# An Alternative Cross Entropy Loss for Learning-to-Rank

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#### **Abstract**

Listwise learning-to-rank methods form a powerful class of ranking algorithms that are widely adopted in applications such as information retrieval. These algorithms learn to rank a set of items by optimizing a loss that is a function of the entire set—as a surrogate to a typically non-differentiable ranking metric. Despite their empirical success, existing listwise methods are based on heuristics and remain theoretically illunderstood. In particular, none of the empiricallysuccessful loss functions are related to ranking metrics. In this work, we propose a cross entropybased learning-to-rank loss function that is theoretically sound and is a convex bound on NDCG, a popular ranking metric. Furthermore, empirical evaluation of an implementation of the proposed method with gradient boosting machines on benchmark learning-to-rank datasets demonstrates the superiority of our proposed formulation over existing algorithms in quality and robustness.

### 1. Introduction

Learning-to-rank or supervised ranking is a central problem in a range of applications including web search, recommendation systems, and question answering. The task is to learn a function that, conditioned on some context, arranges a set of items into an ordered list so as to maximize a given metric. In this work, without loss of generality, we take search as an example where a set of documents (items) are ranked by their relevance to a query (context).

Rather than directly working with permutations, learning-to-rank methods typically approach the ranking problem as one of "score and sort." The objective is then to learn a "scoring" function to measure the relevance of a document with respect to a query. Subsequently, they sort documents in decreasing relevance to form a ranked list. Ideally, the resulting ranked list should maximize a ranking metric.

Popular ranking metrics are instances of the general class of *conditional linear rank statistics* (Clémençon & Vayatis, 2008) that summarize the Receiver Operator Characteristic (ROC) curve. Of particular interest are the ranking statistics that care mostly about the leftmost portion of the ROC curve, corresponding to the top of the ranked list. Mean Reciprocal Rank and Normalized Discounted Cumulative Gain (Järvelin & Kekäläinen, 2002) are two such metrics that are widely used in information retrieval applications.

Ranking metrics, as functions of learning-to-rank scores, are flat almost everywhere; a small perturbation of scores is unlikely to lead to a change in the metric. This property poses a challenge for gradient-based optimization algorithms, making a direct optimization of ranking metrics over a complex hypothesis space infeasible. Addressing this challenge has been the focus of a large body of research (Liu, 2009), with most considering smooth loss functions as surrogates to metrics.

The majority of the proposed surrogate loss functions (Cao et al., 2007; Burges et al., 2005; Burges, 2010; Xia et al., 2008; Joachims, 2006), however, are only loosely related to ranking metrics such as NDCG. ListNet (Cao et al., 2007), as an example, projects labels and scores onto the probability simplex and minimizes the cross-entropy between the resulting distributions. LambdaMART (Burges, 2010; Wu et al., 2010) (denoted as  $\lambda$ MART), as another example, forgoes the loss function altogether and heuristically formulates the gradients.

The heuristic nature of learning-to-rank surrogate loss functions and a lack of theoretical justification for their use have hindered progress in the field. While  $\lambda$ MART remains the state-of-the-art to date, the fact that its loss function—presumed to be smooth—is unknown makes a theoretical analysis of the algorithm difficult. Empirical improvements over existing methods remain marginal for similar reasons.

In this work, we are motivated to help close the gap above. To that end, we present a construction of the cross-entropy loss which we dub XE<sub>NDCG</sub>, that is only slightly different from the ListNet loss, but that enjoys strong theoretical properties. In particular, we prove that our construction is a convex bound on negative (translated and log-transformed) mean NDCG—where NDCG, a utility is turned into a cost by negation—thereby lending credence to its optimization

for the purpose of learning ranking functions. Furthermore, we show that the generalization error bound of  $XE_{NDCG}$  compares favorably with that of  $\lambda$ MART's. Experiments on benchmark learning-to-rank datasets further reveal the empirical superiority of our proposed method. We anticipate the theoretical soundness of our method and its strong connection to ranking metrics enable future research and progress.

Our contributions can be summarized as follows:

- We present a cross entropy-based loss function, dubbed XE<sub>NDCG</sub>, for learning-to-rank and prove that it is a convex bound on negative (translated and log-transformed) mean NDCG;
- We compare model complexity between  $\lambda$ MART and  $XE_{NDCG}$ ;
- We formulate an approximation to the inverse Hessian for XE<sub>NDCG</sub> for optimization with second-order methods; and,
- We optimize  $XE_{NDCG}$  to learn Gradient Boosted Regression Trees (denoted by  $XE_{NDCG}MART$ ) and compare its performance and robustness with  $\lambda MART$  on benchmark learning-to-rank datasets through extensive randomized experiments.

This document is organized as follows. Section 2 reviews existing work on learning-to-rank. In Section 3, we introduce the notation adopted in this work and formulate the problem. Section 4 presents a detailed description of our proposed learning-to-rank loss function and examines its theoretical properties, including a comparison of generalization error bounds. We empirically evaluate our proposed method and report our findings in Section 5. Finally, we conclude this work in Section 6.

#### 2. Related Work

A large class of learning-to-rank methods attempt to optimize pairwise misranking error—a popular ranking statistic in many prioritization problems—by learning to correctly classify pairwise preferences. Examples include RankSVM (Joachims, 2006) and AdaRank (Xu & Li, 2007) which learn margin classifiers, RankNet (Burges et al., 2005) which optimizes a probabilistic loss function, and the P-Norm Push method (Rudin, 2009) which extends the problem to settings where we mostly care about the top of the ranked list. While the so-called "pairwise" methods typically optimize convex upper-bounds of the misranking error, direct optimization methods based on mathematical programming have also been proposed (Rudin & Wang, 2018) albeit for linear hypothesis spaces.

Pairwise learning-to-rank methods, while generally effective, optimize loss functions that are misaligned with more complex ranking statistics such as Expected Reciprocal Rank (Chapelle et al., 2009) or NDCG (Järvelin & Kekäläinen, 2002). This discrepancy has given rise to the so-called "listwise" learning-to-rank methods, where the loss function under optimization is defined over the entire list of items, not just pairs.

Listwise learning-to-rank methods either derive a smooth approximation to ranking metrics or use heuristics to construct smooth surrogate loss functions. Algorithms that represent the first class are SoftRank (Taylor et al., 2008) which takes every score to be the mean of a Gaussian distribution, and ApproxNDCG (Qin et al., 2010) which approximates the indicator function—used in the computation of ranks given scores—with a generalized sigmoid.

The other class of listwise learning-to-rank methods include ListMLE (Xia et al., 2008), ListNet (Cao et al., 2007), and  $\lambda$ MART (Wu et al., 2010; Burges, 2010). ListMLE maximizes the log-likelihood based on the Plackett-Luce probabilistic model, a loss function that is disconnected from ranking metrics. ListNet minimizes the cross-entropy between the ground-truth and score distributions. Though a recent work (Bruch et al., 2019a) establishes a link between the ListNet loss function and NDCG under strict conditions—requiring binary relevance labels—in a general setting, its loss is only loosely related to ranking metrics.

 $\lambda$ MART is a gradient boosting machine (Friedman, 2001) that forgoes the loss function altogether and, instead, directly designs the gradients of its unknown loss function using heuristics. While a recent work (Wang et al., 2018) claims to have found  $\lambda$ MART's loss function, it overlooks an important detail: The reported loss function is not differentiable.

There is abundant evidence to suggest listwise methods are empirically superior to pairwise methods where MRR, ERR, or NDCG is used to determine ranking quality (Wang et al., 2018; Bruch et al., 2019b; Liu, 2009). However, unlike pairwise methods, listwise algorithms remain theoretically ill-understood. Past studies have examined the generalization error bounds for existing surrogate loss functions (Tewari & Chaudhuri, 2015; Chapelle & Wu, 2010; Lan et al., 2009), but little attention has been paid to the validity of such functions which could shed light on their empirical success.

