\partial s_i}{\partial w_k} \left(-\eta \lambda \frac{\partial s_i}{\partial w_k} \right) < 0 \\ \delta s_j &= \frac{\partial s_j}{\partial w_k} \delta w_k = \frac{\partial s_j}{\partial w_k} \left(\eta \lambda \frac{\partial s_j}{\partial w_k} \right) > 0\end{aligned}$$

Thus, every pair generates an equal and opposite λ , and for a given url, all the lambdas are incremented (from contributions from all pairs in which it is a member, where the other member of the pair has a different label). This accumulation is done for every url for a given query; when that calculation is done, the weights are adjusted based on the computed lambdas using a small (stochastic gradient) step.

4.2 LambdaRank: Empirical Optimization of NDCG (or other IR Measures)

Here we briefly describe how we showed empirically that LambdaRank directly optimizes NDCG [12, 7]. Suppose that we have trained a model and that its (learned) parameter values are w_k^* . We can estimate a smoothed version of the gradient empirically by fixing all weights but one (call it w_i), computing how the NDCG (averaged over a large number of training queries) varies, and forming the ratio

$$\frac{\delta M}{\delta w_i} = \frac{M - M^*}{w_i - w_i^*}$$

where for n queries

$$M \equiv \frac{1}{n} \sum_{i=1}^n NDCG(i) \quad (8)$$

and where the i th query has NDCG equal to $NDCG(i)$. Now suppose we plot M as a function of w_i for each i . If we observe that M is a maximum at $w_i = w_i^*$ for every i , then we know that the function has vanishing gradient at the learned values of the weights, $w = w^*$. (Of course, if we zoom in on the graph with sufficient magnification, we'll find that the curves are little step functions; we are considering the gradient at a scale at which the curves are smooth). This is necessary but not sufficient to show that the NDCG is a maximum at $w = w^*$: it could be a saddle point. We could attempt to show that the point is a maximum by showing that the Hessian is negative definite, but that is in several respects computationally challenging. However we can obtain an

arbitrarily tight bound by applying a one-sided Monte Carlo test: choose sufficiently many random directions in weight space, move the weights a little along each such direction, and check that M always decreases as we move away from w^* . Specifically, we choose directions uniformly at random by sampling from a spherical Gaussian. Let p be the fraction of directions that result in M increasing. Then

$$P(\text{We miss an ascent direction despite } n \text{ trials}) = (1 - p)^n$$

Let's call $1 - P$ our confidence. If we require a confidence of 99% (i.e. we choose $\delta = 0.01$ and require $P \leq \delta$), how large must n be, in order that $p \leq p_0$, where we choose $p_0 = 0.01$? We have

$$(1 - p_0)^n \leq \delta \rightarrow n \geq \frac{\log \delta}{\log(1 - p_0)} \quad (9)$$

which gives $n \geq 459$ (i.e. choose 459 random directions and always find that M decreases along those directions; note that larger value of p_0 would require fewer tests). In general we have confidence at least $1 - \delta$ that $p \leq p_0$ provided we perform at least $n = \frac{\log \delta}{\log(1 - p_0)}$ tests.

4.3 When are the Lambdas Actually a Gradient?

Suppose you write down some arbitrary λ 's. Does there necessarily exist a cost for which those λ 's are the gradients? Are there general conditions under which such a cost exists? It's easy to write down expressions for which no function exists for which those expressions are the partial derivatives: for example, there is no $F(x, y)$ for which

$$\frac{\partial F(x, y)}{\partial x} = 1, \quad \frac{\partial F(x, y)}{\partial y} = x$$

It turns out that the necessary and sufficient conditions under which functions $f_1(x_1, \dots, x_n), f_2(x_1, \dots, x_n), \dots, f_n(x_1, \dots, x_n)$ are the partial derivatives of some function F , so that

$$\frac{\partial F}{\partial x_i} = f_i$$

are that

$$\frac{\partial f_i}{\partial x_j} = \frac{\partial f_j}{\partial x_i} \quad (10)$$

under the condition that the domain \mathcal{D} of F be open and star-shaped (in other words, if $x \in \mathcal{D}$, then all points joining x with the origin are also in \mathcal{D}) (see for example [10]). This result is known as the Poincaré lemma. In our case, for a given pair, for any particular values for the model parameters (that is, for a particular sorting of the urls by current model scores), it is easy to write down such a cost: it is the RankNet cost multiplied by Δ_{NDCG} . However the general expression depends in a complicated way on the model parameters, since the model generates the score by which the urls are sorted, and since the λ 's are computed after the sort.

