StochasticRank: Global Optimization of Scale-Free Discrete Functions

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Abstract

In this paper, we introduce a powerful and efficient framework for the direct optimization of ranking metrics. The problem is ill-posed due to the discrete structure of the loss, and to deal with that, we introduce two important techniques: a stochastic smoothing and a novel gradient estimate based on partial integration. We also address the problem of smoothing bias and present a universal solution for a proper debiasing. To guarantee the global convergence of our method, we adopt a recently proposed Stochastic Gradient Langevin Boosting algorithm. Our algorithm is implemented as a part of the CatBoost gradient boosting library and outperforms the existing approaches on several learning to rank datasets. In addition to ranking metrics, our framework applies to any scale-free discreet loss function.

1. Introduction

The quality of ranking algorithms is traditionally measured by ranking quality metrics such as Normalized Discounted Cumulative Gain (NDCG), Expected Reciprocal Rank (ERR), Mean Average Precision (MAP), Mean Reciprocal Rank (MRR), and so on (Sakai, 2013). These metrics are defined on a list of documents sorted by their predicted relevance to a query and capture the utility of that list for users of a search engine, who are more likely to scan documents starting at the top. Direct optimization of ranking metrics is an extremely challenging problem since sorting makes them piecewise constant (as functions of predicted relevances), so they are neither convex nor smooth. Many algorithms were proposed for different ranking objectives in the learning-to-rank (LTR) research field. We refer to Liu (2009) for a systematic overview of some classical methods.

To deal with the discrete structure of a ranking loss, one can use some smooth approximation, which is easier to optimize. This technique lies behind such well-known algorithms as SoftRank (Taylor et al., 2008), ApproxNDCG (Qin et al., 2010), RankNet (Burges, 2010), etc. The obtained smooth function can be optimized by gradient-based methods and, in particular, by Stochastic Gradient Boosting (SGB) that is known to be the learning algorithm behind all state-of-the-art LTR frameworks and is commonly preferred by major search engines (Chapelle & Chang, 2010; Yin et al., 2016). Unfortunately, all known smoothing approaches suffer from bias (see Sections 4.2-4.3) which prevents them from truly direct optimization. Moreover, smoothed ranking loss functions are non-convex, and existing algorithms can guarantee only local optima.

Our ultimate goal is to solve these problems and propose a truly direct LTR algorithm with provable guarantees of global convergence and generalization. We adopt a theoretical approach, so we start with formal definitions of the class of ranking losses and its generalization to scale-free (SF) discrete loss functions (Section 3.2). Our results hold for the general class, which, in addition to all ranking metrics, includes, e.g., a recently proposed loss function for Learning-to-Select-with-Order (Vorobev et al., 2019). Then, to mitigate the discontinuity of the loss, use a stochastic smoothing. We prove that previous smoothing-based approaches are inconsistent with the underlying loss (due to the problem of ties, which we discuss in the next section) and propose a universal solution to this problem (see Section 4). Next, we derive a novel stochastic gradient estimate, which can be applied to the entire class of SF losses (see Section 5). The obtained estimate has low variance and uniformly bounded error, which is crucial for our analysis. Finally, to guarantee a global convergence of the algorithm, we adopt a recently proposed Stochastic Gradient Langevin Boosting (SGLB) algorithm (Ustimenko & Prokhorenkova, 2020). SGLB is based on a well studied Stochastic Gradient Langevin Dynamics (Gelfand et al., 1992; Raginsky et al., 2017; Erdogdu et al., 2018) and converges globally for a wide range of loss functions including non-convex ones. We adapt SGLB to our setting and obtain a gradient boosting algorithm that converges globally for the entire class of SF loss functions with provable generalization guarantees.

To sum up, to the best of our knowledge, the proposed StochasticRank algorithm is the first globally
converging LTR method with proven guarantees that optimizes exactly the underlying ranking quality loss. We implemented StochasticRank within the CatBoost library (Prokhorenkova et al., 2018). Our experiments show that StochasticRank outperforms the existing approaches on several LTR datasets.

2. Related Work

Usually, researches divide all LTR methods into three classes: pointwise, pairwise, and listwise (Liu, 2009).

Pointwise are the earliest and simplest methods: they approximate relevance labels based on simple or ordinal regression or classification in the binary case. Such methods were shown to be ineffective for LTR, since loss functions they optimize (e.g., RMSE for relevance labels) differ significantly from the target ranking metric, e.g., NDCG@k.

Pairwise methods make a step forward and focus on pairwise preferences and thus known to outperform pointwise approaches significantly. Nevertheless, pairwise approaches still suffer from the problem of solving a different task rather than optimizing a ranking quality objective.

Listwise methods try to solve the problem directly by developing either smooth proxies of the target ranking metric like SoftRank (Taylor et al., 2008), BoltzRank (Volkovs & Zemel, 2009), ApproxNDCG (Qin et al., 2010), RankNet (Burges, 2010) or by Majorization-Minimization procedure that builds convex upper bound on the metric on each iteration like LambdamART (Wu et al., 2010), LambdaLoss (Wang et al., 2018), PermuRank (Xu et al., 2010), SVMRank (Cao et al., 2006), etc.

The limitations of the algorithms based on smooth approximations (bias and local optima) were discussed in the previous section. Also, there are listwise approaches that try to optimize the target loss function without smoothing. For instance, DirectRank (Tan et al., 2013) constructs an ensemble of decision trees, where the weights of the leaves are chosen to optimize the original loss. However, due to greediness, this approach can guarantee only local optima. Finally, let us note that algorithms optimizing a convex upper bound instead of the original loss cannot be truly direct since an optimum for the upper bound can potentially be far away from the true optimum. This is nicely illustrated by Nguyen & Sanner (2013) for accuracy optimization.

The issue of smoothing bias mentioned in the introduction is connected to the problem of ties: if predicted relevances of some documents coinide, one has to order them somehow to compute a ranking metric. This situation may occur when two documents have equal features. More importantly, ties are always present in boosting algorithms based on discrete weak learners such as decision trees. Unfortunately, this problem is rarely addressed in papers on LTR. In practice, it is reasonable to use the worst permutation. First, due to strong penalization, it would force an optimization algorithm to avoid ties. Second, in practice, one cannot know how a production system would rank the items and often some attribute negatively correlated with relevance is used (e.g., sorting by a bid in online auction). The importance of using the worst permutation is also discussed in (Rudin & Wang, 2018), and this ordering is adopted in some open-source libraries like CatBoost (Prokhorenkova et al., 2018). An alternative choice is to compute the expected value of a ranking metric for a random permutation. This choice is rarely used in practice, since it is computationally complex and gives non-trivial scores to trivial constant predictions, but is often assumed (explicitly or implicitly) by LTR algorithms (Kustarev et al., 2011).

3. Problem Formalization

3.1. Examples of ranking loss functions

Before we introduce a general class of loss functions, let us define classic ranking losses widely used throughout the literature. These loss functions depend on z, which is a vector of scores produced by the model, and r, which is a vector of relevances to a query. The length of these vectors is denoted by n and can be different for different queries.

Let \( s = \text{argsort}(z) \), i.e., \( s_i \) is the index of a document at \( i \)-th position if documents are ordered according to their scores (if \( z_i = z_j \) for \( j \neq i \), then we place the worst first).

Let us define DCG@k, where \( k \) denotes the number of top documents we are interested in:

\[
\text{DCG@}k(z, r) = \sum_{i=1}^{k} \frac{2^{r_{s_i}} - 1}{\log_2(i + 1)},
\]

where \( r_i \in [0, 4] \) are relevance labels. For each document, the numerator corresponds to gain for the relevance, while the denominator discounts for a lower position. We placed “−” before the loss since we want to minimize it.