## 3. Preliminaries

In this section, we formalize the problem and introduce our notation. To simplify exposition, we write vectors in bold and use subscripts to index their elements (e.g.,  $\gamma_i \in \gamma$ ).

Let  $(x, y) \in \mathcal{X}^m \times \mathcal{Y}^m$  be a training example comprising

of m items and relevance labels where  $\mathcal{X} \subset \mathbb{R}^d$  is the bounded space of items or item-context pairs represented by d-dimensional feature vectors, and  $\mathcal{Y} \subset \mathbb{R}_+$  is the space of relevance labels. For consistency with existing work on listwise learning-to-rank, we refer to each  $x_i \in \mathbf{x}$ ,  $1 \le i \le m$  as a "document." Note, however, that  $x_i$  could be the representation of any general item or item-context pair. We assume the training set  $\Psi$  consists of n such examples.

We denote a learning-to-rank scoring function by  $f: \mathcal{X} \to \mathbb{R}$  and assume  $f \in \mathcal{F}$  where  $\mathcal{F}$  is a compact hypothesis space of bounded functions endowed with the uniform norm. For brevity, we denote  $f(x_i)$  by  $f_i$  and, with a slight abuse of notation, define  $f(x) = (f_1, f_2, \dots, f_m)$ , the vector of scores for m documents in x.

As noted in earlier sections, the goal is to learn a scoring function f that minimizes the empirical risk:

$$\mathcal{L}(f) = \frac{1}{|\Psi|} \sum_{(\boldsymbol{x}, \boldsymbol{y}) \in \Psi} \ell(\boldsymbol{y}, f(\boldsymbol{x})), \tag{1}$$

where  $\ell(\cdot)$  is by assumption a smooth loss function.

**ListNet**: The loss  $\ell$  in ListNet (Cao et al., 2007) first projects labels y and scores f(x) onto the probability simplex to form distributions  $\phi_{\text{ListNet}}$  and  $\rho_{\text{ListNet}}$ , respectively. Given the two distributions, the loss is their distance as measured by cross entropy:

$$\ell(\boldsymbol{y}, f(\boldsymbol{x})) \triangleq -\sum_{i=1}^{m} \phi_{\text{ListNet}}(y_i) \log \rho_{\text{ListNet}}(f_i).$$
 (2)

The distributions  $\phi_{\text{ListNet}}$  and  $\rho_{\text{ListNet}}$  may be understood as encoding the likelihood of document  $x_i$  appearing at the top of the ranked list, referred to as "top one" probability, according to the labels and scores respectively. In the original publication (Cao et al., 2007),  $\phi_{\text{ListNet}}$  and  $\rho_{\text{ListNet}}$  are defined as follows:

$$\phi_{\text{ListNet}}(y_i) = \frac{e^{y_i}}{\sum_{j=1}^m e^{y_j}}, \quad \rho_{\text{ListNet}}(f_i) = \frac{e^{f_i}}{\sum_{j=1}^m e^{f_j}}.$$
(3)

 $\lambda$ MART: The loss  $\ell$  in  $\lambda$ MART is unknown but its gradients with respect to the scoring function are designed as follows:

$$\frac{\partial \ell}{\partial f_i} = \sum_{y_i > y_i} \frac{\partial \ell_{ij}}{\partial f_i} + \sum_{y_k > y_i} \frac{\partial \ell_{ki}}{\partial f_i},\tag{4}$$

where

$$\frac{\partial \ell_{mn}}{\partial f_m} = \frac{-\sigma |\Delta_{\text{NDCG}_{mn}}|}{1 + e^{\sigma(f_m - f_n)}} = -\frac{\partial \ell_{nm}}{\partial f_m},\tag{5}$$

where  $\sigma$  is a hyperparameter and  $\Delta_{\text{NDCG}_{mn}}$  is the change in NDCG if documents at ranks m and n are swapped. Finally, NDCG is defined as follows:

$$NDCG(\boldsymbol{\pi}_f, \boldsymbol{y}) = \frac{DCG(\boldsymbol{\pi}_f, \boldsymbol{y})}{DCG(\boldsymbol{\pi}_y, \boldsymbol{y})},$$
 (6)

where  $\pi_f$  is a ranked list induced by f on x,  $\pi_y$  is the ideal ranked list (where x is sorted by y), and DCG is defined as follows:

$$DCG(\boldsymbol{\pi}, \boldsymbol{y}) = \sum_{i=1}^{m} \frac{2^{y_i} - 1}{\log_2(1 + \boldsymbol{\pi}[i])},$$
 (7)

with  $\pi[i]$  denoting the rank of  $x_i$ .

## 4. Proposed Method

In this section, we show how a slight modification to the ListNet loss function equips the loss with interesting theoretical properties. To avoid conflating implementation details with the loss function itself, we name our proposed loss function  $XE_{NDCG}$ .

**Definition 1.** For a training example  $(x, y) \in \mathcal{X}^m \times \mathcal{Y}^m$  and scores  $f(x) \in \mathbb{R}^m$ , we define  $XE_{NDCG}$  as the cross entropy between score distribution  $\rho$  and a parameterized class of label distributions  $\phi$  defined as follows:

$$\rho(f_i) = \frac{e^{f_i}}{\sum_{j=1}^m e^{f_j}}, \quad \phi(y_i; \, \gamma) = \frac{2^{y_i} - \gamma_i}{\sum_{j=1}^m 2^{y_j} - \gamma_j}$$

where  $\gamma \in [0, 1]^m$ .

In effect, the distribution  $\phi$  allocates a mass in the interval  $[2^{y_r} - 1, 2^{y_r}]$  for each document. As we will explain later, the vector  $\gamma$  plays an important role in certain theoretical properties of our proposed loss function. Note that in general,  $\gamma$  may be unique to each training example (x, y).

#### 4.1. Relationship to NDCG

The difference between  $XE_{NDCG}$  and ListNet is minor but consequential: The change to the definition of  $\phi$  leads to our main result.

**Theorem 1.** XE<sub>NDCG</sub> is an upper-bound on negative (translated and log-transformed) mean Normalized Discounted Cumulative Gain.

Theorem 1 asserts that  $XE_{NDCG}$  is a convex proxy to minimizing negative NDCG (where we turn NDCG which is a utility to a cost by negation). No such analytical link exists between the  $\lambda$ MART, ListNet, or other listwise learning-torank loss functions and ranking metrics.

In proving Theorem 1 we make use of Jensen's inequality when applied to the log function:

$$\log \mathbb{E}[X] \ge \mathbb{E}[\log X],\tag{8}$$

where X is a random variable and  $\mathbb{E}[\cdot]$  denotes expectation. We also use the following bound on ranks that was originally

derived in (Bruch et al., 2019a):

$$\begin{split} \pi[r] &= 1 + \sum_{i \neq r} \mathbbm{1}_{f_i > f_r} = 1 + \sum_{i \neq r} \mathbbm{1}_{f_i - f_r > 0} \\ &\leq 1 + \sum_{i \neq r} e^{(f_i - f_r)} = \sum_{i} e^{(f_i - f_r)} = \frac{\sum_{i} e^{f_i}}{e^{f_r}}, \end{split}$$

where  $\mathbb{I}_p$  is the indicator function taking value 1 when the predicate p is true and 0 otherwise. The above leads to:

$$\frac{1}{\boldsymbol{\pi}[r]} \ge \frac{e^{f_r}}{\sum_i e^{f_i}} = \rho(f_r). \tag{9}$$

*Proof.* Consider  $\mathrm{DCG}(\boldsymbol{\pi_y}, \boldsymbol{y})$ . Using  $\log_2(1+z) \geq 1, \forall z > 1$ :

$$DCG(\boldsymbol{\pi}_{\boldsymbol{y}}, \boldsymbol{y}) = \sum_{i=1}^{m} \frac{2^{y_i} - 1}{\log_2(1 + \boldsymbol{\pi}_{\boldsymbol{y}}[i])} \le \sum_{i=1}^{m} 2^{y_i} - \gamma_i,$$
(10)

for  $0 \le \gamma_i \le 1$ .

