Abstract

Learning to rank has become an important research topic in machine learning. While most learning-to-rank methods learn the ranking functions by minimizing the loss functions, it is the ranking measures (such as NDCG and MAP) that are used to evaluate the performance of the learned ranking functions. In this work, we reveal the relationship between ranking measures and loss functions in learning-to-rank methods, such as Ranking SVM, RankBoost, RankNet, and ListMLE. We show that the loss functions of these methods are upper bounds of the measure-based ranking errors. As a result, the minimization of these loss functions will lead to the maximization of the ranking measures. The key to obtaining this result is to model ranking as a sequence of classification tasks, and define a so-called essential loss for ranking as the weighted sum of the classification errors of individual tasks in the sequence. We have proved that the essential loss is both an upper bound of the measure-based ranking errors, and a lower bound of the loss functions in the aforementioned methods. Our proof technique also suggests a way to modify existing loss functions to make them tighter bounds of the measure-based ranking errors. Experimental results on benchmark datasets show that the modifications can lead to better ranking performances, demonstrating the correctness of our theoretical analysis.

1 Introduction

Learning to rank has become an important research topic in many fields, such as machine learning and information retrieval. The process of learning to rank is as follows. In training, a set of objects and labels representing their rankings (e.g., in terms of multi-level ratings\(^1\)) is given. Then a ranking function is constructed by minimizing a certain loss function on the training data. In testing, given a new set of objects, the ranking function is applied to produce a ranked list of the objects.

Many learning-to-rank methods have been proposed in the literature, with different motivations and formulations. In general, these methods can be divided into three categories [3]. The pointwise approach, such as subset regression [4] and McRank [10], considers each single object the learning instance. The pairwise approach, such as Ranking SVM [7], RankBoost [5], and RankNet [2], regards a pair of objects as the learning instance. The listwise approach, such as ListNet [3] and ListMLE [16], takes the entire ranked list of objects as the learning instance. Almost all these

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\(^1\)The work was performed when the first and the third authors were interns at Microsoft Research Asia.

\(^1\)In information retrieval, such a label represents the relevance of a document to the given query.
methods learn their ranking functions by minimizing certain loss functions, namely the pointwise, pairwise, and listwise losses. On the other hand, however, it is the ranking measures that are used to evaluate the performance of the learned ranking functions. Taking information retrieval as an example, measures such as Normalized Discounted Cumulative Gain (NDCG) [8] and Mean Average Precision (MAP) [1] are widely used, which obviously differ from the loss functions used in the aforementioned methods. In such a situation, a natural question to ask is whether the minimization of the loss functions can really lead to the optimization of the ranking measures.\footnote{Actually people have tried to answer this question. It has been proved in [4] and [10] that the regression and classification based losses used in the pointwise approach are upper bounds of $(1-NDCG)$. However, for the pairwise and listwise approaches, which are regarded as the state-of-the-art of learning to rank [3, 11], limited results have been obtained. The motivation of this work is just to reveal the relationship between ranking measures and the pairwise/listwise losses.}

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It is non-trivial to achieve this goal, however. Note that ranking measures like NDCG and MAP are defined with the labels of objects (i.e., in terms of multi-level ratings). Therefore it is relatively easy to establish the connection between the pointwise losses and the ranking measures, since the pointwise losses are also defined with the labels of objects. In contrast, the pairwise and listwise losses are defined with the partial or total order relations among objects, rather than their individual labels. As a result, it is much more difficult to bridge the gap between the pairwise/listwise losses and the ranking measures.

To tackle the challenge, we propose making a transformation of the labels on objects to a permutation set. All the permutations in the set are consistent with the labels, in the sense that an object with a higher rating is ranked in the permutation before another object with a lower rating. We then define an essential loss for ranking on the permutation set as follows. First, for each permutation, we construct a sequence of classification tasks, with the goal of each task being to distinguish an object from the objects ranked below it in the permutation. Second, the weighted sum of the classification errors of individual tasks in the sequence is computed. Third, the essential loss is defined as the minimum value of the weighted sum over all the permutations in the set.

Our study shows that the essential loss has several nice properties, which help us reveal the relationship between ranking measures and the pairwise/listwise losses. First, it can be proved that the essential loss is an upper bound of measure-based ranking errors such as $(1-NDCG)$ and $(1-MAP)$. Furthermore, the zero value of the essential loss is a sufficient and necessary condition for the zero values of $(1-NDCG)$ and $(1-MAP)$. Second, it can be proved that the pairwise losses in Ranking SVM, RankBoost, and RankNet, and the listwise loss in ListMLE are all upper bounds of the essential loss. As a consequence, we come to the conclusion that the loss functions used in these methods can bound $(1-NDCG)$ and $(1-MAP)$ from above. In other words, the minimization of these loss functions can effectively maximize NDCG and MAP.

The proofs of the above results suggest a way to modify existing pairwise/listwise losses so as to make them tighter bounds of $(1-NDCG)$. We hypothesize that tighter bounds will lead to better ranking performances; we tested this hypothesis using benchmark datasets. The experimental results show that the methods minimizing the modified losses can outperform the original methods, as well as many other baseline methods. This seems to validate the correctness of our theoretical analysis.

2 Related work

In this section, we review the widely-used loss functions in learning to rank, ranking measures in information retrieval, and previous work on the relationship between loss functions and ranking measures.
2.1 Loss functions in learning to rank

Let \( x = \{x_1, \cdots, x_n\} \) be the objects to be ranked. Suppose the labels of the objects are given as multi-level ratings \( L = \{l(1), \ldots, l(n)\} \), where \( l(i) \in \{r_1, \ldots, r_K\} \) denotes the label of \( x_i \) [11]. Without loss of generality, we assume \( l(i) \in \{0, 1, \ldots, K - 1\} \) and name the corresponding labels as \( K \)-level ratings. If \( l(i) > l(j) \), then \( x_i \) should be ranked before \( x_j \). Let \( F \) be the function class and \( f \in F \) be a ranking function. The optimal ranking function is learned from the training data by minimizing a certain loss function defined on the objects, their labels, and the ranking function. Several approaches have been proposed to learn the optimal ranking function.