NDCG@k is a normalized variant of DCG@k:

\[
\text{NDCG@}k(z, r) = \frac{\text{DCG@}k(z, r)}{\max_{z' \in \mathbb{R}^n} \text{DCG@}k(z', r)}.
\]

ERR@k assumes that \( r_j \in [0, 1] \):

\[
\text{ERR@}k(z, r) = -\sum_{i=1}^{\min(n, k)} r_{s_i} \prod_{j=1}^{i-1} (1 - r_{s_j}).
\]

MRR is used for binary relevance labels \( r_j \in \{0, 1\} \):

\[
\text{MRR}(z, r) = -\sum_{i=1}^{n} \frac{r_{s_i}}{\prod_{j=1}^{i-1} (1 - r_{s_j})}.
\]
Finally, let us define a loss function for the LSO (learning to select with order) problem introduced by Vorobeiv et al. (2019), which is not exactly a ranking metric, but has a similar structure. The order of elements is predefined, but the list of documents to be included is determined by $\{z_i>0\}_{i=1}^n \in \{0,1\}^n$:

$$
DCG-RR(z,r) = -\sum_{i=1}^n \frac{r_i \mathbb{1}_{\{z_i>0\}}}{1 + \sum_{j<i} \mathbb{1}_{\{z_j>0\}}}.
$$

### 3.2. Generalized ranking loss functions

To develop a stochastic ranking theory, we first formalize the start of a very general class of scale-free (SF) discrete loss functions. Further by ξ we denote a vector of contexts, which may include relevance and any other factors affecting the quality value (like query type or document topic).

**Definition 1.** A function $L(z, \xi) : \prod_{n>0} \mathbb{R}^n \times \Xi_n \to \mathbb{R}$ is called Scale-Free Discrete Loss Function iff the following conditions hold:

- **Uniform boundedness:** There exists a constant $l > 0$ such that $|L(z, \xi)| \leq l$ holds $\forall n, \forall \xi \in \Xi_n, \forall z \in \mathbb{R}^n$.
- **Discreteness on subspaces:** For each $n \in \mathbb{N}$ and linear subspace $V \subset \mathbb{R}^n$ there exist convex open subsets $U_1, \ldots, U_k \subset V, k = k(n,V)$ (w.r.t. induced topology on $V$), mutually disjoint $U_i \cap U_j = \emptyset$ for $i \neq j$ with everywhere dense union $\bigcup_{U_i} = V$ ($X$ denotes a closure of $X$ w.r.t. the ambient topology), such that for any $\xi \in \Xi_n$ and $i \leq k$ holds $L(z, \xi)|_{U_i} \equiv \text{const(i, } \xi, V);$  
- **Jumps regularity:** By reusing $U_i$ defined above, for any $z \notin \bigcup_{U_i}$ either of the following holds:  
  $$
  \lim_{z' \to z} L(z', \xi) < L(z, \xi) \leq \lim_{z \to z} \sup L(z', \xi),
  $$
  $$
  \lim_{z' \to z} L(z', \xi) = L(z, \xi) = \lim_{z \to z} \sup L(z', \xi),
  $$
  where $z'$ means $z' \notin \bigcup_{U_i}, z' \to z$.
- **Scalar freeness:** For any $n > 0, \xi \in \Xi_n, z \in \mathbb{R}^n, \lambda > 0$ holds $L(\lambda z, \xi) = L(z, \xi)$.

We denote the class of all SF discrete loss functions by $\mathcal{R}_0$. Informally speaking, $\mathcal{R}_0$ is a class of bounded discrete functions on a sphere. The jumps regularity property is needed to exclude breaking points from $\arg \min L$. It is easy to see that all loss functions defined in Section 3.1, including the LSO loss DCG-RR, belong to $\mathcal{R}_0$.

Our method out-of-box can be applied to any SF discrete loss function. However, to guarantee a global convergence, we need to use a consistent smoothing (see Section 4.3), which has to be chosen based on properties of a particular metric. We developed a general solution for the whole class of ranking loss functions which we now define.

Assume that $\Xi_n = \mathbb{R}^n \times \Xi_n'$ and $\xi \in \Xi_n$ is a tuple $(r, \xi')$, where $r \in \mathbb{R}^n$ is a vector of relevances. As discussed in Section 2, a particular definition of a ranking loss depends on tie resolution. When some documents have equal scores, we may either use the worst permutation (the choice commonly adapted in practice) or compute the average over all orderings (the option usually assumed by LTR algorithms).

The definition below assumes the worst permutation.

**Definition 2.** A function $L(z, \xi) \in \mathcal{R}_0$ is a Ranking Loss Function iff the following properties hold:

- **Relevance monotones:** For each $n > 0$ and $z, r \in \mathbb{R}^n, \xi \in \Xi_n$, there exists $\epsilon_1 > 0$ such that $\forall \epsilon \in (0, \epsilon_0)$:
  $$
  \exists \delta = \delta(\epsilon, r, z > 0) > 0 \text{ such that } \forall z' : ||z' - z|| < \delta
  $$
  $$
  \lim_{z' \to z} L(z'', \xi) = L(z' - cr, \xi).
  $$
  $\text{Informally, } -r \text{ is the worst direction for the loss function, i.e., near a breaking point with } z_i = z_j \text{ but } r_i > r_j \text{ for some } i, j, \text{ it is better to have } z_i > z_j.$
- **Strong upper semi-continuity (s.u.s.c.):** For each $n > 0$ and $z, r \in \mathbb{R}^n$:
  $$
  \lim_{z' \to z} L(z', \xi) = L(z, \xi).
  $$
  $\text{Informally, this means that if do not know how to rank two items (i.e., } z_i = z_j \text{ for } i \neq j \text{, then we shall rank them by placing the worst one by the relevance first.}$
- **Translation invariance:** For any $n > 0, r, z \in \mathbb{R}^n, \lambda, \xi \in \Xi_n$:
  $$
  \lambda \in \mathbb{R} \text{ holds: } L(z + \lambda \xi, \xi) \equiv L(z, \xi), \text{ where } \xi := (1, \ldots, 1) \in \mathbb{R}^n.
  $$
- **Pairwise decision boundary:** Partition of the space for discreteness on subspaces $\{U_i\}$ for $\mathbb{R}^n$ can be obtained as connected components of $\mathbb{R}^n \setminus \bigcup_{i,j} \{z : z_i - z_j = 0\}$, similarly for an arbitrary subspace $V$.

We denote this class of functions by $\mathcal{R}_1$. It is easy to see that $\mathcal{R}_1$ includes all ranking losses defined in Section 3.1, but not the LSO loss DCG-RR.

Let us now define a class $\mathcal{R}_{1,\text{opt}}$, where instead of the worst ranking for ties, we consider the expected loss of a random ranking. For this, we replace the s.u.s.c. condition by:

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1This property is assumed only to be consistent with the learning to rank literature and can be omitted.

2This condition can also be removed, but it simplifies the analysis of smoothing bias.
1983
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of the ap-

We will show that under some restrictive conditions (that are commonly assumed in the LTR literature), it does not matter which of the two definitions we use (\(R_1\) or \(R_{1\text{soft}}\)) as they coincide almost surely and have equal \(\arg\ min\ L\) sets. However, we will explain why these conditions do not hold in practice and in general the minimizers for \(R_1\) and \(R_{1\text{soft}}\) do not coincide.

3.3. Model assumptions

We assume that for each \(n > 0\) and \(\xi \in \Xi_n\) there is a model \(f_\xi(\theta) : \mathbb{R}^m \to \mathbb{R}^n\) such that \(f_\xi(\theta) = \Phi_\xi\theta\) for some matrix \(\Phi_\xi \in \mathbb{R}^{m \times n}\), where \(m \in \mathbb{N}\) denotes the number of parameters of the model (i.e., \(\theta\) is independent from \(\xi\)). Typically, each row of \(\Phi_\xi\) is a feature vector. Gradient boosting over decision trees satisfies this assumption. Indeed, let us consider all possible trees of a fixed depth formed by a finite number of binary splits that obtained by binarization of the initial feature vectors. To get a linear model, we say that \(\theta\) is a vector of leaf weights of these trees and \(\Phi_\xi\) is a binary matrix formed by binarized feature vectors.

We will also assume that \(\langle 1_n, z \rangle_2 = 0\). Indeed, instead of \(z = f_\xi(\theta)\) we can define the model as \(z = f_\xi(\theta) - \frac{1}{\lambda} \Phi_\xi T f_\xi(\theta) 1_n\), which is equivalent due to the translation invariance property.