Turning to  $DCG(\pi_f, y)$  and using  $1 + z \le 2^z$  for a positive integer z or equivalently  $\log_2(1 + z) \le z$ , we have the following:

$$DCG(\pi_{f}, \mathbf{y}) = \sum_{r} \frac{2^{y_{r}} - 1}{\log_{2}(1 + \pi_{f}[r])} \ge \sum_{r} \frac{2^{y_{r}} - 1}{\pi_{f}[r]}$$

$$\ge \sum_{r} (2^{y_{r}} - 1)\rho(f_{r}) = \left[\sum_{r} 2^{y_{r}}\rho(f_{r})\right] - 1$$

$$\ge \left[\sum_{r} (2^{y_{r}} - \gamma_{r})\rho(f_{r})\right] - 1,$$
(11)

where the second inequality holds by Equation (9).

Finally, consider a translation (by a constant) and log-transformation of mean NDCG, NDCG, as follows:

$$\overline{\overline{\text{NDCG}}} \triangleq \log \big( \overline{\text{NDCG}} + \frac{1}{|\Psi|} \sum_{(\boldsymbol{x}, \boldsymbol{y})} \frac{1}{\text{DCG}(\boldsymbol{\pi}_{\boldsymbol{y}}, \boldsymbol{y})} \big).$$

Given the monotonicity of  $\log(\cdot)$ , the maximizer of  $\overline{NDCG}$  also maximizes  $\overline{NDCG}$ . We now proceed as follows:

$$\overline{\overline{\text{NDCG}}} = \log \frac{1}{|\Psi|} \sum_{(\boldsymbol{x}, \boldsymbol{y})} \frac{1}{\text{DCG}(\boldsymbol{\pi}_{\boldsymbol{y}}, \boldsymbol{y})} \left[ \text{DCG}(\boldsymbol{\pi}_{f}, \boldsymbol{y}) + 1 \right]$$

$$\geq \log \frac{1}{|\Psi|} \sum_{(\boldsymbol{x}, \boldsymbol{y})} \frac{1}{\sum_{j} 2^{y_{j}} - \gamma_{j}} \left[ \text{DCG}(\boldsymbol{\pi}_{f}, \boldsymbol{y}) + 1 \right]$$

$$\geq \log \frac{1}{|\Psi|} \sum_{(\boldsymbol{x}, \boldsymbol{y})} \sum_{r} \phi(y_{r}) \rho(f_{r}) \tag{12}$$

$$\geq \frac{1}{|\Psi|} \sum_{(r,y)} \sum_{r} \phi(y_r) \log \rho(f_r), \tag{13}$$

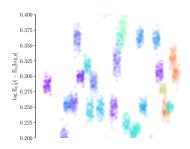


Figure 1. A simulation of the effect of  $\gamma$  on the Jensen gap. Each cloud of points represents a training example with m=100 documents, for which we sample scores from [0,1] and labels from 0–4 with smaller probabilities for larger labels. Each point reports the Jensen gap obtained by using a different  $\gamma$ . In particular, we sample  $\gamma$  uniformly from  $[0,1]^m$  to define  $\phi$ . The vertically stretched clouds illustrate the impact of the resulting distribution  $\phi$  on the Jensen gap.

where the first inequality holds by Equation (10), the second inequality by Equation (11), the third inequality by Definition 1, and the last inequality by repeated applications of Equation (8). Finally, negating both sides completes the proof.  $\Box$ 

#### 4.2. Effect of $\gamma$

In the proof of Theorem 1, we made use of Jensen's inequality as defined in Equation (8). In particular, the inequality from Equation (12) to Equation (13) holds by repeated applications of Jensen's inequality, the last of which involves:

$$\log \mathbb{E}_{\phi}[\rho(f_r)] = \log \sum_{r} \phi(y_r) \rho(f_r)$$
$$\geq \sum_{r} \phi(y_r) \log \rho(f_r) = \mathbb{E}_{\phi}[\log \rho(f_r)].$$

The gap between the RHS and LHS in the above—known as the Jensen gap—contributes to the tightness of the bound on the ranking metric. This gap, and therefore the tightness of the resulting bound, can be controlled by the distribution  $\phi$ . This is illustrated in Figure 1 with simulated data points. The tightest bound can be achieved by minimizing the following constrained optimization problem per training example (x, y) given scores f(x):

$$\begin{split} & \underset{\gamma}{\text{minimize}} & & \log \sum_r \phi(y_r) \rho(f_r) - \sum_r \phi(y_r) \log \rho(f_r) \\ & \text{such that} & & \phi(y_r) = \frac{2^{y_r} - \gamma_r}{\sum_j 2^{y_j} - \gamma_j}. \end{split}$$

In addition to its effect on the Jensen gap,  $\gamma$  affects the tightness of the bounds in Equations (10) and (11). Solving these optimization problems jointly per training example at

every step of training, however, is nontrivial. In this work, as we will elaborate later in Section 5, we reduce the problem of choosing  $\gamma$  to a more tractable optimization problem by treating it as a hyperparameter that may be tuned on a validation dataset.

#### 4.3. Comparison with $\lambda$ MART

In this section, we compare  $XE_{NDCG}$  with  $\lambda MART$  in terms of model complexity and generalization error. In what follows, we proceed under the strong assumption that the loss optimized by  $\lambda MART$  in fact exists. That is, we assume that there exists a differentiable function that satisfies Equation (4).

We begin with an examination of the Lipschitz constant of the two algorithms—an upper-bound on the variation a function can exhibit. Intuitively, functions with a smaller Lipschiz constant are simpler because they vary at a slower rate, and thus generalize better.

**Proposition 1.** The  $\lambda$ MART loss is  $\sigma m^2$ -Lipschitz with respect to  $\|\cdot\|_{\infty}$ .

*Proof.* Recall the definition of the Lipschitz constant for a differentiable function h(.):

$$Lip_h = \sup_{\|f - f'\|} \frac{|h(f) - h(f')|}{\|f - f'\|}$$
$$= \sup_{\|f - f'\|} \frac{|\nabla_f h(f'')(f - f')|}{\|f - f'\|} = \|\nabla_f h(f)\|_*,$$

where the second equality holds by the Mean Value Theorem and the last equality by definition of the dual norm,  $\|\cdot\|_*$ . Therefore, to derive the Lipschitz constant of a function with respect to the infinity norm, it is sufficient to calculate the  $L_1$  norm of its gradient. Given that  $\lambda$ MART's loss function is unknown, we resort to this strategy to derive its Lipschitz constant.

Observe that the terms in Equation (5) are bounded by  $\sigma$  and Equation (4) has at most m such terms. As such, we have that,

$$\left|\frac{\partial \ell}{\partial f_i}\right| \le \sigma m.$$

Then,

$$\|\nabla_f \ell\|_1 = \sum_{i=1}^m \left| \frac{\partial \ell}{\partial f_i} \right| \le \sum_{i=1}^m \sigma m = \sigma m^2$$

which completes the proof.

**Proposition 2.**  $XE_{NDCG}$  is 2-Lipschitz with respect to  $\|\cdot\|_{\infty}$ .

*Proof.* We present the proof in the appendix due to space constraints.  $\Box$ 

In order to put this difference into perspective, we use the results above to derive bounds on the generalization error of the two algorithms. But first we need the following result.