In the pointwise approach, the loss function is defined on the basis of single objects. For example, in subset regression [4], the loss function is as follows,

\[
L'(f; x, L) = \sum_{i=1}^{n} (f(x_i) - l(i))^2.
\]

(1)

In the pairwise approach, the loss function is defined on the basis of pairs of objects whose labels are different. For example, the loss functions of Ranking SVM [7], RankBoost [5], and RankNet [2] all have the following form,

\[
L^p(f; x, L) = \sum_{i=1}^{n} \sum_{j=1, j < i}^{n} \phi(f(x_i) - f(x_j)),
\]

(2)

where the \( \phi \) functions are hinge function \( (\phi(z) = (1 - z)_+) \), exponential function \( (\phi(z) = e^{-z}) \), and logistic function \( (\phi(z) = \log(1 + e^{-z})) \) respectively, for the three algorithms.

In the listwise approach, the loss function is defined on the basis of all the \( n \) objects. For example, in ListMLE [16], the following loss function is used,

\[
L^l(f; x, y) = \sum_{s=1}^{n} \left( -f(x_{y(s)}) + \ln \left( \sum_{i=1}^{n} \exp(f(x_{y(i)})) \right) \right),
\]

(3)

where \( y \) is a randomly selected permutation (i.e., ranked list) that satisfies the following condition: for any two objects \( x_i \) and \( x_j \), if \( l(i) > l(j) \), then \( x_i \) is ranked before \( x_j \) in \( y \). Notation \( y(i) \) represents the index of the object ranked at the \( i \)-th position in \( y \).

2.2 Ranking measures

Several ranking measures have been proposed in the literature to evaluate the performance of a ranking function. Here we introduce two of them, NDCG [8] and MAP[1], which are popularly used in information retrieval.

NDCG is defined with respect to \( K \)-level ratings \( L \),

\[
NDCG(f; x, L) = \frac{1}{N_n} \sum_{r=1}^{n} G(l(\pi_f(r))) D(r),
\]

where \( \pi_f \) is the ranked list produced by ranking function \( f \), \( G \) is an increasing function (named the gain function), \( D \) is a decreasing function (named the position discount function), and \( N_n = \max_{\pi} \sum_{r=1}^{n} G(l(\pi(r))) D(r) \). In practice, one usually sets \( G(z) = 2^z - 1; D(z) = \frac{1}{\log_2(1 + z)} \) if \( z \leq C \), and \( D(z) = 0 \) if \( z > C \) (\( C \) is a fixed integer).

MAP is defined with respect to \( 2 \)-level ratings as follows,

\[
MAP(f; x, L) = \frac{1}{n_1} \sum_{s \leq s \leq n} \frac{\sum_{i:s(l(\pi_f(i)) = 1)} I(l(\pi_f(i)) = 1)}{s},
\]

(4)

where \( I(\cdot) \) is the indicator function, and \( n_1 \) is the number of objects with label 1. When the labels are given in terms of \( K \)-level ratings (\( K > 2 \)), a common practice of using MAP is to fix a level \( k^* \), and regard all the objects whose ratings are lower than \( k^* \) as having label 0, and regard the other objects as having label 1 [11].

From the definitions of NDCG and MAP, we can see that their maximum values are both one. Therefore, we can consider \( (1 - \text{NDCG}) \) and \( (1 - \text{MAP}) \) as ranking errors. For ease of reference, we call them measure-based ranking errors.

\footnote{For example, for information retrieval, \( x \) represents the documents associated with a given query.}
2.3 Previous bounds

For the pointwise approach, the following results have been obtained in [4] and [10].\footnote{Note that the bounds given in the original papers of [4] and [10] are with respect to DCG. Here we give their equivalent forms in terms of NDCG, and set $P(\{x,y\}) = \delta_{y(i)}(\cdot)$ in the bound of [4], for ease of comparison.}
The regression based pointwise loss is an upper bound of $(1 - \text{NDCG})$,
\[
1 - \text{NDCG}(f; x, \mathcal{L}) \leq \frac{1}{N_n} \left( \sum_{i=1}^{n} D(i)^2 \right)^{1/2} \left( \frac{L' \sum_{i=1}^{n} I_{i(\hat{l}(i))}}{2} \right)^{1/2}.
\]
The classification based pointwise loss is also an upper bound of $(1 - \text{NDCG})$,
\[
1 - \text{NDCG}(f; x, \mathcal{L}) \leq \frac{15\sqrt{2}}{N_n} \left( \sum_{i=1}^{n} D(i)^2 - n \prod_{i=1}^{n} D(i)^{2/n} \right)^{1/2} \left( \sum_{i=1}^{n} I_{i(\hat{l}(i))} \right)^{1/2},
\]
where $\hat{l}(i)$ is the label of object $x_i$ predicted by the classifier, in the setting of 5-level ratings.
For the pairwise approach, the following result has been obtained [9],
\[
1 - \text{MAP}(f; x, \mathcal{L}) \leq 1 - \frac{1}{n_1} (L''(f; x, \mathcal{L}) + C_{n_1+1}^{-1} \sum_{i=1}^{n_1} \sqrt{l})^2.
\]
According to the above results, minimizing the regression and classification based pointwise losses will minimize $(1 - \text{NDCG})$. Note that the zero values of these two losses are sufficient but not necessary conditions for the zero value of $(1 - \text{NDCG})$. That is, when $(1 - \text{NDCG})$ is zero, the loss functions may still be very large [10]. For the pairwise losses, the result is even weaker: their zero values are even not sufficient for the zero value of $(1 - \text{MAP})$.