3.4. Data Distribution

Assume that we are given some distribution \(\xi \sim D\) on \(\Xi := \bigoplus_{n>0} \Xi_n\) meaning that \(\xi\) also incorporates information about the number of items \(n\) implicitly, i.e., for \(\xi \in \Xi\) there exists a unique number \(n > 0\) so that \(\xi \in \Xi_n\). \(D\) is some unknown distribution, e.g., the distribution of queries submitted to a search system. We are given a finite i.i.d. sample \(\xi_1, \ldots, \xi_N \sim D\) that corresponds to the train set. We denote by \(D_N := \frac{1}{N} \sum_{i=1}^N \delta_{\xi_i}\), the empirical distribution.

3.5. Optimization target

Assumptions and definitions above allow us to define the expected (generalized) ranking quality for the function \(L \in \mathcal{R}_0\) with respect to \(\xi \sim D\) and model parameters \(\theta \in \mathbb{R}^m\): 
\[
\mathcal{L}(\theta) := \mathbb{E}_{\xi \sim D} L(f_\xi(\theta), \xi) .
\]

The reason for why it is possible lies within stability of global minimizers even for discontinuous functions as for \(N \gg 1\) an almost minimizer of \(\mathcal{L}(\theta)\) should be an almost minimizer of \(\mathcal{L}(\theta)\) (Arstein & Wets, 1999).

Thus, we need to find a global minimizer of \(\mathcal{L}_N\). Due to the discrete structure, we can ignore sets with zero Lebesgue measure. Recall that essential infimum (ess inf) is infimum that ignores the sets of zero measure and \(\text{int} U\) denotes an open interior of the set \(U\).

**Definition 3.** For any function \(\mathcal{L}(\theta) : \mathbb{R}^m \to \mathbb{R}\) with \(\mathcal{L}_* := \text{ess inf}_{\theta \in \mathbb{R}^m} \mathcal{L}(\theta) > -\infty\) define the set: \(\text{arg min} \mathcal{L}(\theta) := \text{int} \{\theta \in \mathbb{R}^m : \mathcal{L}(\theta) = \mathcal{L}_*\}\).

We need this unusual definition because of the discrete structure of our loss: we want to exclude breaking points from \(\text{arg min}\). One can see that despite \(L(\cdot, \cdot)\) satisfies Jumps regularity, the function \(\mathcal{L}_N(\theta)\) does not have to.

**Statement 1.** The set \(\text{arg min}_{\theta \in \mathbb{R}^m} \mathcal{L}_N(\theta)\) is not empty.

The proof is straightforward (see Section A of the appendix).

4. Stochastic smoothing

4.1. Smoothing of scores

Discrete structure of ranking loss functions prevents their effective optimization. Hence, some smoothing is needed and a natural approach for this is mollification (Ermoliev et al., 1995; Dolecki et al., 1983), i.e., adding randomness to parameters. We refer to Section B.1 of the appendix for the formal definition and the reasons why this approach is not applicable in our case. Thus, instead of acting on the level of parameters \(\theta\), we act on the level of scores \(z: L^z_\xi(z, \sigma) := \mathbb{E} L(z + \sigma \varepsilon, \xi)\), where \(\sigma \varepsilon\) has p.d.f. \(\sigma^{-n} \pi(\sigma^{-1} z)\). After that we compose \(\mathbb{E} L(f(\theta) + \sigma \varepsilon, \xi)\). We multiply the noise by \(\sigma\) to preserve Scalar-Freeness in a sense that \(L^z_\xi(\lambda z, \lambda \sigma) = L^z_\xi(z, \sigma) \forall \lambda > 0\).

In the linear case \(f(\theta) = \Phi \theta\), if \(\text{rk} \Phi = n\), it is not hard to show the convergence of minimizers. However, in general, we cannot assume \(\text{rk} \Phi = n\). In particular, this property is violated in the presence of ties which always occur in gradient boosting due to its discrete nature. As a result, a smoothing bias is induced that alters the set of minimizers.
4.2. Simple Example of Smoothing Bias

Within this section, for simplicity we assume that we are dealing with one function $L(z) := L(z, \xi) : \mathbb{R}^n \to \mathbb{R}$ for some arbitrary fixed $n$ and $\xi \in \Xi_n$. Denote $\Phi = \Phi_\xi \in \mathbb{R}^{m \times n}$ and $L(\theta) := L(\Phi_\theta)$. To clearly see how the smoothing bias is introduced, consider the case when $\text{im} (\Phi) \subset \mathbb{R}^n \setminus \cup_{i=1}^M U_i$ where $U_i$ is from the Discreteness on subspaces assumption for $V = \mathbb{R}^n$. Denote by $c_1, \ldots, c_k \in \mathbb{R}$ the values of $L(z)$ on the corresponding subsets $U_i$. Consider the functions $L(\theta)$ and $L^e(\theta) := \lim_{\sigma \to 0} \|z(\Phi_\theta + \sigma e)\|_2$. The value of $L^e(\theta)$ is fully determined by $\pi$, $c_1, \ldots, c_k$ and the subsets $U_1, \ldots, U_k$ in the following way: $L^e(\theta) = \sum_i \alpha_i c_i$, where $\alpha_i = \alpha_i(\pi, \theta, U_1, \ldots, U_k) = \lim_{\sigma \to 0} \|z(\Phi_\theta + \sigma e)\|_2(\pi, \sigma, U_i)$, $\alpha_i \geq 0$, $\sum_i \alpha_i = 1$.

In contrast, the value $L(\theta)$ depends on the values $c_1, \ldots, c_k$ much weaker: for fixed $\pi$ consider the values $c_1', \ldots, c_k'$, that corresponds to $U_i$ such that $\Phi_\theta \in U_i$, then the only limitation we have is $\min c_i' < L(\theta) \leq \max c_i'$. This is required by Jumps regularity), which clearly allows more flexibility than the linear combination defined above.

In LTR, the issue of smoothing bias is connected to the problems of ties: the situation when $z_i = z_j$ and $r_i \neq r_j$ is often called a tie.

4.3. Consistent smoothing

**Definition 4.** We say that the family of distributions $\pi_\xi(z) : \prod_{n>0} \mathbb{R}^n \times \Xi_n \to \mathbb{R}^+$ is a consistent smoothing for $L(z, \xi) \in \mathcal{R}_0$ and for model $f_\xi$ iff for each $n > 0$, $\xi \in \Xi_n$ the following limit holds almost surely locally uniform in $\theta$: $L(f_\xi(\theta), \xi) = \lim_{\sigma \to 0} L^{\xi}_{\xi}(f_\xi(\theta), \sigma)$.

If $\pi$ is smooth enough and consistent, then the function $L^{\xi}_{\xi}(\theta, \sigma) := \frac{1}{N} \sum_{i=1}^N L^{\xi}_{\xi}(f_\xi(\theta), \sigma)$ is also smooth and almost surely locally uniformly approximates the discrete loss $L_N(\theta)$ as $\sigma \to 0$.

To optimize ranking losses, it is important to find a consistent smoothing $\pi$ for functions in $\mathcal{R}_1$. Fortunately, we can do this with an arbitrary precision by shifting the normal distribution by $-\mu r$ for large enough $\mu$. Relevance monotones ans s.u.s.c. imply the following pointwise limit: $L(z, r) = \lim_{\mu \to \infty} \lim_{\sigma \to 0} \mathbb{E}_{z \sim N(-\mu r, \sigma I)} L(z + \sigma e, \xi)$.

This can be strengthened to the following theorem, which is proven in Section B.2 of the appendix.

**Theorem 1.** $\pi_{1, \mu, 0} = N(-\mu r, I_n)$ is a consistent smoothing for $\mathcal{R}_1$ as $\mu \to \infty$. Formally, $\forall \theta$ except zero measure $\exists \delta > 0 \forall \epsilon > 0 \exists \mu > 0 \exists \sigma_0 > 0$ such that $\forall \sigma \in (0, \sigma_0)$ and $\forall \theta : \|\theta - \theta'\| < \delta$ holds $|L^{\xi}_{\xi}(f_\xi(\theta'), \sigma) - L^{\xi}_{\xi}(f_\xi(\theta'), \xi)| < \epsilon$.