**Theorem 2.** Let  $\mathcal{F}$  be a compact space of bounded functions from  $\mathcal{X}$  to [0,1],  $n=|\Psi|$  be the number of training examples,  $Lip_{\ell}$  the Lipschitz constant of loss function  $\ell$ , and  $\mathfrak{N}(\frac{\epsilon}{4Lip_{\ell}},\mathcal{F},\|\cdot\|_{\infty})$  the covering number of  $\mathcal{F}$  by  $L_{\infty}$  balls of radius  $\frac{\epsilon}{4Lip_{\ell}}$ . The following generalization error bound holds:

$$\mathcal{P}\{\mathcal{E}(f) \le \epsilon\} \ge 1 - 2\mathfrak{N}(\frac{\epsilon}{4Lip_{\ell}}, \mathcal{F}, \|\cdot\|_{\infty}) exp(\frac{-2n\epsilon^2}{Lip_{\ell}^2}),$$

where the generalization error  $\mathcal{E}$  is defined as follows:

$$\mathcal{E}(f) \triangleq \mathbb{E}_{\mathcal{X}^m \times \mathcal{Y}^m} [\ell(\boldsymbol{y}, f(\boldsymbol{x}))] - \frac{1}{n} \sum_{(\boldsymbol{x}, \boldsymbol{y}) \in \Psi} \ell(\boldsymbol{y}, f(\boldsymbol{x})).$$

*Proof.* Based on the proofs in (Cucker & Smale, 2002; Rudin, 2009) and, for completeness, presented in the appendix.  $\Box$ 

The dependence of the generalization error bound on the Lipschitz constant suggests that unlike  $\lambda \text{MART}$ ,  $\text{XE}_{\text{NDCG}}$ 's generalization error does not degrade as the number of documents per training example increases. Given  $\lambda \text{MART}$ 's higher complexity, we hypothesize that the algorithm is less robust to noise or in settings where the number of documents per training example is large.

We note that, the independence of the ListNet generalization error bound from m was also reported in (Tewari & Chaudhuri, 2015) for linear models, but we present the (structure of the) bounds here to allow a direct comparison between  $\lambda$ MART and  $XE_{NDCG}$ .

## 4.4. Approximating the Inverse Hessian

In this work, we fix the hypothesis space,  $\mathcal{F}$ , to Gradient Boosted Regression Trees. This is, in part, because we are interested in a fair comparison of ListNet,  $XE_{NDCG}$ , and  $\lambda$ MART in isolation of other factors, as explained in Section 5. As most GBRT learning algorithms use second-order optimization methods (e.g., Newton's), however, we must approximate the inverse Hessian for ListNet and  $XE_{NDCG}$ .

Unfortunately,  $XE_{NDCG}$  as defined in Definition 1 results in a Hessian that is singular, making the loss incompatible with a straightforward implementation of Newton's second-order method. We resolve this technical difficulty by making a small adjustment to the formulation of the loss function.

Let us re-define the score distribution,  $\rho$ , from Definition 1 as follows for a negligible  $\epsilon > 0$ :

$$\rho(f_i) = \frac{e^{f_i}}{\sum_{j=1}^m e^{f_j} + \epsilon}.$$
 (14)

In effect, we take away a small probability mass,  $\rho(f_{m+1}) = \epsilon/(\sum e^{f_j} + \epsilon)$ , from the score distribution for a nonexistent,  $m+1^{\text{th}}$  document with label probability  $\phi(f_{m+1})=0$ . The gradients of the loss will take the following form:

$$\frac{\partial \ell}{\partial f_r} = \frac{\partial}{\partial f_r} \left[ \sum_i (-\phi(y_i)f_i) + \log(\sum_j e^{f_j} + \epsilon) \right]$$
$$= -\phi_r + \rho_r,$$

where  $\phi_r = \phi(y_r)$  and  $\rho_r = \rho(f_r)$ . The Hessian looks as follows:

$$H_{ij} = \begin{cases} \rho_i (1 - \rho_i), & i = j \\ -\rho_i \rho_j, & i \neq j \end{cases}$$

Claim 1. The Hessian, as defined above, is positive definite.

*Proof.* A complete proof may be found in the appendix. Observe that H is strictly diagonally dominant:

$$|H_{kk}| = \rho_k (1 - \rho_k) = \rho_k (1 - \frac{e^{f_k}}{\sum e^{f_j} + \epsilon})$$
$$= \rho_k \frac{\sum_{j \neq k} e^{f_j} + \epsilon}{\sum e^{f_j} + \epsilon} > \rho_k \sum_{j \neq k} \rho_j = \sum_{j \neq k} |H_{kj}|.$$

By the properties of strictly diagonally dominant matrices and the fact that the diagonal elements of H are positive, we have that  $H \succ 0$  and therefore invertible.

We now turn to approximating the inverse of H as required. Write H=D(I-S) where I is the identity matrix, D is a diagonal matrix where  $D_{ii}=\rho_i(1-\rho_i)$  and S is a square matrix where,

$$S_{ij} = \begin{cases} 0, & i = j \\ \rho_j/(1 - \rho_i), & i \neq j \end{cases}.$$

Claim 2. The spectral radius of S is strictly less than 1.

*Proof.* A complete proof is presented in the appendix. S is a square matrix with nonnegative entries. By the Perron-Frobenious theorem, its spectral radius is bounded above by the maximum row-wise sum of entries, which, in S, is strictly less than 1.

Claim 2 allows us to apply Neumann's result to approximate  $(I - S)^{-1}$  as follows:

$$(I-S)^{-1} = \sum_{k=0}^{\infty} S^k \approx I + S + S^2.$$

Using this result, we may approximate  $H^{-1}$  as follows:

$$H^{-1} = (I - S)^{-1}D^{-1} \approx (I + S + S^2)D^{-1}$$

With that, we can finally calculate the update rule in Newton's method which requires the quantity  $H^{-1}\nabla$ :

$$\begin{split} &(H^{-1}\nabla)_k = \sum_i H_{ki}^{-1}\nabla_i \\ &\approx \sum_i (I+S+S^2)_{ki}(D^{-1}\nabla)_i \\ &= \sum_i (I+S+S^2)_{ki} \frac{-\phi_i + \rho_i}{\rho_i(1-\rho_i)} \\ &= \underbrace{\frac{-\phi_k + \rho_k}{\rho_k(1-\rho_k)}}_{(ID^{-1}\nabla)_k} + \underbrace{\frac{1}{1-\rho_k} \sum_{i\neq k} \frac{-\phi_i + \rho_i}{1-\rho_i}}_{(SD^{-1}\nabla)_k} + \underbrace{\sum_{i\neq k} \frac{\rho_i(SD^{-1}\nabla)_i}{1-\rho_k}}_{\rho_k(1-\rho_k)} \\ &= \underbrace{\frac{-\phi_k + \rho_k + \rho_k \sum_{i\neq k} \frac{-\phi_i + \rho_i}{1-\rho_i} + \rho_k \sum_{i\neq k} \rho_i(SD^{-1}\nabla)_i}_{\rho_k(1-\rho_k)}. \end{split}$$

## 5. Experiments

We are largely interested in a comparison of (a) the overall performance of ListNet,  $\lambda$ MART, and  $XE_{NDCG}$  on benchmark learning-to-rank datasets, and (b) the robustness of these models to various types and degrees of noise as a proxy to comparing their complexity. In this section, we describe our experimental setup and report our empirical findings.

#### 5.1. Datasets

We conduct experiments on two publicly available benchmark datasets: MSLR Web30K (Qin & Liu, 2013) and Yahoo! Learning to Rank Challenge Set 1 (Chapelle & Chang, 2011). Web30K contains roughly 30,000 example, with an average of 120 documents per example. Documents are represented by 136 numeric features. Yahoo! also has about 30,000 examples but the average number of documents per example is 24 and each document is represented by 519 features. Documents in both datasets are labeled with graded relevance from 0 to 4 with larger labels indicating a higher relevance.