To the best of our knowledge, there was no other theoretical result for the pairwise/listwise losses. Given that the pairwise and listwise approaches are regarded as the state-of-the-art in learning to rank [3, 11], it is very meaningful and important to perform more comprehensive analysis on these two approaches.

3 Main results

In this section, we present our main results on the relationship between ranking measures and the pairwise/listwise losses. The basic conclusion is that many pairwise and listwise losses are upper bounds of a quantity which we call the essential loss, and the essential loss is an upper bound of both $(1 - \text{NDCG})$ and $(1 - \text{MAP})$. Furthermore, the zero value of the essential loss is a sufficient and necessary condition for the zero values of $(1 - \text{NDCG})$ and $(1 - \text{MAP})$.

3.1 Essential loss: ranking as a sequence of classifications

In this subsection, we describe the essential loss for ranking.

First, we propose an alternative representation of the labels of objects (i.e., multi-level ratings). The basic idea is to construct a permutation set, with all the permutations in the set being consistent with the labels. The definition that a permutation is consistent with multi-level ratings is given as below. Furthermore,

**Definition 1.** Given multi-level ratings $\mathcal{L}$ and permutation $y$, we say $y$ is consistent with $\mathcal{L}$, if for all $i, s \in \{1, \ldots, n\}$ satisfying $i < s$, we always have $l(y(i)) \geq l(y(s))$, where $y(i)$ represents the index of the object that is ranked at the $i$-th position in $y$. We denote $Y_{\mathcal{L}} = \{y|y$ is consistent with $\mathcal{L}\}$.

According to the definition, it is clear that the NDCG and MAP of a ranking function equal one, if and only if the ranked list (permutation) given by the ranking function is consistent with the labels.

Second, given each permutation $y \in Y_{\mathcal{L}}$, we decompose the ranking of objects $x$ into several sequential steps. For each step $s$, we distinguish $x_{y(s)}$, the object ranked at the $s$-th position in $y$, from all the other objects ranked below the $s$-th position in $y$, using ranking function $f$. Specifically, we
denote $x(s) = \{x_y(s), \ldots, x_y(n)\}$ and define a classifier based on $f$, whose target output is $y(s)$,

$$T_f(x(s)) = \arg \max_{j \in \{y(s), \ldots, y(n)\}} f(x_j).$$

(5)

It is clear that there are $n - s$ possible outputs of this classifier, i.e., $\{y(s), \ldots, y(n)\}$. The 0-1 loss for this classification task can be written as follows, where the second equality is based on the definition of $T_f$,

$$l_s(f; x(s), y(s)) = l(T_f(x(s)) \neq y(s)) = 1 - \prod_{i=s+1}^{n} I(f(x_{y(i)}) > f(x_{y(i)})).$$

We give a simple example in Figure 1 to illustrate the aforementioned process of decomposition.

Suppose there are three objects, $A$, $B$, and $C$, and a permutation $y = (A, B, C)$. Suppose the output of the ranking function for these objects is $(2, 3, 1)$, and accordingly the predicted ranked list is $\pi = (B, A, C)$. At step one of the decomposition, the ranking function predicts object $B$ to be on the top of the list. However, $A$ should be on the top according to $y$. Therefore, a prediction error occurs. For step two, we remove $A$ from both $y$ and $\pi$. Then the ranking function predicts object $B$ to be on the top of the remaining list. This is in accordance with $y$ and there is no prediction error. After that, we further remove object $B$, and it is easy to verify there is no prediction error in step three either. Overall, the ranking function makes one error in this sequence of classification tasks.

Third, we assign a non-negative weight $\beta(s) (s = 1, \ldots, n - 1)$ to the classification task at the $s$-th step, representing its importance to the entire sequence. We compute the weighted sum of the classification errors of all individual tasks,

$$L_\beta(f; x, y) \overset{\Delta}{=} \sum_{s=1}^{n-1} \beta(s) \left(1 - \prod_{i=s+1}^{n} I(f(x_{y(i)}) > f(x_{y(i)}))\right),$$

(6)

and then define the minimum value of the weighted sum over all the permutations in $Y_L$ as the essential loss for ranking.

$$L_\beta(f; x, L) = \min_{y \in Y_L} L_\beta(f; x, y).$$

(7)

According to the above definition of the essential loss, we can obtain its following nice property. Denote the ranked list produced by $f$ as $\pi_f$. Then it is easy to verify that,

$$L_\beta(f; x, L) = 0 \iff \exists y \in Y_L\text{ satisfying } L_\beta(f; x, y) = 0 \iff \pi_f = y \in Y_L.$$

In other words, the essential loss is zero if and only if the permutation given by the ranking function is consistent with the labels. Further considering the discussions on the consistent permutation at the beginning of this subsection, we can come to the conclusion that the zero value of the essential loss is a sufficient and necessary condition for the zero values of $(1$-NDCG) and $(1$-MAP).

### 3.2 Essential loss: upper bound of measure-based ranking errors

In this subsection, we show that the essential loss is an upper bound of $(1$-NDCG) and $(1$-MAP), when specific weights $\beta(s)$ are used.

**Lemma 1.** Given 2-level rating data $(x, L)$, for $\forall f$, we have,

$$L_{\beta_2}(f; x, L) = n_1 - i_0 + 1,$$

where $i_0$ denotes the position of the first object with label 0 in $\pi_f$ and $\beta_2(s) \equiv 1$. 
Proof. We consider the modeling of ranking as a sequence of classifications.

First of all, it is easy to see that \( i_0 \leq n_1 + 1 \). For \( \forall y \in Y_L \), since \( \ell(\pi_f(i_0)) = 0 \), we have \( y(s) \neq \pi_f(i_0) \) for \( \forall s \in \{1, \ldots, n_1\} \). That is, the object \( x_{\pi_f(i_0)} \) will not be removed in the first \( n_1 \) steps.