5 MART

LambdaMART combines MART [8] and LambdaRank. To understand LambdaMART we first review MART. Since MART is a boosted tree model in which the output of the model is a linear combination of the outputs of a set of regression trees, we first briefly review regression trees. Suppose we are given a data set $\{x_i, y_i\}$, $i = 1, \dots, m$ where $x_i \in \mathcal{R}^d$ and the labels $y_i \in \mathcal{R}$. For a given vector x_i we index its feature values by x_{ij} , $j = 1, \dots, d$. Consider first a regression stump, consisting of a root node and two leaf nodes, where directed arcs connect the root to each leaf. We think of all the data as residing on the root node, and for a given feature, we loop through all samples and find the threshold t such that, if all samples with $x_{ij} \leq t$ fall to the left child node, and the rest fall to the right child node, then the sum

$$S_j \equiv \sum_{i \in L} (y_i - \mu_L)^2 + \sum_{i \in R} (y_i - \mu_R)^2 \quad (11)$$

is minimized. Here L (R) is the sets of indices of samples that fall to the left (right), and μ_L (μ_R) is the mean of the values of the labels of the set of samples that fall to the left (right). (The dependence on j in the sum appears in L , R and in μ_L , μ_R). S_j is then computed for all choices of feature j and all choices of threshold for that feature, and the split (the choice of a particular feature j and threshold t) is chosen that gives the overall minimal S_j . That split is then attached to the root node. For the two leaf nodes of our stump, a value γ_l , $l = 1, 2$ is computed, which is just the mean of the y 's of the samples that fall there. In a general regression tree, this process is continued $L - 1$ times to form a tree with L leaves³.

³ We are overloading notation (the meaning of L) in just this paragraph.

MART is a class of boosting algorithms that may be viewed as performing gradient descent in function space, using regression trees. The final model again maps an input feature vector $x \in R^d$ to a score $F(x) \in R$. 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). Note, however, that **the underlying model upon which MART is built is the least squares regression tree**, whatever problem MART is solving. MART's output $F(x)$ can be written as

$$F_N(x) = \sum_{i=1}^N \alpha_i f_i(x)$$

where each $f_i(x) \in R$ is a function modeled by a single regression tree and the $\alpha_i \in R$ is the weight associated with the i th regression tree. Both the f_i and the α_i are learned during training. A given tree f_i maps a given x to a real value by passing 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 , $j = 1, \dots, d$ and where the output of the tree is taken to be **a fixed value associated with each leaf, γ_{kn}** , $k = 1, \dots, L$, $n = 1, \dots, N$, where L is the number of leaves and N the number of trees. Given training and validation sets, the user-chosen parameters of the training algorithm are N , a fixed learning rate η (that multiplies every γ_{kn} for every tree), and L . (One could also choose different L for different trees). The γ_{kn} are also learned during training.

Given that, say, n trees have been trained, how should the next tree be trained? MART uses gradient descent to decrease the loss: specifically, the next regression tree models the m derivatives of the cost with respect to the current model score evaluated at each training point: $\frac{\partial C}{\partial F_n}(x_i)$, $i = 1, \dots, m$. Thus:

$$\delta C \approx \frac{\partial C(F_n)}{\partial F_n} \delta F \quad (12)$$

and so $\delta C < 0$ if we take $\delta F = -\eta \frac{\partial C}{\partial F_n}$. Thus each tree models the gradient of the cost with respect to the model score, and the new tree is added to the ensemble with a step size $\eta \gamma_{kn}$. The step sizes γ_{kn} can be computed exactly in some cases, or using Newton's approximation in others. The role of η as an overall learning rate is similar to that in other stochastic gradient descent algorithms: taking a step that is smaller than the optimal step size (i.e. the step size that maximally reduces the cost) acts as a form of regularization for the model that can significantly improve test accuracy.

Clearly, since MART models derivatives, and since LambdaRank works by specifying the derivatives at any point during training, the two algorithms are well matched: LambdaMART is the marriage of the two [11].

To understand MART, let's next examine how it works in detail, for perhaps the simplest supervised learning task: binary classification.

6 MART for Two Class Classification

We follow [8], although we give a somewhat different emphasis here; in particular, we allow a general sigmoid parameter σ (although it turns out that choice of σ does not make affect the model, it's instructive to see why).