From each dataset, we sample training (60%), validation (20%), and test (20%) examples, and train and compare models on the resulting splits. We repeat this procedure 100 times and obtain mean NDCG at different rank cutoffs for each trial. We subsequently compare the ranking quality between pairs of models and determine statistical significance of differences using a paired t-test.

During evaluation, we discard examples with no relevant documents. There are 982 and 1,135 such examples in the Web30K and Yahoo! datasets. The reason for ignoring these examples during evaluation is that their ranking quality can be arbitrarily 0 or 1, and that arbitrary choice skews the mean metrics one way or another.

Table 1. Ranking quality on test sets measured by mean NDCG at rank cutoffs 5 and 10, averaged over 100 randomized trials. In each trial, training, validation, and test sets are sampled from each dataset. The differences at all rank cutoffs between all models are statistically significant according to a paired t-test ( $\alpha = .01$ ).

	WEB30K		YAHOO!	
Model	@5	@10	@5	@10
LISTNET $\lambda$ MART $XE_{NDCG}MART$	47.68 48.08 48.23	49.76 49.94 50.27	71.76 73.00 73.37	76.52 77.49 77.84

#### 5.2. Models

We train  $\lambda$ MART models using LightGBM (Ke et al., 2017). The hyperparameters are guided by previous work (Ke et al., 2017; Wang et al., 2018; Bruch et al., 2019a). For Web30K, max\_bin is 255, learning\_rate is 0.02, num\_leaves is 400, min\_data\_in\_leaf is 50, min\_sum\_hessian\_in\_leaf is set to 0,  $\sigma$  is 1, and lambdamart\_norm is set to false. We do not utilize any regularizing terms because we are interested in a comparison of core algorithms. For Yahoo!, num\_leaves is 200 and min\_data\_in\_leaf is 100. We use NDCG@5 to select the best models on validation sets by fixing early stopping round to 50 up to 500 trees.

We also implemented ListNet and XE<sub>NDCG</sub>MART in Light-GBM, which we intend to open source. As noted earlier, by fixing the hypothesis space to gradient boosted regression trees, we aim to strictly compare the performance of the loss functions and shield our analysis from any effect the hypothesis space may have on convergence and generalization. We use the same hyperparameters above for these algorithms as well

Finally, we must address the choice for  $\gamma$  in XE<sub>NDCG</sub>MART. As explained in Section 4.2, in this work we turn  $\gamma$  into a hyperparameter. In effect, our strategy is similar to the process that led to the visualization in Figure 1: At every iteration and for every training example with m documents, we sample  $\gamma$  uniformly from  $[0, 1]^m$ . We train 10 models in this way and choose the one that performs the best on the validation set.

#### 5.3. Ranking Quality

We compare the ranking quality of the three models under consideration. We report model quality by measuring average NDCG at rank cutoffs 5 and 10. As noted earlier, we also measure statistical significance in the difference between model qualities using a paired t-test with significance level set to  $\alpha = .01$ . Our results are summarized in Table 1.

From Table 1, we observe that ListNet consistently performs poorly across both datasets and the quality gap between List-

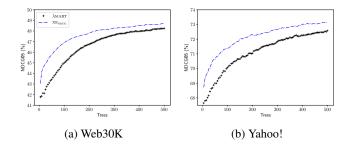


Figure 2. NDCG@5 on validation sets during training of  $\lambda$ MART and  $XE_{NDCG}MART$  in a representative trial.

Net and  $\lambda$ MART is statistically significant at all rank cutoffs. This observation is in agreement with past studies (Bruch et al., 2019a).

On the other hand, our proposed XE<sub>NDCG</sub>MART yields a significant improvement over ListNet. This observation holds consistently across both datasets and rank cutoffs and lends support to our theoretical findings in previous sections.

Not only does  $XE_{NDCG}MART$  outperform ListNet, its performance surpasses that of  $\lambda$ MART's. While  $XE_{NDCG}MART$ 's gain over  $\lambda$ MART is smaller than its gap with ListNet, the differences are statistically significant. This is an encouraging result:  $XE_{NDCG}MART$  is not only theoretically sound and is equipped with better properties, it also performs well empirically compared to the state-of-the-art algorithm.

A notable difference between  $\lambda$ MART and XE<sub>NDCG</sub>MART is in their convergence rate. Figure 2 plots NDCG@5 on validation sets as more trees are added to the ensemble. To avoid clutter, the figure illustrates just one trial (out of 100) but we note that we observe a similar trend across trials. From Figure 2, it is clear that XE<sub>NDCG</sub>MART outperforms  $\lambda$ MART by a wider margin when the number of trees in the ensemble is small. This property is important in latency-sensitive applications where a smaller ensemble is preferred.

#### 5.4. Robustness

We now turn to model robustness where we perform a comparative analysis of the effect of noise on  $\lambda$ MART and XE<sub>NDCG</sub>MART. The robustness of a ranking model to noise is important in practice due to the uncertainty in relevance labels, whether judged by human experts or is collected implicitly by user feedback such as clicks. We expect  $\lambda$ MART to overfit to noise and be less robust due to its higher model complexity—see findings in Section 4.3. As such, we expect the performance of  $\lambda$ MART to degrade at a higher pace than XE<sub>NDCG</sub>MART as we inject more noise into the dataset. We put this hypothesis to test through two types of experiments.

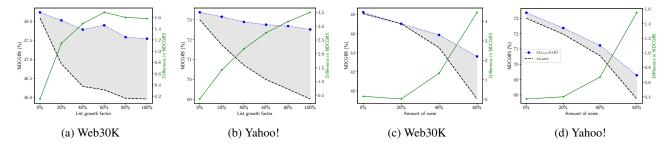


Figure 3. Mean NDCG@5 on test sets, averaged over 100 trials. In each trial, training, validation, and test sets are sampled from the dataset. In (a) and (b), training examples are augmented by additional (randomly sampled) negative documents. For example, the data point at "40%" indicates a 40% increase in the number of documents for every example. In (c) and (d), a percentage of relevance labels are set to a random value. The solid (green) lines show the difference in NDCG@5 between the two models.

In a first series of experiments, we focus on the effect of enlarging the document list per training example by the addition of noise. In particular, we augment document lists for training examples with new negative (i.e., non-relevant) documents using the following process. For every training example (x,y), we sample from the collection of all documents in the training set excluding x to form  $x' = \{\overline{x} \mid (\overline{x}, \overline{y}) \sim (\overline{x}, \overline{y}), (\overline{x}, \overline{y}) \sim \Psi \setminus (x, y)\}$ ). Subsequently, we augment x by adding x' as non-relevant documents:  $(x \oplus x', y \oplus 0)$ , where  $\oplus$  denotes concatenation. Finally, we train models on the resulting training set and evaluate on the (unmodified) test set. As before, we repeat this experiment 100 times.

We illustrate NDCG@5 on the test sets averaged over 100 trials and for various degrees of augmentation in Figures 3a and 3b. The trend confirms our hypothesis: On both datasets, the performance of  $\lambda$ MART degrades more severely as more noise is added to the training set, increasing the number of documents per example (m). This effect is more pronounced on the Yahoo! dataset where m is on average small. We note that the increase in NDCG@5 of XE<sub>NDCG</sub>MART from the 40% mark to 60% on Web30K is not statistically significant.

In another series of experiments we perturb relevance labels in the training set. To that end, for each training example (x, y), we randomly choose a subset of its documents and set their labels (independently) to 0 through 4 with decreasing probabilities: p(0) = .5, p(1) = .2, p(2) = .15, p(3) = .1, p(4) = .05. We train models on the perturbed training set and evaluate on the (unmodified) test set. As before, we repeat this experiment 100 times.

The results are shown in Figures 3c and 3d. As before,  $\lambda$ MART's performance degrades more rapidly with more noise. This behavior is more pronounced on Web30K.