Then, we conduct discussions on \( i_0 \) case by case.

(1) If \( i_0 \leq n_1 \), according to the construction of \( \{x(s)\} \), \( \exists s' \in \{1, 2, \ldots, n_1\} \), satisfies \( T_f(x(s)) = \pi_f(i_0) \) for \( \forall s \in \{s', \ldots, n_1\} \).

- For step \( s \in \{1, \ldots, s' - 1\} \): for \( \forall y \in Y_L \), since there are \( i_0 - 1 \) objects before position \( i_0 \) in \( \pi_f \), there are at most \( i_0 - 1 \) nonrecurring elements in \( \{T_f(x(1)), \ldots, T_f(x(s'-1))\} \). In other words, at least \( s' - i_0 \) elements are recurring. Thus, by the definition of \( \{x(s)\} \), from step 1 to step \( s' - 1 \), there are at least \( s' - i_0 \) steps are incorrect.

- For step \( s \in \{s', \ldots, n_1\} \): \( y(s) \neq \pi_f(i_0) \) for \( \forall y \in Y_L \). So, from step \( s' \) to step \( n_1 \), none step is correct.

To sum up, there is at least a classification error of \( (s' - i_0) + (n_1 - s' + 1) = n_1 - i_0 + 1 \) in the first \( n_1 \) steps. In other words,

\[
L_{\beta_2}(f; x, L) \geq n_1 - i_0 + 1. \quad (8)
\]

We define \( y_{\pi_f} \in Y_L \) as the permutation in which objects are sorted according to their positions in \( \pi_f \). It is not difficult to see that \( s' = i_0 \) and there is no loss before step 0 and after step \( n_1 \). In other words, \( L_{\beta_2}(f; x, y_{\pi_f}) = n_1 - i_0 + 1 \). Considering Eq. (8), we have,

\[
L_{\beta_2}(f; x, L) = n_1 - i_0 + 1.
\]

(2) If \( i_0 = n_1 + 1 \), we have \( \pi_f \in Y_L \), and thus \( L_{\beta_2}(f; x, L) \leq L_{\beta_2}(f; x, \pi_f) = 0 = n_1 - i_0 + 1 \). Considering that the essential loss is non-negative, we have \( L_{\beta_2}(f; x, L) = 0 = n_1 - i_0 + 1 \).

\[ \square \]

Theorem 1. Given \( K \)-level rating data \( (x, L) \) with \( n_k \) objects having label \( k \) and \( \sum_{i=k}^{K} n_i > 0 \), then for \( \forall f \), the following inequalities hold,

1. \( 1 - NDCG(f; x, L) \leq \frac{1}{N_n} L_{\beta_1}(f; x, L) \), where \( \beta_1(s) = G(l(y(s)))\, D(s), \forall y \in Y_L \);

2. \( 1 - MAP(f; x, L) \leq \frac{1}{\sum_{i=k}^{K} n_i} L_{\beta_2}(f; x, L) \), where \( \beta_2(s) \equiv 1 \).

Proof. (1) We now prove the inequality for \((1 - NDCG)\).

First, we reformulate NDCG using the permutation set \( Y_L \). This can be done by changing the index of the sum in NDCG from the rank position \( r \) in \( \pi_f \) to the rank position \( s \) in \( \forall y \in Y_L \). Considering that \( s = y^{-1}(\pi_f(r)) \) and \( r = \pi_f^{-1}(y(s)) \), it is easy to obtain,

\[
NDCG(f; x, L) = \frac{1}{N_n} \sum_{s=1}^{n} G((\pi_f(\pi_f^{-1}(y(s))))\, D(\pi_f^{-1}(y(s)))) = \frac{1}{N_n} \sum_{s=1}^{n} G(l(y(s)))\, D(\pi_f^{-1}(y(s))).
\]

Second, we consider the essential loss case by case. Note that

\[
L_{\beta_1}(f; x, L) = \min_{y \in Y_L} \sum_{s=1}^{n-1} G(l(y(s)))\, D(s)\, (1 - \prod_{i=s+1}^{n} I_{\{\pi_f^{-1}(y(s)) < \pi_f^{-1}(y(i))\}}).
\]

For \( \forall y \in Y_L \), if position \( s \) satisfies \( \prod_{i=s+1}^{n} I_{\{\pi_f^{-1}(y(s)) < \pi_f^{-1}(y(i))\}} = 1 \) (i.e., \( \forall i > s, \pi_f^{-1}(y(s)) < \pi_f^{-1}(y(i)) \)), we have \( \pi_f^{-1}(y(s)) \leq s \). As a consequence, \( D(s) \prod_{i=s+1}^{n} I_{\{\pi_f^{-1}(y(s)) < \pi_f^{-1}(y(i))\}} = \).
3.3 Essential loss: lower bound of loss functions

In this section, we show that many pairwise/listwise losses are upper bounds of the essential loss.

**Lemma 2.** Given $K$-level rating data $(x, \mathcal{L})$, for all $f$, we have,

$$L_\beta(f; x, \mathcal{L}) \leq \max_{y \in Y_\mathcal{L}} \sum_{a=1}^{n-1} \beta(s) a \left(T_f(x_s), y(s)\right).$$

**Proof.** We define $y_{\pi_f} \in Y_\mathcal{L}$ as the permutation in which the objects with the same label are sorted according to their positions in $\pi_f$. We denote $s_{K-1}$ as the position of the first object whose label is not $K-1$. It is easy to see that $s_{K-1} \leq n_{K-1} + 1$, and $l(y_{\pi_f}(s)) = K-1$ for all $s \in \{1, \ldots, n_{K-1}\}$.