By similar arguments, one can show that $N(0, I_n)$ is a consistent smoothing for $\mathcal{R}_1^{\mu, 1}$. Note that in both cases the consistent smoothing is universal for the entire class ($\mathcal{R}_1^{\mu, 1}$), i.e., it is independent from the choice of $f$. Thus, LTR problems require non-trivial smoothing to preserve consistency. However, under some restrictive assumptions on the loss and on the model, any smoothing $\pi$ is consistent. Recall that $L_N(\theta) = \frac{1}{N} \sum_{i=1}^N L(\Phi_\xi, \theta, \xi)$ and assume $L(z, \xi) \in \mathcal{R}_0$. The following theorem is proven in Section B.3 of the appendix.

**Theorem 2.** Consider open and convex subsets $U_i := U_i \cap \text{im} \Phi_\xi$. If $\forall i \exists j$ s.t. $U^i_j \neq 0$ and $\bigcup_i U^i = \text{im} \Phi_\xi$, then any smoothing $\pi$ is consistent for $L_N(\theta)$.

In early literature on LTR, all authors used such conditions implicitly by assuming that predictions for all items are different. In contrast, we do not assume this as it never holds in practice (e.g., when two documents have equal features). As a result, in existing approaches, a smoothing bias is present in the LTR case, in contrast to, e.g., the LSO case (see the discussion in Section B.4).

4.4. Scale-Free Acceleration

It is intuitively clear that for a scale-free function it is better to have a scalar-free approximation. However, for each $\lambda > 0$ we have $L^{\xi}(\lambda z, \sigma) = L^{\xi}(z, \lambda^{-1} \sigma)$, i.e., the smoothed function is no longer scale-free. To enforce scale-freeness, we take a vector $z'$ with $\|z'\|_2 > 0$ and define $L^{\xi}(\lambda z, \sigma|z') := L^{\xi}_{\xi} \left( z', \frac{\|z\|_2}{\|z'\|_2} \sigma \right)$.

Such smoothing we call Scale-Free Acceleration (SFA). The obtained function is indeed scale-free: $L^{\xi}_{\xi}(\lambda z, \sigma|z') \equiv L^{\xi}_{\xi}(z, \sigma|z') \forall \lambda > 0$.

Denote $\tilde{\sigma}(z) := \left( \frac{\|z\|_2}{\|z'\|_2} \right) \sigma$. In our optimization, we will be interested only in the case when $z' = z_i$ is the vector of predictions obtained on $t$-th iteration of the optimization algorithm. So, we have $\tilde{\sigma}(z_i) = \sigma$. Hence, SFA does not change the scale $\sigma$.

One can imagine a sphere of radius $R = \|z'\|_2$, where we restrict $L^{\xi}_{\xi}(z, \sigma)$ and homogenize it along the rays from the origin to infinity to obtain a scalar-free function.

4.5. Smoothing properties

Finally, let us place some regularity assumptions on $\pi$ on which our optimization method relies. Consider a family of distributions with p.d.f. $\pi_\xi(z)$ with $\xi \in \Xi_n$ for some $n > 0$, $z \in \mathbb{R}^n$. We place the following assumptions on $\pi_{\xi}(z)$:
• Continuous differentiability: \( \pi_{\xi}(z) \) is \( C^{(1)}(\mathbb{R}^n) \), i.e., is differentiable with a continuous derivative.

• Uniformly bounded derivative: \( \forall n \in \mathbb{N}, \forall \xi \in \Xi_\alpha \) we have \( \| \nabla_z \pi_{\xi} \|_2 = O(1) \) uniformly in \( z \in \mathbb{R}^n \).

• Derivative Decay: \( \forall n \in \mathbb{N} \) we have \( \| \nabla_z \pi_{\xi} \|_2 = O(\|z\|_2^{-n+2}) \) as \( \|z\|_2 \rightarrow \infty \).

• Tractable conditional expectations: conditional densities \( \pi_{\xi}^j(z_j) := \pi_{\xi}(z_1, \ldots, z_j) \) are easy to compute.\(^3\)

Clearly, \( \mathcal{N}(-\mu_r, I_N) \) satisfies these assumptions \( \forall \mu \geq 0 \).

5. Coordinate Conditional Sampling

5.1. Gradient Estimate

In the previous section, we required that we can easily compute \( \pi_{\xi}^j(z_j) \). This property allows us to do the following trick: we decompose \( \pi_{\xi}(z) = \pi_{\xi}(z_j) \pi_{\xi}(z_{\bar{j}}) \) with \( \pi_{\xi}(z_{\bar{j}}) \) being the marginal distribution for \( z_{\bar{j}} \). Then, we can represent \( \mathcal{L}_{\xi}(z, \sigma) = \mathcal{L}_{\xi}^j \pi_{\xi}^j \pi_{\xi}^{\bar{j}} \). Note that convolution is an associative operation that commutes with differentiation and, henceforth,

\[
\frac{\partial}{\partial z_j} \mathcal{L}_{\xi}(z, \sigma) = \left( \frac{\partial}{\partial z_j} \mathcal{L}_{\xi}^j \pi_{\xi}^j \right) \pi_{\xi}^{\bar{j}}.
\]

Note that we differentiate by \( z_j \), the convolution by the same \( z_j \). So, if we want to estimate the gradient unbiasedly, we need to sample \( \varepsilon_{j, \bar{j}} \sim \pi_{\xi}^{\bar{j}} \) and then compute exactly 

\[
\left( \frac{\partial}{\partial z_j} \mathcal{L}_{\xi}^j \pi_{\xi}^j \right) ((z_j, z_{\bar{j}} + \varepsilon_{j, \bar{j}})).
\]

The resulting estimate would be unbiased by construction. The following lemma suggests how to deal with \( \frac{\partial}{\partial z_j} \mathcal{L}_{\xi}^j \pi_{\xi}^j \). For \( \mathcal{L}_{\xi}^j \) the above formula becomes:

\[
\frac{\partial}{\partial z_j} \mathcal{L}_{\xi}^j(z, \sigma) = -\sigma^{-1}.
\]

\[
\mathbb{E}_{\varepsilon_{j, \bar{j}} \sim \pi_{\xi}^{\bar{j}}} \sum_{s=1}^{k'} \Delta l_j(b_s) \pi_{\xi}^j(\sigma^{-1}(b_s - z_j)),
\]

where \( k' \) and \( b_s = b_s(z_{\bar{j}} + \sigma \varepsilon_{j, \bar{j}}) \) are from Lemma 1.

Corollary 1. For LTR the above formula becomes:

\[
-\sigma^{-1}, \mathbb{E}_{\varepsilon_{j, \bar{j}} \sim \pi_{\xi}^{\bar{j}}} \sum_{s=1}^{k'} \Delta l_j(z_s + \sigma \varepsilon_s) \pi_{\xi}^j(\sigma^{-1}(z_s - z_j) + \varepsilon_s).
\]

Uniform boundedness of \( \Delta l_j \) and \( \pi \) implies the following.

Statement 2. The estimate is uniformly bounded by \( O(\sigma^{-1}) \).

Proceeding analogously with each coordinate \( j \in \{1, \ldots, n\} \), we obtain an unbiased estimate of \( \nabla_z \mathcal{L}_{\xi}^j(z, \sigma) \) that is uniformly bounded, in contrast to the obvious estimate \( \mathcal{L}(z + \sigma \varepsilon) - \mathcal{L}(z) \varepsilon \) (Nesterov & Spokoiny, 2017) obtained by the log-derivative trick for the normal distribution that is also known as REINFORCE (Williams, 1992). Uniform boundedness is crucial since without it we would not be able to claim the global convergence. We call such estimate Conditional Coordinate Sampling (CCS) and denote it by \( \nabla_{\text{CCS}} \mathcal{L}_{\xi}^j(z, \sigma) \).