We have included additional experiments in the appendix that explore the robustness of  $\lambda$ MART and  $XE_{NDCG}MART$  to

noise in a click dataset simulated from Yahoo! and Web30K. The results from those experiments additionally support our hypothesis that  $XE_{NDCG}MART$  is a more robust algorithm.

## 6. Conclusion

In this work, we presented a novel "listwise" learning-to-rank loss function,  $XE_{NDCG}$ , that, unlike existing methods bounds NDCG—a popular ranking metric—in a general setting. We contrasted our proposed loss function with  $\lambda$ MART and showed its superior theoretical properties. In particular, we showed that the loss function optimized by  $\lambda$ MART (if it exists), has a higher complexity with a Lipschitz constant that is a function of the number of documents, m. In contrast, the complexity of  $XE_{NDCG}$  is invariant to m.

Furthermore, we proposed a model that optimizes  $XE_{NDCG}$  to learn an ensemble of gradient-boosted decision trees which we refer to as  $XE_{NDCG}MART$ . Through extensive experiments on two benchmark learning-to-rank datasets, we demonstrated the superiority of our proposed method over ListNet and  $\lambda MART$  in terms of quality and robustness. We showed that,  $XE_{NDCG}MART$  is less sensitive to the number of documents and is more robust in the presence of noise. Finally, our experiments suggest that the performance gap between  $XE_{NDCG}MART$  and  $\lambda MART$  widens if we constrain the size of the learned ensemble. Better performance with fewer trees is important for latency-sensitive applications.

As a future direction, we are interested in an examination of the tightness of the presented bound and its effect on the convergence of  $XE_{NDCG}$ . In particular, in this work, we cast the problem presented in Section 4.2 as one of hyperparameter tuning. However, more effective strategies for solving  $\gamma$ 's and obtaining tighter bounds during boosting remain unexplored. Furthermore, given its robustness to label noise (implicit and explicit), we are also interested in studying  $XE_{NDCG}$  in an online learning setting.

#### References

- Bruch, S., Wang, X., Bendersky, M., and Najork, M. An analysis of the softmax cross entropy loss for learning-to-rank with binary relevance. In *Proceedings of the 2019 ACM SIGIR International Conference on the Theory of Information Retrieval*, 2019a.
- Bruch, S., Zoghi, M., Bendersky, M., and Najork, M. Revisiting approximate metric optimization in the age of deep neural networks. In *Proceedings of the 42nd International ACM SIGIR Conference on Research and Development in Information Retrieval*, 2019b.
- Burges, C., Shaked, T., Renshaw, E., Lazier, A., Deeds, M., Hamilton, N., and Hullender, G. Learning to rank using gradient descent. In *Proceedings of the 22nd In*ternational Conference on Machine Learning, pp. 89–96, 2005.
- Burges, C. J. From RankNet to LambdaRank to LambdaMART: An overview. Technical Report MSR-TR-2010-82, Microsoft Research, 2010.
- Cao, Z., Qin, T., Liu, T.-Y., Tsai, M.-F., and Li, H. Learning to rank: from pairwise approach to listwise approach. In *Proceedings of the 24th International Conference on Machine Learning*, pp. 129–136, 2007.
- Chapelle, O. and Chang, Y. Yahoo! learning to rank challenge overview. pp. 1–24, 2011.
- Chapelle, O. and Wu, M. Gradient descent optimization of smoothed information retrieval metrics. *Information Retrieval*, 13(3):216–235, June 2010.
- Chapelle, O., Metzler, D., Zhang, Y., and Grinspan, P. Expected reciprocal rank for graded relevance. In *Proceedings of the 18th ACM Conference on Information and Knowledge Management*, pp. 621–630, 2009.
- Clémençon, S. and Vayatis, N. Empirical performance maximization for linear rank statistics. In *Proceedings of the 21st International Conference on Neural Information Processing Systems*, pp. 305–312, 2008.
- Craswell, N., Zoeter, O., Taylor, M., and Ramsey, B. An experimental comparison of click position-bias models. In *Proceedings of the 2008 International Conference on Web Search and Data Mining*, pp. 87–94, 2008.
- Cucker, F. and Smale, S. On the mathematical foundations of learning. *Bulletin of the American Mathematical Society*, 39:1–49, 2002.
- Friedman, J. H. Greedy function approximation: a gradient boosting machine. *Annals of Statistics*, 29(5):1189–1232, 2001.

- Järvelin, K. and Kekäläinen, J. Cumulated gain-based evaluation of ir techniques. *ACM Transactions on Information Systems*, 20(4):422–446, 2002.
- Joachims, T. Training linear syms in linear time. In *Proceedings of the 12th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pp. 217–226, 2006.
- Joachims, T., Swaminathan, A., and Schnabel, T. Unbiased learning-to-rank with biased feedback. In *Proceedings of the 10th ACM International Conference on Web Search and Data Mining*, pp. 781–789, 2017.
- Ke, G., Meng, Q., Finley, T., Wang, T., Chen, W., Ma, W., Ye, Q., and Liu, T.-Y. Lightgbm: A highly efficient gradient boosting decision tree. In Advances in Neural Information Processing Systems 30, pp. 3146–3154. 2017.
- Lan, Y., Liu, T.-Y., Ma, Z., and Li, H. Generalization analysis of listwise learning-to-rank algorithms. In *Proceedings of the 26th Annual International Conference on Machine Learning*, pp. 577–584, 2009.
- Liu, T.-Y. Learning to rank for information retrieval. *Foundations and Trends in Information Retrieval*, 3(3):225–331, 2009.
- Qin, T. and Liu, T.-Y. Introducing LETOR 4.0 datasets, 2013.
- Qin, T., Liu, T.-Y., and Li, H. A general approximation framework for direct optimization of information retrieval measures. *Information Retrieval*, 13(4):375–397, 2010.
- Rudin, C. The p-norm push: A simple convex ranking algorithm that concentrates at the top of the list. *Journal of Machine Learning Research*, 10:2233–2271, December 2009.
- Rudin, C. and Wang, Y. Direct learning to rank and rerank. In *Proceedings of Artificial Intelligence and Statistics AISTATS*, 2018.
- Taylor, M., Guiver, J., Robertson, S., and Minka, T. Softrank: Optimizing non-smooth rank metrics. In *Proceed*ings of the 1st International Conference on Web Search and Data Mining, pp. 77–86, 2008.
- Tewari, A. and Chaudhuri, S. Generalization error bounds for learning to rank: Does the length of document lists matter? In *Proceedings of the 32nd International Conference on Machine Learning*, pp. 315–323, 2015.
- Wang, X., Li, C., Golbandi, N., Bendersky, M., and Najork, M. The lambdaloss framework for ranking metric optimization. In *Proceedings of the 27th ACM International Conference on Information and Knowledge Management*, pp. 1313–1322, 2018.

- Wu, Q., Burges, C. J., Svore, K. M., and Gao, J. Adapting boosting for information retrieval measures. *Information Retrieval*, 13(3):254–270, 2010.
- Xia, F., Liu, T.-Y., Wang, J., Zhang, W., and Li, H. Listwise approach to learning to rank: theory and algorithm.
  In *Proceedings of the 25th International Conference on Machine Learning*, pp. 1192–1199, 2008.
- Xu, J. and Li, H. Adarank: A boosting algorithm for information retrieval. In *Proceedings of the 30th Annual International ACM SIGIR Conference on Research and Development in Information Retrieval*, pp. 391–398, 2007.

## A. Proof of Proposition 2

**Proposition.**  $XE_{NDCG}$  is 2-Lipschitz with respect to  $\|\cdot\|_{\infty}$ .

*Proof.* We follow the proof of Proposition 1.

Recall that the cost function  $\ell(\cdot)$  for  $XE_{NDCG}$  is defined as follows:

$$\ell(\boldsymbol{y}, f(\boldsymbol{x})) \triangleq -\sum \phi(y_i) \log \rho(f_i),$$

where  $\phi$  and  $\rho$  form probability distributions over labels  $\boldsymbol{y}$  and scores  $f(\boldsymbol{x})$  respectively, and  $f_i = f(x_i)$ .