- If $s_{K-1} \leq n_{K-1}$,
  - For $1 \leq s < s_{K-1}$, by the definition of $y_{\pi_f}$, we have $y_{\pi_f}(s) = T_f(x_s) = \pi_f(s)$ for all $s \in \{1, \ldots, s_{K-1} - 1\}$. Considering $l(\pi_f(s)) = K-1$, the following equations hold,
    $$I_{(T_f(x_s) \neq y_{\pi_f}(s))} = 0 = I_{(l(T_f(x_s)) \neq K-1)} = I_{(l(T_f(x_s)) \neq l(y_{\pi_f}(s)))}. $$
  - For $s_{K-1} \leq s \leq n_{K-1}$, $T_f(x_s) = \pi_f(s_{K-1})$ for all $s \in \{s_{K-1}, \ldots, n_{K-1}\}$. Therefore, $l(T_f(x_s)) = l(\pi_f(s_{K-1})) \neq K-1$ and $T_f(x_s) \neq y_{\pi_f}(s)$. Considering all of this, we have,
    $$I_{(T_f(x_s) \neq y_{\pi_f}(s))} = 1 = I_{(l(T_f(x_s)) \neq K-1)} = I_{(l(T_f(x_s)) \neq l(y_{\pi_f}(s)))}. $$

- If $s_{K-1} = n_{K-1} + 1$, for all $s \in \{1, 2, \ldots, n_{K-1}\}$, all the indicator functions will take value zero by the definition of $y_{\pi_f}$. 

\[ \]
Now, all the objects which ratings are higher than $l(\pi(s_{K-1}))$ are removed from both $\pi_f$ and $y_{\pi_f}$. Then we denote $s(\pi(s_{K-1}))$ as the position of the first object after position $s_{K-1}$ whose label is not $l(\pi(s_{K-1}))$ in the remaining list of $\pi_f$. With similar discussions as above, we can get the same results with those regarding the label $K - 1$. The above process can be iterated until only the objects with label 0 are left in both $\pi_f$ and $y_{\pi_f}$. In that case, all the indicator functions will take value zero.

To sum up, the above discussions show that $\forall s \in \{1, 2, ..., n - 1\}$, 

$$I_{\tau_1}(x(s)) = I_{\tau_1}(y(s)) = I_{\tau_1}(y_{\pi_f}(s)),$$

And we can obtain the result as below,

$$L_{\beta}(f; x, \mathcal{L}) = \max_{s=1}^{n-1} \beta(s)I_{\tau_1}(x(s)) = \sum_{s=1}^{n-1} \beta(s)I_{\tau_1}(x(s)) \geq \max_{s=1}^{n-1} \beta(s)\phi(T_f(x(s)), y(s)).$$

**Theorem 2.** The pairwise losses in Ranking SVM, RankBoost, and RankNet, and the listwise loss in ListMLE are all upper bounds of the essential loss, i.e.,

1. $L_{\beta}(f; x, \mathcal{L}) \leq \max_{1 \leq s \leq n-1} \beta(s)L(f; x, \mathcal{L})$;
2. $L_{\beta}(f; x, \mathcal{L}) \leq \frac{1}{\ln 2} \max_{1 \leq s \leq n-1} \beta(s)L(f; x, y)$, $\forall y \in \mathcal{Y}_e$.

**Proof.** (1) We now prove the inequality for the pairwise losses.

First, we reformulate the pairwise losses using permutation set $Y_e$,

$$L(f; x, \mathcal{L}) = \sum_{i=1}^{n-1} \sum_{\pi \in \pi_{n-1}} \phi(f(y_{\pi(i)}), f(y_{\pi(i+1)})),$$

where $y$ is an arbitrary permutation in $Y_e$, $a(i, j) = 1$ if $l(i) = l(j)$; $a(i, j) = 0$ otherwise. Note that only those pairs whose first object has a larger label than the second one are counted in the pairwise loss. Thus, the value of the pairwise loss is equal for $\forall y \in Y_e$.

Second, we consider the value of $a(T_f(x(s)), y(s))$ case by case. For $\forall y$ and $\forall s \in \{1, 2, ..., n - 1\}$, if $a(T_f(x(s)), y(s)) = 1$ (i.e., $\exists y(i) > s$, satisfying $l(y(i)) \neq l(y(s))$ and $f(x(y(s))) > f(x(y(i))))$ considering that function $\phi$ in Ranking SVM, RankBoost and RankNet are all non-negative, non-increasing, and $\phi(0) = 1$, we have,

$$\sum_{i=s+1}^{n} a(y(i), y(s))\phi(f(y_{\pi(i)})) \geq a(y(i), y(s))\phi(f(x_{\pi(i)})) = \phi(f(x_{\pi(i)})) - f(x_{\pi(i)})) > 1 = a(T_f(x(s)), y(s)).$$

If $a(T_f(x(s)), y(s)) = 0$, it is clear that $\sum_{i=s+1}^{n} a(y(i), y(s))\phi(f(x_{\pi(i)})) \geq 0 = a(T_f(x(s)), y(s)).$ Therefore,

$$\sum_{i=s+1}^{n} a(y(i), y(s))\phi(f(x_{\pi(i)})) \geq \sum_{s=1}^{n-1} \beta(s)a(T_f(x(s)), y(s)).$$

Third, by Lemma 2 the following inequality holds,

$$L_{\beta}(f; x, \mathcal{L}) \leq \max_{y \in \mathcal{Y}_e} \sum_{s=1}^{n-1} \beta(s)a(T_f(x(s)), y(s)).$$