Note that for each coordinate when estimating \( \nabla_{\text{CCS}} \mathcal{L}_{\xi}^j(z, \sigma) \) we use the shared noise vector \( \varepsilon \sim \pi_{\xi} \), i.e., the components of the gradient can have non-trivial covariation, but due to the uniform boundness the covariation is also uniformly bounded by \( O(\sigma^{-1}) \).

5.2. SFA Gradient Estimate

It is not hard to generalize CCS to SFA. In Section C.4 of the appendix we derive the following theorem.

Theorem 3. The derivative \( \frac{\partial}{\partial z_j} \mathcal{L}_{\xi}^j(z, \sigma) \) is equal to:

\[
-\sigma^{-1}, \mathbb{E}_{\varepsilon_{j, \bar{j}} \sim \pi_{\xi}^{\bar{j}}} \sum_{s=1}^{k'} \Delta l_j(b_s) \pi_{\xi}^j(\sigma^{-1}(b_s - z_j)),
\]

where \( k' \) and \( b_s = b_s(z_{\bar{j}} + \sigma \varepsilon_{j, \bar{j}}) \) are from Lemma 1.

Corollary 2. Unbiased CCS estimate for SFA can be obtained by orthogonalizing \( \nabla_{\text{CCS}} \mathcal{L}_{\xi}^j(z, \sigma) \) and \( z \).

Since orthogonalization reduces the norm of the estimate, it is necessarily reduces the variance, so we obtain the following corollary.

Corollary 3. SFA CCS estimate has lower variance than original CCS.

The intuition for orthogonalization is based on Scalar-freeness: the function \( L(z, \xi) \) does not change along \( z \) direction, so the direction \( z \) in the gradient \( \nabla_z \mathcal{L}_{\xi}^j \) does not contribute to \( \hat{L}(z, \xi) \) optimization.
As we need to deal with possibility of \( z = z' = 0 \), we introduce a parameter \( \nu > 0 \) and replace \( \|z\|_2 \) by \( \|z\|_2 + \nu \):

\[
\hat{\nabla}_{CC} L^\gamma_F(z, \sigma | z', \nu) := \hat{\nabla}_{CC} L^\gamma_F(z, \hat{\sigma}) - \left\langle \hat{\nabla}_{CC} L^\gamma_F(z, \hat{\sigma}), \|z\|_2 + \nu / 2 \right\rangle.
\]

**Lemma 2. Bias of SFA CCS estimate is uniformly bounded**

\[
|\mathbb{E}\hat{\nabla}_{CC} L^\gamma_F(z, \sigma_0 | z', \nu) - \nabla_{CC} L^\gamma_F(z, \hat{\sigma})| = O\left(\frac{1}{\|z\| + \nu}\right).
\]

As a consequence, if \( \nu \to \infty \) or \( \|z\| \to \infty \) then the estimate asymptotically unbiased.

Thus, for convergence analysis we consider only \( \hat{\nabla}_{CC} L^\gamma_F(z, \sigma) \) since the estimate \( \hat{\nabla}_{CC} L^\gamma_F(z, \sigma_0 | z', \nu) \) can be made unbiased by varying parameter \( \nu > 0 \). In practice, we consider \( \hat{\nabla}_{CC} L^\gamma_F(z, \sigma_0 | z', \nu) \) with fixed \( \nu = 10^{-2} \) as we observed that this parameter performs well enough. Moreover, SFA can be seen as bias-variance trade-off controlled by \( \nu > 0 \) for CCS estimate of \( \nabla_{CC} L^\gamma_F(z, \sigma) \). For practical comparison of \( \hat{\nabla}_{CC} L^\gamma_F(z, \sigma) \) and \( \hat{\nabla}_{CC} L^\gamma_F(z, \sigma_0 | z', \nu) \) see Section 7, where we show that SFA gives a significant improvement.

**6. Global Optimization by Diffusion**

6.1. SGLB

Previously, we discussed the importance of global optimization of \( \mathcal{L}_N(\theta) \). As we will show in this section this can be achieved by global optimization of smoothed \( \mathcal{L}^\gamma_N(\theta, \sigma) \) for \( \sigma = 1 \) if smoothing is consistent using the recently proposed Stochastic Gradient Langevin Boosting (SGLB) (Ustimenko & Prokhorenkova 2020). SGLB is easy to apply: essentially, each iteration of standard SGB is modified via model shrinkage and adding Gaussian noise to gradients. However, the obtained algorithm is backed by strong theoretical results, see Ustimenko & Prokhorenkova (2020) for the details and the appendix (Section E.1) for a brief sketch. The global convergence is implied by the fact that as \( t \to \infty \), the stationary distribution \( p_\beta(F) \) of the predictions \( F = (f_{E_1}(\theta), \ldots, f_{E_N}(\theta)) \) concentrates around the global optima of implicitly regularized loss

\[
\mathcal{L}^\gamma_N(F, \sigma, \gamma) = \mathcal{L}_N^\gamma(F, \sigma) + \frac{\gamma}{2} \|F\|_2^2,
\]

where \( \Gamma \) is implicitly defined regularization matrix. More formally, \( p_\beta(F) \propto \exp\left(-\beta \mathcal{L}^\gamma_N(F, \sigma, \gamma)\right) \).

Global convergence of SGLB requires Lipshitz smoothness and continuity (Ustimenko & Prokhorenkova, 2020). We can ensure this for the entire \( \mathcal{T}_0 \), which allows us to claim the following theorem (see Section E.2 for the proof).

**Theorem 5.** SGLB method applied to \( \mathcal{L}^\gamma_N(F, \sigma) \) converges globally to the optima of \( \mathcal{L}_N(F) \equiv \mathcal{L}_N(\theta) \) when used with CCS estimate.

The following statement ensures that we can safely fix \( \sigma = 1 \) and fit only \( \gamma \) parameter, and we would not lose any possible solution.

**Statement 3.** \( \mathbb{E}_{F \sim p_\beta} \mathcal{L}_N(F) = \mathbb{E}_{F' \sim p'_\beta} \mathcal{L}_N(F') \), where \( p_\beta \) corresponds to \( (\sigma, \gamma) \) and \( p'_\beta \) to \( (1, \sigma^{-2} \gamma) \).

**Proof.** Due to Scalar-freeness, we can write \( \mathcal{L}_N(F, \sigma) \equiv \mathcal{L}_N(\sigma^{-1} F, 1) \) and \( \frac{\gamma}{2} \|F\|_2^2 \equiv \frac{\gamma^2}{2} \|\sigma^{-1} F\|_2^2 \). Finally, due to Scalar-freeness, the change \( F' = \sigma^{-1} F \) does not change the value of \( \mathcal{L}_N(F) \equiv \mathcal{L}_N(F') \) and thus the expectation does not change. \( \square \)

6.2. Generalization

Ustimenko & Prokhorenkova (2020) related the generalization gap with the uniform spectral gap parameter \( \lambda_* \geq 0 \) for the distribution \( p_\beta(\theta) := \frac{\exp(-\beta \mathcal{L}(\theta, \sigma, \gamma))}{\int_{\mathcal{T}} \exp(-\beta \mathcal{L}(\theta, \sigma, \gamma)) d\theta} \) (see Raginsky et al. (2017) for the definition of uniform spectral gap). Here \( p_\beta(\theta) \) represents the limiting (as learning rate goes to zero) distribution of the parameters vector \( \theta \) and is induced by the distribution \( p_\beta(F) \propto \exp(-\beta \mathcal{L}(F, \sigma, \gamma)) \) using the relation \( F = \Phi(\theta) \). The following theorem is proven in the appendix.

**Theorem 6.** The generalization gap \( \|\mathbb{E}_{\theta \sim p_\beta(\theta)} \mathcal{L}^\gamma(\theta, \sigma) - \mathbb{E}_{\theta \sim p_\beta(\theta)} \mathcal{L}_N^\gamma(\theta, \sigma)\| \) can be bounded by:

\[
O \left( (\beta + 2d + \frac{d^2}{\beta}) \exp(O(\frac{\beta}{\gamma^2 N})) \right).
\]

7. Experiments

**Datasets** For our experiments, we use the following publicly available data sets. First, we use the data from YAHOO! Learning to Rank Challenge (Chapelle & Chang, 2010): there are two datasets, each is pre-divided into training, validation and testing parts. The other datasets are WEB10K and WEB30K released by Microsoft (Qin & Liu, 2013). Following (Wang et al., 2018), we use Fold 1 for these two datasets.