Observe that the derivative of the cost function  $\ell$  with respect to a score  $f_r$  is:

$$\begin{split} \frac{\partial \ell}{\partial f_r} &= \frac{\partial}{\partial f_r} \left[ -\sum_i \phi(y_i) (f_i - \log \sum_j e^{f_j}) \right] \\ &= \frac{\partial}{\partial f_r} \left[ \left( \sum_i -\phi(y_i) f_i \right) + \log \sum_j e^{f_j} \right] \\ &= -\phi(y_r) + \frac{e^{f_r}}{\sum_j e^{f_j}} = -\phi(y_r) + \rho(f_r). \end{split}$$

By triangle inequality,

$$\left|\frac{\partial \ell}{\partial f_r}\right| \le \phi(y_r) + \rho(f_r)$$

Then,

$$\|\nabla_f \ell\|_1 = \sum \left|\frac{\partial \ell}{\partial f_i}\right| \le \sum (\phi(y_r) + \rho(f_r)) = 2$$

as required.

## B. Proof of Theorem 2

**Theorem.** Let  $\mathcal{F}$  be a compact space of bounded functions from  $\mathcal{X}$  to [0,1],  $^1 n = |\Psi|$  be the number of training examples,  $Lip_{\ell}$  the Lipschitz constant of loss function  $\ell$ , and  $\mathfrak{N}(\frac{\epsilon}{4Lip_{\ell}}, \mathcal{F}, \|\cdot\|_{\infty})$  the covering number of  $\mathcal{F}$  by  $L_{\infty}$  balls of radius  $\frac{\epsilon}{4Lip_{\ell}}$ . The following generalization error bound holds:

$$\mathcal{P}\{\mathcal{E}(f) \leq \epsilon\} \geq 1 - 2\mathfrak{N}(\frac{\epsilon}{4Lip_{\ell}}, \mathcal{F}, \|\cdot\|_{\infty}) exp(\frac{-2n\epsilon^{2}}{Lip_{\ell}^{2}}),$$

where the generalization error  $\mathcal{E}$  is defined as follows:

$$\mathcal{E}(f) \triangleq \underset{\mathcal{X}^m \times \mathcal{Y}^m}{\mathbb{E}} [\ell(\boldsymbol{y}, f(\boldsymbol{x}))] - \frac{1}{n} \sum_{(\boldsymbol{x}, \boldsymbol{y}) \in \Psi} \ell(\boldsymbol{y}, f(\boldsymbol{x})).$$

*Proof.* Based on the proofs in (Cucker & Smale, 2002; Rudin, 2009). At a high level, the proof can be sketched as follows: Consider a cover of  $\mathcal F$  with  $\epsilon$ -balls with respect to  $\|\cdot\|_\infty$  and let  $\mathfrak N_\epsilon$  be its covering number (i.e., the number of elements in the smallest such cover). That is, we assume there exists  $\mathfrak N_\epsilon$  balls centered on  $f^r$ s for  $1 \le r \le \mathfrak N_\epsilon$  that cover  $\mathcal F$ . In Lemma B.2, we show that if the radius of the balls is sufficiently small, it matters little which f we choose to represent each ball; the generalization error does not change much within each ball. We then proceed to work with the centers  $f^r$ s and find a probabilistic generalization bound within each ball for  $f^r$ s. Finally, we use the union bound to derive a bound on the entire cover. But first we need the following lemma.

<sup>&</sup>lt;sup>1</sup>The  $\lambda$ MART loss is invariant to a translation of scores. Scaling the scores is equivalent to scaling the generalized sigmoid's hyperparameter,  $\sigma$ , by a scalar and the gradients by inverse of that scalar, which subsequently does not affect the Lipschitz constant of the loss. As such, any (bounded) function produced by  $\lambda$ MART can be translated and scaled into the [0, 1] interval without loss of generality.

**Lemma B.1.** For any  $f, f' \in \mathcal{F}$ ,  $\mathcal{E}(f) - \mathcal{E}(f') \leq 2Lip_{\ell}||f - f'||_{\infty}$ .

Proof.

$$\begin{split} \mathcal{E}(f) - \mathcal{E}(f') &= [\underset{\mathcal{X}^m \times \mathcal{Y}^m}{\mathbb{E}}[\ell(\boldsymbol{y}, f(\boldsymbol{x}))] - \frac{1}{n} \sum_{(\boldsymbol{x}, \boldsymbol{y}) \in \Psi} \ell(\boldsymbol{y}, f(\boldsymbol{x}))] - \\ & [\underset{\mathcal{X}^m \times \mathcal{Y}^m}{\mathbb{E}}[\ell(\boldsymbol{y}, f'(\boldsymbol{x}))] - \frac{1}{n} \sum_{(\boldsymbol{x}, \boldsymbol{y}) \in \Psi} \ell(\boldsymbol{y}, f'(\boldsymbol{x}))] \\ &= \underset{\mathcal{X}^m \times \mathcal{Y}^m}{\mathbb{E}}[|\ell(\boldsymbol{y}, f(\boldsymbol{x})) - \ell(\boldsymbol{y}, f'(\boldsymbol{x}))|] + \\ & \frac{1}{n} \sum_{(\boldsymbol{x}, \boldsymbol{y}) \in \Psi} |\ell(\boldsymbol{y}, f(\boldsymbol{x})) - \ell(\boldsymbol{y}, f'(\boldsymbol{x}))| \\ & \leq Lip_{\ell} \|f - f'\|_{\infty} + Lip_{\ell} \|f - f'\|_{\infty} \end{aligned} \tag{by Lipschitz continuity)} \\ &= 2Lip_{\ell} \|f - f'\|_{\infty}. \end{split}$$

**Lemma B.2.** Consider an  $L_{\infty}$  ball,  $N(f^*)$  in  $\mathcal{F}$  centered at  $f^*$  with radius  $\frac{\epsilon}{4Lip_{\ell}}$ . We have that:

$$\mathbb{P}\{\sup_{f\in N(f^*)}\mathcal{E}(f)\geq \epsilon\}\leq \mathbb{P}\{\mathcal{E}(f^*)\geq \frac{\epsilon}{2}\}.$$

Proof.

$$\begin{split} \sup_{f \in N(f^*)} \mathcal{E}(f) - \mathcal{E}(f^*) &\leq 2Lip_{\ell} \sup_{f \in N(f^*)} \|f - f^*\| \\ &\leq 2Lip_{\ell} \frac{\epsilon}{4Lip_{\ell}} = \frac{\epsilon}{2}. \end{split} \tag{by Lemma B.1}$$

The above means:

$$\sup_{f \in N(f^*)} \mathcal{E}(f) \ge \epsilon \Rightarrow \mathcal{E}(f^*) \ge \frac{\epsilon}{2}.$$

The claim follows.