We choose labels $y_i \in \{\pm 1\}$ (this has the advantage that $y_i^2 = 1$, which will be used later). The model score for sample $x \in \mathcal{X}^n$ is denoted $F(x)$. To keep notation brief, denote the modeled conditional probabilities by $P_+ \equiv P(y = 1|x)$ and $P_- \equiv P(y = -1|x)$, and define indicators $I_+(x_i) = 1$ if $y_i = 1$, 0 otherwise, and $I_-(x_i) = 1$ if $y_i = -1$, 0 otherwise. We use the cross-entropy loss function (the negative binomial log-likelihood):

$$L(y, F) = -I_+ \log P_+ - I_- \log P_-$$

(Note the similarity to the RankNet loss). Logistic regression models the log odds. So if $F_N(x)$ is the model output, we choose (the factor of $\frac{1}{2}$ here is included to match [8]):

$$F_N(x) = \frac{1}{2} \log\left(\frac{P_+}{P_-}\right) \quad (13)$$

or

$$P_+ = \frac{1}{1 + e^{-2\sigma F_N(x)}}, \quad P_- = 1 - P_+ = \frac{1}{1 + e^{2\sigma F_N(x)}}$$

which gives

$$L(y, F_N) = \log(1 + e^{-2y\sigma F_N}) \quad (14)$$

The gradients of the cost with respect to the model scores (called pseudoresponses in [8]) are:

$$\bar{y}_i = - \left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)} \right]_{F(x)=F_{m-1}(x)} = \frac{2y_i\sigma}{1 + e^{2y_i\sigma F_{m-1}(x)}}$$

These are the exact analogs of the Lambda gradients in LambdaRank (and in fact are the gradients in LambdaMART). They are the values that the regression tree is modeling. Denoting the set of samples that land in the j th leaf node of the m th tree by R_{jm} , we want to find an approximately optimal step for each leaf, that is, the values that minimize the loss:

$$\gamma_{jm} = \arg \min_{\gamma} \sum_{x_i \in R_{jm}} \log \left(1 + e^{-2y_i\sigma(F_{m-1}(x_i) + \gamma)} \right) \equiv \arg \min_{\gamma} g(\gamma)$$

The Newton approximation is used to find γ : for a function $g(\gamma)$, a Newton-Raphson step towards the extremum of g is

$$\gamma_{n+1} = \gamma_n - \frac{g'(\gamma_n)}{g''(\gamma_n)}$$

Here we start from $\gamma = 0$ and take just one step. Again let's simplify the expressions by collapsing notation: define $S_i(\gamma) \equiv 1 + e^{-2v_i} \equiv 1 + e^{-2y_i\sigma(F_{m-1}(x)+\gamma)}$. We want to compute

$$\arg \min_{\gamma} g(\gamma) \equiv \arg \min_{\gamma} \sum_{x_i \in R_{jm}} \log S_i(\gamma)$$

Now

$$\begin{aligned} g' &= \sum_{x_i \in R_{jm}} \frac{1}{S_i} (-2y_i\sigma e^{-2v_i}) \\ g'' &= \sum_{x_i \in R_{jm}} \frac{-1}{S_i^2} (-2y_i\sigma e^{-2v_i})^2 - \frac{2y_i\sigma}{S_i} (-2y_i\sigma) e^{-2v_i} \\ &= \sum_{x_i \in R_{jm}} \frac{4}{S_i^2} y_i^2 \sigma^2 e^{-2v_i} \end{aligned}$$

But

$$\bar{y}_i \equiv \frac{2y_i\sigma}{1 + e^{2y_iF}} \Rightarrow g' = \sum_{x_i \in R_{jm}} -\frac{2y_i\sigma}{e^{2v_i} S_i} = \sum_{x_i \in R_{jm}} -\bar{y}_i$$

Also

$$g'' = \sum_{x_i \in R_{jm}} \frac{4y_i^2 \sigma^2}{(1 + e^{2v_i})^2} e^{2v_i}$$

Since $y_i^2 = 1$ we have

$$|\bar{y}_i| = \frac{2\sigma}{1 + e^{2v_i}}$$

so

$$|\bar{y}_i|(2\sigma - |\bar{y}_i|) = \frac{4\sigma^2 e^{2v_i}}{(1 + e^{2v_i})^2}$$

giving simply

$$\gamma_{jm} = -\frac{g'}{g''} = \frac{\sum_{x_i \in R_{jm}} \bar{y}_i}{\sum_{x_i \in R_{jm}} |\bar{y}_i|(2\sigma - |\bar{y}_i|)}$$

(This corresponds to Algorithm 5 in [8]). Note that this step combines both the estimate of the gradient (the numerator) and the usual gradient descent step size (in

this case, $1/g''$). To include a learning rate r , we just multiply each leaf value γ_{jm} by r .