**Metrics** The first metric we use is NDCG@5, which is very common in LTR research. The second one is MRR, which is a well-known click-based metric. Recall that MRR requires binary labels, so we binarize each label by \( \bar{y}_i := \mathbb{1}_{\{y_i > 0\}} \). Notably, while MRR is frequently used in online evaluations, it is much less studied compared to NDCG@k and there are no effective approaches designed for it. Fortunately, our method can be easily adapted to any ranking metric via a combination of SGLB with Coordinate Conditional Seeded smoothing by Gaussian noise.
Baselines As baseline approaches, we consider the well-known LambdaMART framework optimized for NDCG@k (Wu et al., 2010), NDCG-Loss2++ from LambdaLoss framework (Wang et al., 2018), and SoftRank (Taylor et al., 2008). As in (Wang et al., 2018), we set the parameter \( \mu \) to be equal to 5 for NDCG-Loss2++. According to our experiments, NDCG-Loss2++ performed significantly better than NDCG-Loss2, which agrees (Wang et al., 2018).

Framework We implemented all approaches in CatBoost, which is an open-source gradient boosting library outperforming the most popular alternatives like XGBoost (Chen & Guestrin, 2016) and LightGBM (Ke et al., 2017) for various tasks (Prokhorenkova et al., 2018). LambdaMART can be easily adapted for optimizing MRR, so we implemented both versions. In contrast, LambdaLoss is specifically designed for NDCG and cannot be easily modified for MRR. For SoftRank we used CCS to estimate gradients, since the original computation and memory demanding approach is infeasible in gradient boosting, which requires all gradients to be estimated at each iteration.

Parameter tuning For all algorithms, we set the maximal number of trees to 1000. We tune the hyperparameters using 500 iterations of random search and select the best combination according to the validation set, the details are given in the appendix (Section F).

Results The results are shown in Table 1. One can see that StochasticRank (SR-\( R_1^{soft} \)) outperforms the baseline approaches on all datasets. In all cases, the difference with the closest baseline is statistically significant with p-value < 0.05 measured by the paired one-tailed z-test. Also, in most of the cases, SR-\( R_1^{soft} \) outperforms SR-\( R_1^{soft} \), which clearly demonstrates the advantage of unbiased smoothing, which takes into account tie resolution policy, over standard smoothing approaches.

In Table 2, we show the improvement we get from each feature of our algorithm using the Yahoo datasets and NDCG metrics. We see that CCS is significantly better than REINFORCE, while SFA gives an additional significant performance boost. SGLB and consistent smoothing further improve NDCG. We note that for both REINFORCE and CCS we use one sample per gradient estimation since the most time consuming operation for both estimates is sorting (see Section D of the appendix for fast evaluation of CCS).

### Table 1. Experimental results

| Method      | Data set     | NDCG@5 | MRR  |
|-------------|--------------|--------|------|
| \( \lambda \)-MART | Yahoo Set 1 | 74.53  | 90.21|
| \( \lambda \)-Loss | Yahoo Set 1 | 74.73  | -    |
| SoftRank    | Yahoo Set 1 | 71.98  | 90.17|
| SR-\( R_1^{soft} \) | Yahoo Set 1 | 74.68  | 91.07|
| SoftRank    | Yahoo Set 2 | 72.08  | 92.72|
| SR-\( R_1^{soft} \) | Yahoo Set 2 | 73.95  | 93.16|
| \( \lambda \)-MART | WEB10K | 48.22  | 81.85|
| \( \lambda \)-Loss | WEB10K | 48.33  | -    |
| SoftRank    | WEB10K      | 42.82  | 81.38|
| SR-\( R_1^{soft} \) | WEB10K | 48.19  | 83.08|
| SoftRank    | WEB30K      | 43.46  | 82.73|
| SR-\( R_1^{soft} \) | WEB30K | 49.59  | 85.01|

### Table 2. Comparison of the algorithm’s features on Yahoo Set 1

| Features | NDCG@5 |
|----------|--------|
| REINFORCE| 70.74  |
| CCS      | 71.89  |
| CCS+SFA  | 74.55  |
| CCS+SFA+SGLB (SR-\( R_1^{soft} \)) | 74.68 |
| CCS+SFA+SGLB+\( \pi_\mu \) (SR-\( R_1 \)) | 74.92 |

Using XGBoost and LightGBM (Ke et al., 2017) for various tasks (Prokhorenkova et al., 2018). LambdaMART can be easily adapted for optimizing MRR.

On Yahoo Set 1, NDCG-Loss2++ (R-\( R_1^{soft} \)) outperforms the closest baseline (SR-\( R_1^{soft} \)), which clearly demonstrates the advantage of unbiased smoothing, which takes into account tie resolution policy, over standard smoothing approaches.

In Table 2, we show the improvement we get from each feature of our algorithm using the Yahoo datasets and NDCG metrics. We see that CCS is significantly better than REINFORCE, while SFA gives an additional significant performance boost. SGLB and consistent smoothing further improve NDCG. We note that for both REINFORCE and CCS we use one sample per gradient estimation since the most time consuming operation for both estimates is sorting (see Section D of the appendix for fast evaluation of CCS).

### 8. Conclusion

In this paper, we proposed the first truly direct LTR algorithm. We formally proved that this algorithm converges globally to the minimizer of the target loss function. This is possible due to the combination of three techniques: unbiased smoothing for consistency between the original and smooth losses, SGLB for global optimization via gradi-

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| CCS+SFA+SGLB+\( \pi_\mu \) (SR-\( R_1 \)) | 74.92 |
ent boosting, and CCS gradient estimate with uniformly bounded error and low variance, which is required for SGLB to be applied. Our experiments clearly illustrate that the new algorithm outperforms state-of-the-art LTR methods.

Appendix

A. Proof of Statement 1

Let us prove that the set arg minθ∈ℝm L_N(θ) is not empty. Consider U_{ij} being open and convex sets for V_i = imΦ_{ξ_i} (see Discreteness on subspaces in Definition 1 in the main text). Then, we have that U'_{ij} = Φ^{-1}_{ξ_i}U_{ij} ⊂ ℝ^m are also open and convex. Henceforth, the function L_N can be written as (ignoring the sets of zero measure):

L_N(θ) = N^{-1} \sum_{j_1=1}^{k_1} \cdots \sum_{j_N=1}^{k_N} c_{j_1,\ldots,j_N} Φ_{\theta} \cap \bigcap_{i=1}^{N} U'_{ij_i}.

Henceforth, the function L_N is also discrete with open convex sets U_ξ := \bigcap_{i=1}^N U'_{ij_i} on the whole space ℝ^m; henceforth, its arg min is one of these sets or their union.

B. Stochastic smoothing

B.1. Mollification

A natural approach for smoothing is mollification (Ermoliev et al., 1995; Dolecki et al., 1983): choose a smooth enough distribution with p.d.f. π(θ), consider the family of distributions π_δ(θ) = δ^{-m}π(δ^{-1}θ), and let L_N(θ, δ) := L_N * π_δ := E_{ξ \sim π} L_N(θ + δξ). Then, the minimizers’ of L_N(θ, δ) convergence to one of L_N(θ). Unfortunately, despite theoretical soundness, it is hard to derive efficient gradient estimates even in the linear case f_{ξ}(θ) = Φ_{ξ}, θ. Moreover, in the gradient boosting setting, we do not have an access to all possible coordinates of θ at each iteration. Henceforth, we cannot use mollification approach directly.

Thus, instead of acting on the level of parameters θ, we act on the level of scores z: L^N_{ξ}(z, σ) := zL(z + σξ, ξ), where σ has p.d.f. σ^{-m}π(σ^{-1}z). After that, we compose E_L(f(θ) + σξ, ξ). We multiply the noise by σ to preserve Scalar-Freeness in a sense that L^N_{ξ}(ξ, σ) = L^N_{ξ}(ξ, σ) ∀λ > 0.