Finally, we turn to proving the main result. Define  $S = \frac{1}{n} \sum_{(\boldsymbol{x}, \boldsymbol{y}) \in \Psi} \ell(\boldsymbol{y}, f(\boldsymbol{x}))$ . The largest possible change in S due to a replacement of  $(\boldsymbol{x}, \boldsymbol{y})$  with another training example  $(\boldsymbol{x}', \boldsymbol{y}')$  is bounded by:

$$\frac{1}{n}Lip_{\ell}||f(\boldsymbol{x}) - f(\boldsymbol{x}')||_{\infty} \leq \frac{1}{n}Lip_{\ell}\sup_{x,x'\in\mathcal{X}}||f(\boldsymbol{x}) - f(\boldsymbol{x}')||_{\infty} \leq \frac{1}{n}Lip_{\ell}.$$

Using McDiarmid's inequality:

$$\mathcal{P}\{|\mathbb{E}[S] - S| \ge \epsilon\} \le 2exp(\frac{-2\epsilon^2}{n(\frac{1}{n}Lip_{\ell})^2}).$$

Finally, using Lemma B.2 and the union bound over the entire cover, we obtain:

$$\begin{split} \mathcal{P}\{\sup_{f}\mathcal{E}(f) \geq \epsilon\} &\leq \mathfrak{N}(\frac{\epsilon}{4Lip_{\ell}}, \mathcal{F}, \|\cdot\|_{\infty}) \mathcal{P}\{\mathcal{E}(f^{r}) \geq \frac{\epsilon}{2}\} \\ &\leq 2\mathfrak{N}(\frac{\epsilon}{4Lip_{\ell}}, \mathcal{F}, \|\cdot\|_{\infty}) exp(\frac{-2n\epsilon^{2}}{Lip_{\ell}^{2}}) \end{split}$$

## C. Proof of Claim 1

Using  $\rho_r = \rho(f_r) = e^{f_r}/(\sum e^{f_j} + \epsilon)$  to denote the score probability of the  $r^{\text{th}}$  document, the Hessian can be written as follows:

$$H_{ij} = \begin{cases} \rho_i (1 - \rho_i), & i = j \\ -\rho_i \rho_j, & i \neq j \end{cases}$$

Claim. The Hessian, as defined above, is positive definite.

*Proof.* We first prove that H is strictly diagonally dominant. By definition, a square matrix A is said to be strictly diagonally dominant if the following holds for all i:

$$|A_{ii}| > \sum_{j \neq i} |A_{ij}|.$$

Observe that:

$$|H_{kk}| = \rho_k (1 - \rho_k) = \rho_k (1 - \frac{e^{f_k}}{\sum e^{f_j} + \epsilon})$$
$$= \rho_k \frac{\sum_{j \neq k} e^{f_j} + \epsilon}{\sum e^{f_j} + \epsilon} > \rho_k \sum_{j \neq k} \rho_j = \sum_{j \neq k} |H_{kj}|.$$

Using this property, we now prove nonsingularity of H by contradiction. Assume there exists a vector  $\mathbf{u} \neq \mathbf{0}$  such that  $H\mathbf{u} = \mathbf{0}$ . Let i be the index of the  $u_i$  with the largest magnitude:  $i = \arg\max_i |u_i|$ . Then:

$$\begin{split} \sum_{j} H_{ij} u_{j} &= 0 \Rightarrow H_{ii} u_{i} = -\sum_{j \neq i} H_{ij} u_{j} \overset{u_{i} \neq 0}{\Rightarrow} \\ H_{ii} &= -\sum_{j \neq i} \frac{u_{j}}{u_{i}} H_{ij} \Rightarrow \\ |H_{ii}| &\leq \sum_{j \neq i} |\frac{u_{j}}{u_{i}} H_{ij}| \Rightarrow \\ |H_{ii}| &\leq \sum_{j \neq i} |H_{ij}|, \end{split}$$

which is a contradiction. This concludes the proof for nonsingularity of the Hessian, which is already sufficient for subsequent results. However, as a consequence of the Gershgorin circle theorem it can further be shown that, because the diagonal elements of H are strictly positive, H is positive definite.

## D. Proof of Claim 2

Use  $\rho_r = \rho(f_r) = e^{f_r}/(\sum e^{f_j} + \epsilon)$  to denote the score probability of the  $r^{\text{th}}$  document. The nonnegative, square matrix S in Claim 2 is defined as follows:

$$S_{ij} = \begin{cases} 0, & i = j \\ \rho_j/(1 - \rho_i), & i \neq j \end{cases}.$$

**Claim.** The spectral radius of S is strictly less than 1.

*Proof.* Note that, for all eigenvalues  $\lambda_i$ ,  $1 \le i \le n$  of an  $n \times n$  matrix A, their corresponding eigenvectors  $u_i$ , and for any induced operator norm  $\|\cdot\|$  we have that:

$$||A|| = \sup_{\boldsymbol{x}} \frac{||A\boldsymbol{x}||}{||\boldsymbol{x}||} \ge \frac{||A\boldsymbol{u}_i||}{||\boldsymbol{u}_i||} = \frac{||\lambda_i \boldsymbol{u}_i||}{||\boldsymbol{u}_i||} = |\lambda_i|, \ \forall i.$$

This is, in particular, true for the infinity norm:

$$||A||_{\infty} = \max_{i} \sum_{j} |A_{ij}|.$$

The inequality above holds for the spectral radius of A which is defined as the largest absolute value of A's eigenvalues:  $\max_i |\lambda_i|$ . Therefore, we have that the spectral radius of S is bounded above by:

$$\max_{i} \sum_{j} |S_{ij}| = \max_{i} \sum_{j} \frac{\rho_{j}}{1 - \rho_{i}} = \max_{i} \frac{\sum_{j \neq i} \rho_{j}}{1 - \rho_{i}}$$
$$= \max_{i} \frac{1 - \rho_{i} - \epsilon'}{1 - \rho_{i}} = \max_{i} 1 - \frac{\epsilon'}{1 - \rho_{i}} < 1,$$

where  $\epsilon' = \epsilon / \sum e^{f_k} + \epsilon$ . That completes the proof.

## E. Additional Experiments on Robustness

In Section 5.4, we examined the behavior of  $\lambda$ MART and XE<sub>NDCG</sub>MART in the presence of noise on datasets with explicit relevance judgments (i.e., where relevance of every document is determined by human judges). In this section, we provide an analysis of the robustness of  $\lambda$ MART and XE<sub>NDCG</sub>MART on a simulated click dataset where noise occurs more naturally (e.g., where a user clicks a non-relevant document by accident).

We follow the procedure proposed in (Joachims et al., 2017) to simulate a user in the cascade click model (Craswell et al., 2008). In the cascade click model, when presented with a ranked list of documents, a user scans the list sequentially from the top and clicks on each document according to a *click probability* distribution—the probability that a document is clicked given its relevance label. We assume the user is persistent in that they continue to examine the list until either a document is clicked or they reach the end of the list.

We construct click datasets as follows. We first create training and validation splits using the procedure of Section 5.1. Given a training (or validation) example (x, y) consisting of m documents and relevance labels, we shuffle its elements and sequentially scan the resulting list to produce clicks using the cascade click model. We stop at the first occurrence of a click and return the list up to the first click as an "impression." We create 10 impressions per training example to form our click dataset. Finally, we train ranking models on the click dataset and evaluate on the original (non-click) test set. We repeat this experiment 20 times and measure mean NDCG.

In our experiments, we adjust the click probability of non-relevant documents to simulate noise in the training set. We begin with click probabilities set to (.05, .3, .5, .7, .95) for relevance labels 0 through 4, respectively. That is, in this setting, a non-relevant document (with relevance label 0) is clicked 5% of the time. In subsequent experiments, we increase the click probability of non-relevant documents by .05.

The results of our experiments on Web30K and Yahoo! are illustrated in Figure 4. Clearly, the performance of  $XE_{NDCG}MART$  on the test sets is consistently better than  $\lambda MART$  for all levels of noise in the training set. We note that all differences are statistically significant according to a paired *t*-test (significance level  $\alpha = .01$ ). Additionally, as with previous experiments, the performance of  $XE_{NDCG}MART$  is more robust to noise: its performance degrades more slowly than  $\lambda MART$ .

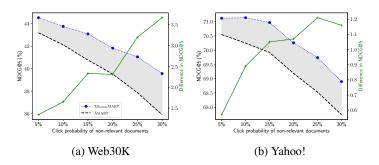


Figure 4. Mean NDCG@5 on test sets, averaged over 20 trials. In each trial, training and validation sets are turned into clicks using the cascade click model and a random base ranker. The horizontal axis indicates the click probability of non-relevant documents. The solid (green) lines show the difference in NDCG@5 between the two models.