It's interesting that for this algorithm, the value of σ makes no difference. The Newton step γ_{jm} is proportional to $1/\sigma$. Since $F_m(x) = F_{m-1}(x) + \gamma$, and since F appears with an overall factor of σ in the loss, the σ 's just cancel in the loss function.

6.1 Extending to Unbalanced Data Sets

For completeness we include a discussion on how to extend the algorithm to cases where the data is very unbalanced (e.g. far more positive examples than negative).

If n_+ (n_-) is the total number of positive (negative) examples, for unbalanced data a useful way to count errors is:

$$\text{error rate} = \frac{\text{number false positives}}{2n_-} + \frac{\text{number false negatives}}{2n_+}$$

The factor of two in the denominator is just to scale so that the maximum error rate is one. We still use logistic regression (model the log odds) but instead use the balanced loss:

$$L_B(y, F) = -\frac{I_+}{n_+} \log P_+ - \frac{I_-}{n_-} \log P_- = \left(\frac{I_+}{n_+} + \frac{I_-}{n_-} \right) \log(1 + e^{-2y\sigma F})$$

The equations are similar to before. The gradients y_i are replaced by

$$\bar{z}_i = - \left[\frac{\partial L_B(y_i, F(x_i))}{\partial F(x_i)} \right]_{F(x)=F_{m-1}(x)} = \bar{y}_i \left(\frac{I_+}{n_+} + \frac{I_-}{n_-} \right)$$

and the Newton step becomes

$$\gamma_{jm}^B = -\frac{g'}{g''} = \frac{\sum_{x_i \in R_{jm}} \bar{y}_i \left(\frac{I_+}{n_+} + \frac{I_-}{n_-} \right)}{\sum_{x_i \in R_{jm}} |\bar{y}_i| (2\sigma - |\bar{y}_i|) \left(\frac{I_+}{n_+} + \frac{I_-}{n_-} \right)} \quad (15)$$

(Note that this is not the same as the previous Newton step with \bar{y}_i replaced by \bar{z}_i .)

7 LambdaMART

To implement LambdaMART we just use MART, specifying appropriate gradients and the Newton step. The gradients \bar{y}_i are easy: they are just the λ_i . As always in MART, least squares is used to compute the splits. In LambdaMART, each tree models the λ_i for the entire dataset (not just for a single query). To compute the Newton step, we collect some results from above: for any given pair of urls U_i and U_j such that $U_i \triangleright U_j$, then after the urls have been sorted by score, the λ_{ij} 's are defined as (see Eq. (4))

$$\lambda_{ij} = \frac{-\sigma|\Delta Z_{ij}|}{1 + e^{\sigma(s_i - s_j)}},$$

where we write the utility difference generated by swapping the rank positions of U_i and U_j as Z_{ij} (for example, Z might be NDCG). We also have

$$\lambda_i = \sum_{j:\{i,j\} \in I} \lambda_{ij} - \sum_{j:\{j,i\} \in I} \lambda_{ij}$$

To simplify notation, let's denote the above sum operation as follows:

$$\sum_{\{i,j\} \in I} \lambda_{ij} \equiv \sum_{j:\{i,j\} \in I} \lambda_{ij} - \sum_{j:\{j,i\} \in I} \lambda_{ij}$$

Thus, for any given state of the model (i.e. for any particular set of scores), and for a particular url U_i , we can write down a utility function for which λ_i is the derivative of that utility⁴

$$C = \sum_{\{i,j\} \in I} |\Delta Z_{ij}| \log \left(1 + e^{-\sigma(s_i - s_j)} \right)$$

so that

$$\frac{\partial C}{\partial s_i} = \sum_{\{i,j\} \in I} \frac{-\sigma|\Delta Z_{ij}|}{1 + e^{\sigma(s_i - s_j)}} \equiv \sum_{\{i,j\} \in I} -\sigma|\Delta Z_{ij}| \rho_{ij}$$

where we've defined

$$\rho_{ij} \equiv \frac{1}{1 + e^{\sigma(s_i - s_j)}} = \frac{-\lambda_{ij}}{\sigma|Z_{ij}|}$$

Then

$$\frac{\partial^2 C}{\partial s_i^2} = \sum_{\{i,j\} \in I} \sigma^2 |\Delta Z_{ij}| \rho_{ij} (1 - \rho_{ij})$$

⁴ We switch back to utilities here but use C to match previous notation.