In the linear case f(θ) = Φθ, if rkΦ = n, it is not hard to show the convergence of minimizers. Indeed, we can obtain mollification by "bypassing" the noise from scores to parameters by multiplying on Φ^{-1}. However, in general, we cannot assume rkΦ = n.

B.2. Proof of Theorem 1

The trick is to proceed with L(f_{ξ}(θ), ξ_i) and to show that there exists an open and dense set U_{ξ_i} ⊂ ℝ^m such that the convergence is locally uniform as σ → 0, μ → ∞, σμ → 0.

Let us proceed with proving the existence of such U_{ξ_i}∀i. Let us define

U_{ξ_i} := \{θ ∈ ℝ^m : ∀j \neq j' (f_{ξ_i}(θ)_j = f_{ξ_i}(θ)$_{j'}$) ⇒ ∀θ' ∈ ℝ^m (f_{ξ_i}(θ')_j = f_{ξ_i}(θ')$_{j'}$) \}.

Clearly, the set is not empty, open and dense. Now, take an arbitrary θ ∈ U_{ξ_i}. Consider z = f_{ξ_i}(θ) and divide the set {1, …, n_i} into disjoint subsets J_1, …, J_k such that all components z_j corresponding to one group are equal and all components z_j corresponding to different J’s are different. Clearly, we need to “resolve” only those which are equal: for small enough σ ≈ 0, σμ ≈ 0 we obtain that even after adding the noise f_{ξ_i}(θ’) − σμ + σξ the order of J’s is preserved with high probability uniformly in some vicinity of θ, whilst for large enough μ ≳ 1 we obtain the worst case permutation of z_j corresponding to the one group with high probability uniformly on the whole U_{ξ_i}. Thus, we obtain locally uniform convergence E_L(f_{ξ_i}(θ) −
B.3. Proof of Theorem 2

Clearly, the conditions of the theorem imply that for general \( \theta \) w.l.o.g. we can assume that \( \Phi_\xi \theta \in U_{ij} \), for some indexes \( j_i \). Henceforth, after adding the noise with \( \sigma \to 0 \) we must obtain locally uniform approximation since the functions \( L(z, \xi_j) \) are locally constant in a vicinity of \( z = \Phi_\xi \theta \forall i \).

**Theorem 7.** In gradient boosting if \( L(\cdot, \cdot) \in R_0 \) is coming from the LSO problem, then any smoothing is consistent.

**Proof.** Conditions from Theorem 2 of the main text translate into condition that \( \langle \Phi_\xi \theta \rangle_j \neq 0 \) for all \( j \) and for all \( \theta \) almost surely. This can be enforced by adding a free constant to the linear model, but in the gradient boosting setting this condition is essentially satisfied: consider \( \theta = 1_m \), then \( \langle \Phi_\xi 1_m \rangle_j \geq 1 \forall j \) since the matrix \( \Phi_\xi \) is 0-1 matrix and have at least one “1” in each row (every item fell to at least one leaf of each tree). Henceforth, for any general \( \theta \) we can assume another general \( \theta = \theta + \nu 1_m \), where \( \nu \) is any random variable with absolute continuous p.d.f. which in turn imply \( \langle \Phi_\xi \theta \rangle_j \neq 0 \) almost surely. Henceforth, Theorem 2 holds ensuring consistent smoothing.

C. Coordinate Conditional Sampling

C.1. Proof of Lemma 1

Consider a line \( H = \{(z_j, z_{\mathbb{R}}) : \forall z_j \in \mathbb{R}\} \) and subsets \( U_1, \ldots, U_k \) for \( k = k(n, \mathbb{R}^n) \) from the Discretness on subspaces assumption for \( V = \mathbb{R}^n \). Then \( U_i \cap H = (a_i, b_i) \times \{z_{\mathbb{R}}\} \) due to openness and convexity of \( U_i \) for \( a_i, b_i \in \mathbb{R} \cup \{\pm \infty\} \). Moreover, \( (U_i \cap H) \cap (U_i \cap H) = \emptyset \) \( \forall i \neq i' \) and, by ignoring sets of zero measure, we can assume that \( \bigcup_i (a_i, b_i) \times \{z_{\mathbb{R}}\} = H \). After that, we can take all finite \( \{b_1, \ldots, b_k\} \cap \mathbb{R} \) as breaking points.

C.2. Proof of Theorem 3

Observe that \( L * \pi^j_\xi \) tautologically equals \( l_j * \pi^j_\xi \) and the convolution is distributive with respect to summation, so we can write:

\[
L * \pi^j_\xi = \sum_{s=1}^{k'} \Delta l_j(b_s) \mathbb{1}_{(z_j \leq b_s)} * \pi^j_\xi + \text{const}(z_{\mathbb{R}}).
\]

The convolution \( \mathbb{1}_{(z_j \leq b_s)} * \pi^j_\xi \) is equal to \( \mathbb{P}_\xi(z_j + \sigma \varepsilon_j < b_s | \varepsilon_j) := \sigma^{-1} \int_{\mathbb{R}} \mathbb{1}_{(z_j + \sigma \varepsilon_j \leq b_s)} \pi^j_\xi(\sigma^{-1} \varepsilon_j) d\varepsilon_j \), allowing us to rewrite:

\[
L * \pi^j_\xi = \sum_{s=1}^{k'} \Delta l_j(b_s) \mathbb{1}_{(z_j \leq b_s)} + \sigma^{-1} \sum_{s=1}^{k'} \Delta l_j(b_s) \pi^j_\xi(\sigma^{-1} (b_s - z_j)) + \text{const}(z_{\mathbb{R}}).
\]

The above formula is ready for differentiation since each term is actually a \( C(2)(\mathbb{R}) \) function by the variable \( z_j \):

\[
\frac{\partial}{\partial z_j} L * \pi^j_\xi = -\sigma^{-1} \sum_{s=1}^{k'} \Delta l_j(b_s) \pi^j_\xi(\sigma^{-1} (b_s - z_j)).
\]

After the convolution with \( \pi^j_\xi \) we finally get the required formula.

C.3. Proof of Corollary 1

For LTR, all these \( b_s \) actually lay in \( \{z_1, \ldots, z_n\} \subset \mathbb{R} \) due to Pairwise decision boundary assumption and, henceforth, we do not need to compute them, we just need to take coordinates of \( z \in \mathbb{R}^n \) as breaking points and note that if some of \( z_s \) is not a breaking point for \( L(z, \xi) \), then essentially \( \Delta l_j(z_s) = 0 \). Then we can write

\[
\frac{\partial}{\partial z_j} L * \pi^j_\xi = -\sigma^{-1} \sum_{s=1}^{n} \Delta l_j(z_s) \pi^j_\xi(\sigma^{-1} (z_s - z_j)).
\]

For LSO, we can actually take \( k' = 1 \) and \( b_1 = 0 \) and simplify the formula to:

\[
l_j(z_j) = \Delta l_j \mathbb{1}_{(z_j \leq 0)} + \text{const}(z_{\mathbb{R}}).
\]

C.4. Proof of Theorem 4

**Lemma 3.** The function \( L^\pi_\xi(z, \sigma) \) satisfies the following linear first order Partial Differential Equation (PDE):

\[
\frac{\partial}{\partial \sigma} L^\pi_\xi(z, \sigma) = -\sigma^{-1} (\nabla_z L^\pi_\xi(z, \sigma), z).2.
\]

**Proof.** The proof is a direct consequence of Scalar Freenees: we need just to differentiate the equality \( L^\pi_\xi(\alpha z, \alpha \sigma) = L^\pi_\xi(z, \sigma) \) (holding for \( \alpha > 0 \)) by \( \alpha \) and set \( \alpha = 1 \).
By Fubini theorem we can pass the differentiation $\frac{\partial}{\partial \sigma}$ to inside the integral and obtain:

$$\frac{\partial}{\partial \sigma} L^\pi(z, \sigma) = -n \sigma^{-n-1} \int \limits_{\mathbb{R}^n} L(z + \varepsilon, \xi) \pi(\sigma^{-1} \varepsilon) d\varepsilon - \sigma^{-n-2} \int \limits_{\mathbb{R}^n} L(z + \varepsilon, \xi) \langle \nabla \pi(\sigma^{-1} \varepsilon), \varepsilon \rangle d\varepsilon.$$