Considering inequality (10) and noticing that the pairwise losses are equal for $\forall y \in Y_e$, we have

$$L_{\beta}(f; x, \mathcal{L}) \leq \max_{y \in \mathcal{Y}_e} \sum_{s=1}^{n-1} \beta(s) \sum_{i=s+1}^{n} a(y(i), y(s))\phi(f(x_{\pi(i)})) \geq \sum_{s=1}^{n-1} \beta(s)a(T_f(x(s)), y(s)) \leq \frac{1}{\ln 2} \max_{1 \leq s \leq n-1} \beta(s)L(f; x, \mathcal{L})$$.
(2) We then prove the inequality for the loss function of ListMLE. Again, we prove the result case by case. Consider the loss of ListMLE in Eq. (3). For \( \forall y \) and \( \forall s \in \{1, 2, \ldots, n-1\} \), if \( I(T_f(x_s) \neq y(s)) = 1 \) (i.e., \( \exists i_0 > s \) satisfying \( f(x_{y(i_0)}) > f(x_{y(s)}) \)), then \( e^{f(x_{y(s)})} < \frac{1}{2} \sum_{i=s}^{n} e^{f(x_{y(i)})} \). Therefore, we have \( -\ln \frac{e^{f(x_{y(s)})}}{\sum_{i=s}^{n} e^{f(x_{y(i)})}} > \ln 2 = \ln 2 I(T_f(x_s) \neq y(s)) \). If \( I(T_f(x_s) \neq y(s)) = 0 \), then it is clear \( -\ln \frac{e^{f(x_{y(s)})}}{\sum_{i=s}^{n} e^{f(x_{y(i)})}} > 0 = \ln 2 I(T_f(x_s) \neq y(s)) \). To sum up, we have,

\[
\sum_{s=1}^{n-1} \beta(s) \left(-\ln \frac{e^{f(x_{y(s)})}}{\sum_{i=s}^{n} e^{f(x_{y(i)})}}\right) > \sum_{s=1}^{n-1} \beta(s) \ln 2 I(T_f(x_s) \neq y(s)) \geq \ln 2 \min_{y \in Y \mathcal{L}} L_{\beta}(\pi_f, y) = \ln 2 L_{\beta}(\pi_f, \mathcal{L}).
\]

By further relaxing the inequality, we obtain the following result,

\[
L_{\beta}(f; x, \mathcal{L}) \leq \frac{1}{\ln 2} \left( \max_{1 \leq s \leq n-1} \beta(s) \right) L(f; x, y), \forall y \in \mathcal{Y}. \]

3.4 Summary

We have the following inequalities by combining the results obtained in the previous subsections.

(1) The pairwise losses in Ranking SVM, RankBoost, and RankNet are upper bounds of \((1 - \text{NDCG})\) and \((1 - \text{MAP})\).

\[
1 - \text{NDCG}(f; x, \mathcal{L}) \leq \frac{G(K - 1)D(1)}{N_n} L^p(f; x, \mathcal{L});
\]

\[
1 - \text{MAP}(f; x, \mathcal{L}) \leq \frac{1}{\sum_{i=k^*}^{n} n_i} L^p(f; x, \mathcal{L}).
\]

(2) The listwise loss in ListMLE is an upper bound of \((1 - \text{NDCG})\) and \((1 - \text{MAP})\).

\[
1 - \text{NDCG}(f; x, \mathcal{L}) \leq \frac{G(K - 1)D(1)}{N_n \ln 2} L^l(f; x, y), \forall y \in \mathcal{Y};
\]

\[
1 - \text{MAP}(f; x, \mathcal{L}) \leq \frac{1}{\ln 2 \sum_{i=k^*}^{n} n_i} L^l(f; x, y), \forall y \in \mathcal{Y}.
\]

For clarity and simplicity, we assume there is no tie in the predicted rank list in the previous sections. The following theorem shows that the main results still hold without this assumption.

**Theorem 3.** Given \( K \)-level rating data \((x, \mathcal{L})\), for \( \forall f \), and arbitrary \( \pi \) which is randomly selected from the permutations produced by \( f \), the following inequalities hold.

\[
1 - \text{NDCG}(\pi, \mathcal{L}) \leq \frac{G(K - 1)D(1)}{N_n} L^p(f; x, \mathcal{L});
\]

\[
1 - \text{MAP}(\pi, \mathcal{L}) \leq \frac{1}{\sum_{i=k^*}^{n} n_i} L^p(f; x, \mathcal{L});
\]

\[
1 - \text{NDCG}(\pi, \mathcal{L}) \leq \frac{G(K - 1)D(1)}{N_n \ln 2} L^l(f; x, y), \forall y \in \mathcal{Y};
\]

\[
1 - \text{MAP}(\pi, \mathcal{L}) \leq \frac{1}{\ln 2 \sum_{i=k^*}^{n} n_i} L^l(f; x, y), \forall y \in \mathcal{Y}.
\]

**Proof.** The proof is similar with the proofs in the paper. Here we just give the sketch.

Firstly, we give some notations.

- \( \Pi_f = \{ \pi | \pi \text{ is consistent with the ranking score } f(x) \} \).

- \( T_n(x(s)) = \arg \max_{j \in \{y(s), \ldots, y(n)\}} (n - \pi^{-1}(j)) \)

and it is clear that, \( n - \pi^{-1}(i) \neq n - \pi^{-1}(j) \) for \( \forall i \neq j \).
Secondly, we can obtain the following by replacing $\pi_f$ with $\forall \pi \in \Pi_f$ in Theorem 1.

$$1 - \text{NDCG}(\pi, \mathcal{L}) \leq \max_{\pi \in \Pi_f} (1 - \text{NDCG}(\pi, \mathcal{L})) \leq \max_{\pi \in \Pi_f} \frac{1}{N_{n_i}} L_{\beta_1}(\pi, \mathcal{L})$$

$$1 - \text{MAP}(\pi, \mathcal{L}) \leq \max_{\pi \in \Pi_f} (1 - \text{MAP}(\pi, \mathcal{L})) \leq \max_{\pi \in \Pi_f} \frac{1}{\sum_{i=k}^{K} n_i} L_{\beta_2}(\pi, \mathcal{L})$$

where $\beta_1(s) = G(l(y(s)))^D(s), \forall y \in \mathcal{Y}_L$, and $\beta_2(s) \equiv 1$.