(using $\frac{e^x}{(1+e^x)^2} = \left(1 - \frac{1}{1+e^x}\right) \frac{1}{1+e^x}$) and the Newton step size for the k th leaf of the m th tree is

$$\gamma_{km} = \frac{\sum_{x_i \in R_{km}} \frac{\partial C}{\partial s_i}}{\sum_{x_i \in R_{km}} \frac{\partial^2 C}{\partial s_i^2}} = \frac{-\sum_{x_i \in R_{km}} \sum_{\{i,j\} \Rightarrow I} |\Delta Z_{ij}| \rho_{ij}}{\sum_{x_i \in R_{km}} \sum_{\{i,j\} \Rightarrow I} |\Delta Z_{ij}| \sigma \rho_{ij} (1 - \rho_{ij})}$$

(note the change in sign since here we are maximizing). In an implementation it is convenient to simply compute ρ_{ij} for each sample x_i ; then computing γ_{km} for any particular leaf node just involves performing the sums and dividing. Note that, just as for logistic regression, for a given learning rate η , the choice of σ will make no difference to the training, since the γ_{km} 's scale as $1/\sigma$, the model score is always incremented by $\eta \gamma_{km}$, and the scores always appear multiplied by σ .

We summarize the LambdaMART algorithm schematically below. As pointed out in [11], one can easily perform model adaptation by starting with the scores given by an initial base model.

Algorithm: LambdaMART

```

set number of trees  $N$ , number of training samples  $m$ , number of leaves per tree  $L$ ,
learning rate  $\eta$ 
for  $i = 0$  to  $m$  do
     $F_0(x_i) = \text{BaseModel}(x_i)$  //If BaseModel is empty, set  $F_0(x_i) = 0$ 
end for
for  $k = 1$  to  $N$  do
    for  $i = 0$  to  $m$  do
         $y_i = \lambda_i$ 
         $w_i = \frac{\partial y_i}{\partial F_{k-1}(x_i)}$ 
    end for
     $\{R_{lk}\}_{l=1}^L$  // Create  $L$  leaf tree on  $\{x_i, y_i\}_{i=1}^m$ 
     $\gamma_k = \frac{\sum_{x_i \in R_{lk}} y_i}{\sum_{x_i \in R_{lk}} w_i}$  // Assign leaf values based on Newton step.
     $F_k(x_i) = F_{k-1}(x_i) + \eta \sum_l \gamma_{lk} I(x_i \in R_{lk})$  // Take step with learning rate  $\eta$ .
end for

```

Finally it's useful to compare how LambdaRank and LambdaMART update their parameters. LambdaRank updates all the weights after each query is examined. The decisions (splits at the nodes) in LambdaMART, on the other hand, are computed using all the data that falls to that node, and **so LambdaMART updates only a few parameters at a time** (namely, the split values for the current leaf nodes), but using all the data (since every x_i lands in some leaf). This means in particular that LambdaMART is able to choose splits and leaf values that may decrease the utility for some queries, as long as the overall utility increases.

7.1 A Final Note: How to Optimally Combine Rankers

We end with the following note: [11] contains a relatively simple method for linearly combining two rankers such that out of all possible linear combinations, the resulting ranker gets the highest possible NDCG (in fact this can be done for any IR measure). The key trick is to note that if s_i^1 are the outputs of the first ranker (for a given query), and s_i^2 those of the second, then the output of the combined ranker can be written $\alpha s_i^1 + (1 - \alpha)s_i^2$, and as α sweeps through its values (say, from 0 to 1), then the NDCG will only change a finite number of times. We can simply (and quite efficiently) keep track of each change and keep the α that gives the best combined NDCG. However it should also be noted that one can achieve a similar goal (without the guarantee of optimality, however) by simply training a linear (or nonlinear) LambdaRank model using the previous model scores as inputs. This usually gives equally good results and is easier to extend to several models.

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