Thirdly, we prove the following hold for $\forall \pi \in \Pi_f$.

$$L_{\beta}(\pi, \mathcal{L}) \leq \left( \max_{1 \leq s \leq n-1} \beta(s) \right) L^p(f; \mathbf{x}, \mathcal{L});$$

$$L_{\beta}(\pi, \mathcal{L}) \leq \frac{1}{\ln 2} \left( \max_{1 \leq s \leq n-1} \beta(s) \right) L^p(f; \mathbf{x}, \mathcal{L}), \forall y \in \mathcal{Y}_L.$$

We prove it in detail just as the proof of Theorem 2 in the paper. The differences lie in that some "$>$" turn into "$\geq"$. We give the whole proof for integrity. Please pay attention to the differences.

• For the pairwise losses, we consider the value of $\alpha(T_{\pi}(\mathbf{x}(s)), y(s))$ case by case.

For $\forall y$ and $\forall s \in \{1, 2, ..., n - 1\}$, if $\alpha(T_{\pi}(\mathbf{x}(s)), y(s)) = 1$ (i.e., $\exists i_0 > s$ s.t. $l(y(i_0)) \neq l(y(s))$ and $f(x_{y(i_0)}) \geq f(x_{y(s)})$), considering $\phi$ in Ranking SVM, RankBoost and RankNet are all non-negative, non-increasing and $\phi(0) = 1$, we have,

$$\sum_{i=s+1}^{n} \alpha(y(i), y(s))\phi(f(x_{y(s)}) - f(x_{y(i)}))$$

$$\geq \alpha(y(i_0), y(s))\phi(f(x_{y(s)}) - f(x_{y(i_0)})) = \phi(f(x_{y(s)}) - f(x_{y(i_0)})) \geq 1 = \alpha(T_{\pi}(\mathbf{x}(s)), y(s)).$$

If $\alpha(T_{\pi}(\mathbf{x}(s)), y(s)) = 0$, it is clear that $\sum_{i=s+1}^{n} \alpha(y(i), y(s))\phi(f(x_{y(s)}) - f(x_{y(i)})) \geq 0 = \alpha(T_{\pi}(\mathbf{x}(s)), y(s))$. Therefore,

$$\sum_{s=1}^{n-1} \beta(s) \sum_{i=s+1}^{n} \alpha(y(i), y(s))\phi(f(x_{y(s)}) - f(x_{y(i)})) \geq \sum_{s=1}^{n-1} \beta(s)\alpha(T_{\pi}(\mathbf{x}(s)), y(s)). \quad (10)$$

The following inequality can be proved by replacing $\pi_f$ by $\pi$ in Proposition 2,

$$L_{\beta}(\pi, \mathcal{L}) \leq \max_{y \in \mathcal{Y}_L} \sum_{s=1}^{n-1} \beta(s)\alpha(T_{\pi}(\mathbf{x}(s)), y(s)).$$

Considering inequality (10) and noticing that the pairwise losses are equal for $\forall y \in \mathcal{Y}_L$, we have

$$L_{\beta}(\pi, \mathcal{L}) \leq \max_{y \in \mathcal{Y}_L} \sum_{s=1}^{n-1} \beta(s) \sum_{i=s+1}^{n} \alpha(y(i), y(s))\phi(f(x_{y(s)}) - f(x_{y(i)})) \leq \left( \max_{1 \leq s \leq n-1} \beta(s) \right) L^p(f; \mathbf{x}, \mathcal{L}).$$
• For ListMLE loss, we prove the result case by case again. For \( \forall y \) and \( \forall s \in \{1, 2, ..., n-1\} \), if \( I_{\{T_n(x_s), \neq y(s)\}} = 1 \) (i.e., \( \exists \hat{y} \) > \( \forall y \)), then we have, 

\[
\frac{1}{2} \sum_{i=s}^{n} e^{f(x_y(i))} \geq \sum_{i=s}^{n} e^{f(x_y(i))} \geq 2 \ln 2 L_{\beta}(f; x, y), \forall y \in Y_c.
\]

By further relaxing the inequality, we obtain the following results,

\[
L_{\beta}(\pi, \mathcal{L}) \leq \frac{1}{\ln 2} \left( \max_{1 \leq s \leq n-1} \beta(s) \right) L^I(f; x, y), \forall y \in Y_c.
\]

Finally, we sum all the results up and obtain this theorem.

4 Discussion

The proofs of Theorems 1 and 2 actually suggest a way to improve existing loss functions. The key idea is to introduce weights related to \( \beta_1(s) \) to the loss functions so as to make them tighter bounds of \((1-\text{NDCG})\).

Specifically, we introduce weights to the pairwise and listwise losses in the following way,

\[
\tilde{L}^p(f; x, \mathcal{L}) = \sum_{s=1}^{n-1} G(l(y(s))) D \left( 1 + \sum_{k=l(y(s)) + 1}^{K-1} \frac{1}{n_k} \right) \sum_{i=s+1}^{n} a(y(i), y(s)) \phi(f(x_y(i)) - f(x_y(s))), \forall y \in Y_c;
\]

\[
\tilde{L}^I(f; x, y) = \sum_{s=1}^{n-1} G(l(y(s))) D(s) \left( -f(x_y(s)) + \ln \left( \sum_{i=s}^{n} \exp(f(x_y(i))) \right) \right).
\]

The following Proposition shows that the above weighted losses are still upper bounds of \((1-\text{NDCG})\) and they are lower bounds of the original pairwise and listwise losses. In other words, the above weighted loss functions are tighter bounds of \((1-\text{NDCG})\) than existing loss functions.

**Proposition 1.** Given K-level rating data \((x, \mathcal{L})\), for \( \forall f \), we have,

1. \( 1 - \text{NDCG}(f; x, \mathcal{L}) \leq \frac{1}{N_n} \tilde{L}^p(f; x, \mathcal{L}) \leq \frac{G(K-1)D(1)}{N_n} L^p(f; x, \mathcal{L}). \)

2. \( 1 - \text{NDCG}(f; x, \mathcal{L}) \leq \frac{1}{N_n \ln 2} \tilde{L}^I(f; x, y) \leq \frac{G(K-1)D(1)}{N_n \ln 2} L^I(f; x, y), \forall y \in Y_c. \)

**Proof.** It is easy to understand the second “\( \leq \)" in inequalities (1) and (2), since the gain function \( G(z) \) is an increasing function and the discount function \( D(z) \) is a decreasing function.

Now we mainly give the proof for the first "\( \leq \)" in the inequalities.

First, for the loss function of ListMLE, according to Theorem 1 and the proof of Theorem 2, we have,

\[
1 - \text{NDCG}(f; x, \mathcal{L}) \leq \frac{1}{N_n} L_{\beta_1}(f; x, \mathcal{L}) \leq \frac{1}{N_n} \sum_{s=1}^{n-1} \beta_1(s) \left( -\ln \left( \frac{e^{f(x_y(s))}}{\sum_{i=s}^{n} e^{f(x_y(i))}} \right) \right) = \frac{1}{N_n} \tilde{L}^I(f; x, y),
\]

where \( \beta_1(s) = G(l(y(s))) D(s), \forall y \in Y_c. \)

Second, for the pairwise losses, according to Theorem 1 and the proof of Theorem 2, we have,

\[
1 - \text{NDCG}(f; x, \mathcal{L}) \leq \frac{1}{N_n} L_{\beta_1}(f; x, \mathcal{L}) \leq \frac{1}{N_n} \max_{y \in Y_c} \sum_{s=1}^{n-1} \beta_1(s) \sum_{i=s+1}^{n} a(y(i), y(s)) \phi \left( f(x_y(i)) - f(x_y(s)) \right).
\]
Table 1: Ranking accuracy on OHSUMED

<table>
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<tr>
<th>Methods</th>
<th>NDCG@5</th>
<th>RankNet</th>
<th>W-RankNet</th>
<th>ListMLE</th>
<th>W-ListMLE</th>
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<td>0.4868</td>
<td>0.4471</td>
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<table>
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<th>Regression</th>
<th>Ranking SVM</th>
<th>RankBoost</th>
<th>FRank</th>
<th>ListNet</th>
<th>SVM MAP</th>
</tr>
</thead>
<tbody>
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<td>0.4414</td>
<td>0.4604</td>
<td>0.4347</td>
<td>0.4453</td>
<td>0.4516</td>
<td></td>
</tr>
</tbody>
</table>

Note that for \(\forall y \in Y_L\) and \(\forall s \in \{1, 2, ..., n-1\}\), all the objects whose ratings are higher than \(l(y(s))\) are ranked before object \(y(s)\) in \(y\). Therefore, \(s \geq 1 + \sum_{k=l(y(s))+1}^{K-1} n_k\). Considering that \(D(z)\) is a decreasing function, we have \(D(s) \leq D(1 + \sum_{k=l(y(s))+1}^{K-1} n_k)\) and \(\beta_1(s) = G(l(y(s)))D(s) \leq G(l(y(s)))D(1 + \sum_{k=l(y(s))+1}^{K-1} n_k)\).

Therefore, the following inequality holds,

\[
1 - NDCG(f; x, L) \leq \max_{y \in Y_L} \frac{1}{N_n} \sum_{s=1}^{n-1} G(l(y(s)))D(1 + \sum_{k=l(y(s))+1}^{K-1} n_k) \sum_{i=s+1}^{n} a(y(i), y(s))\phi(f(x_y(s)) - f(x_y(i)))
\]

\[
= \frac{1}{N_n} \tilde{L}_p(f; x, L).
\]

Note that the “\(\leq\)" holds since the value of \(\tilde{L}_p\) is equal for \(\forall y \in Y_L\). This is because only those pairs whose first object has a larger label than the second one are counted and the weights are only determined by the label of the first object.

We tested the effectiveness of the weighted loss functions on the OHSUMED dataset in LETOR 3.0.\(^6\) We took RankNet and ListMLE as example algorithms. The methods that minimize the weighted loss functions are referred to as W-RankNet and W-ListMLE. From Table 1, we can see that (1) W-RankNet and W-ListMLE significantly outperform RankNet and ListMLE. (2) W-RankNet and W-ListMLE also outperform other baselines on LETOR such as Regression, Ranking SVM, RankBoost, FRank [15], ListNet and SVMMAP [17]. These experimental results seem to indicate that optimizing tighter bounds of the ranking measures can lead to better ranking performances.

5 Conclusion and future work

In this work, we have proved that many pairwise/listwise losses in learning to rank are actually upper bounds of measure-based ranking errors. We have also shown a way to improve existing methods by introducing appropriate weights to their loss functions. Experimental results have validated our theoretical analysis. As for the future work, we plan to consider the following issues.

(1) We have modeled ranking as a sequence of classifications, when defining the essential loss. We believe this modeling has its general implication for ranking, and will explore its other usages.

(2) We have taken NDCG and MAP as two examples in this work. We will study whether the essential loss is an upper bound of other measure-based ranking errors.

(3) We have taken the loss functions in Ranking SVM, RankBoost, RankNet and ListMLE as examples in this study. We plan to investigate the loss functions in other pairwise and listwise ranking methods, such as RankCosine [13], ListNet [3], FRank [15] and QBRank [18].

(4) While we have mainly discussed the upper-bound relationship in this work, we will study whether loss functions in existing learning-to-rank methods are statistically consistent with the essential loss and the measure-based ranking errors.

\(^6\)http://research.microsoft.com/˜letor
References