Consider the variable $\varepsilon' = \sigma^{-1} \varepsilon$, then we arrive at

$$\frac{\partial}{\partial \sigma} L^\pi(z, \sigma) = -n \sigma^{-1} \int \limits_{\mathbb{R}^n} L(z + \sigma \varepsilon, \xi) \pi(\varepsilon) d\varepsilon - \sigma^{-1} \int \limits_{\mathbb{R}^n} L(z + \sigma \varepsilon, \xi) \langle \nabla \pi(\varepsilon), \varepsilon \rangle d\varepsilon.$$

Taking the absolute value of both sides and using the triangle inequality, we derive

$$\left| \frac{\partial}{\partial \sigma} L^\pi(z, \sigma) \right| \leq nl \sigma^{-1} + l \sigma^{-1} \int \limits_{\mathbb{R}^n} \| \nabla \pi(\varepsilon) \|_2 \| \varepsilon \|_2 d\varepsilon,$$

where $l = \sup_z |L(z, \xi)| < \infty$ by Boundness assumption and the last integral is well defined by the Derivative Decay assumption.

**Corollary 4.** $\sup_z \left| \langle \nabla_z L^\pi(z, \xi), \sigma \rangle \right| = O(1)$ independently from $\sigma$.

**Proof.** Immediate consequence of the previous lemma.

Now assume that $\sigma = \sigma(z)$ is differentiable and non-zero at $z$. The following lemma describes $\nabla_z L^\pi(z, \sigma(z))$ in terms of $\nabla_z L^\pi(z, \sigma) := \nabla_z L^\pi(z, \sigma(z)) |_{\sigma = \sigma(z)}$.

**Lemma 5.** The following formula holds:

$$\nabla_z L^\pi(z, \sigma(z)) = \nabla_z L^\pi(z, \sigma) - \langle \nabla_z L^\pi(z, \sigma), \nabla_z \log \sigma(z) \rangle.$$

**Proof.** Consider writing

$$\nabla_z L^\pi(z, \sigma(z)) = \nabla_z L^\pi(z, \sigma) + \frac{\partial}{\partial \sigma} L^\pi(z, \sigma(z)) \nabla_z \sigma(z).$$

Then by Lemma 3 we obtain the formula.

**D. Fast ranking metrics computation**

We need to be able to compute $L(z', z_{\setminus s_i} + \sigma \varepsilon_{\setminus s_i}, \xi)$ for an arbitrary $z' \in \mathbb{R}$ and a position $i$ where $s \in S_n$ represents $s := \text{argsort}(z + \sigma \varepsilon)$ for the CCS estimate (note that there is no ambiguity in computing argsort since with probability one $z_{j_1} + \sigma \varepsilon_{j_1} \neq z_{j_2} + \sigma \varepsilon_{j_2}$ for $j_1 \neq j_2$). Moreover, argsort requires $O(n \log n)$ operations.

Typically, the evaluation of $L(\cdots)$ costs $O(n)$, e.g., for ERR. Fortunately, for many losses it is possible to exploit the structure of the loss that allows to evaluate $L$ in $O(1)$ operations using some precomputed shared cumulative statistics related to the loss which can be computed in $O(n)$ operations and $O(n)$ memory.

For all $L \in \mathcal{R}_1$ in the worst case we need $O(n^2)$ evaluations of $L$ to compute the CCS (for each of $n$ coordinates to sum up at most $n$ evaluations). Thus, the overall worst case asymptotic of the algorithm would be $O(n \log n + n + n^2) = O(n^2)$ if the evaluation costs $O(1)$.

For the sake of simplicity, we generalize both of NDCG@k and ERR into one class of losses:

$$L(z, \xi) = - \sum_{i=1}^n w_i g(r_{s_i}) \prod_{j=1}^{i-1} d_{s_j}, \quad (8)$$

where $W = \{ w_i \}_{i=1}^n$ are some predefined positions’ weights typically picked as $\frac{1}{\log_{\log \log n}(1 + i^{\gamma})}$ for NDCG@k and $\frac{1}{i}$ for ERR; $D = \{ d_i \}_{i=1}^n$ is typically picked as $d_i = 1 \forall i$ for -NDCG@k and $d_i = 1 - r_i \forall i$ for ERR; and finally we define $g(r) = r$ for $r \in [0, 1]$ and $g(r) = \frac{r^{\gamma-1}}{1 + \gamma - 1}$ for $r \in \{0, 1, 2, 3, 4\}$.

First, we need to define and compute the following cumulative product:

$$p_m = d_{s_{m-1}} p_{m-1} = \prod_{j=1}^{m-1} d_{s_j} \text{ if } m > 1,$$

where $p_1 = 1$. Denote $P := \{ p_i \}_{i=1}^n$. Next, we use them we define the following cumulative sums:

$$S_{m}^{\text{sup}} = S_{m-1}^{\text{sup}} + w_m g(r_{s_m}) p_m \text{ if } m > 1,$$

$$S_{m}^{\text{mid}} = S_{m-1}^{\text{mid}} + w_m g(r_{s_m}) p_m \text{ if } m > 0,$$

$$S_{m}^{\text{low}} = S_{m-1}^{\text{low}} + w_m g(r_{s_m}) p_m \text{ if } m > 0,$$

where $S_0^{\text{sup}} = S_0^{\text{mid}} = S_0^{\text{low}} = 0$

All these cumulative statistics can be computed at the same time while we compute $L(z + \sigma \varepsilon, \xi)$. Note that we need additional $O(n)$ memory to store the statistics.

Now fix position $i$ and score $z'$. Express $L(z', z_{\setminus s_i} + \sigma \varepsilon_{\setminus s_i}, \xi)$ as $L(z', z_{\setminus s_i} + \sigma \varepsilon_{\setminus s_i}, \xi) - L(z + \sigma \varepsilon, \xi) + L(z + \sigma \varepsilon, \xi)$. Thus, we need to compute $L(z', z_{\setminus s_i} + \sigma \varepsilon_{\setminus s_i}, \xi) - L(z + \sigma \varepsilon, \xi)$.

If $z' > z_{s_i} + \sigma \varepsilon_{s_i}$, we define $i' := i$; otherwise, define $i' := i - 1$ — this variable represents the new position of the $s_i$-th document in $z + \sigma \varepsilon$. Also, if $z' > z_{s_i} + \sigma \varepsilon_{s_i}$, we
define:
\[ T^{low} = S_{i}^{mid} - S_{i}^{low}, \]
\[ T^{up} = d_{s_i}^{-1}(S_{i}^{up} - S_{i}^{low}), \]
\[ w = w_ip_i, \]
\[ w' = w_{i-1}d_{s_i}^{-1}p_i. \]

Otherwise, define:
\[ T^{low} = d_{s_i}(S_{i}^{low} - S_{i-1}^{low}), \]
\[ T^{up} = S_{i}^{mid} - S_{i-1}^{mid}, \]
\[ w = w_ip_i, \]
\[ w' = w_{i-1}p_i. \]

Then, we calculate \( L(z', z_{\epsilon_{s_i}} + \sigma \epsilon_{s_i}, \xi) - L(z + \epsilon, \xi) \) as \( g(r_{s_i})(w - w') - (T^{up} - T^{low}) \). The meaning of the formula is simple: we measure the change of gain of the \( s_i \)-th document if we change its score to \( z' \) from \( z_{s_i} + \epsilon_{s_i} \) minus the difference of gains of all documents on positions from \( i' \) up to \( i - 1 \), if \( i' < i \), and from \( i + 1 \) up to \( i' + 1 \), if \( i' > i \).

The above formulas can be verified directly by evaluating the cases when \( z' > z_{s_i} + \epsilon_{s_i} \) or \( z' < z_{s_i} + \epsilon_{s_i} \) and expanding \( S_{n}^{star} \) as \( \sum_{i} w_i \epsilon_{s_i} g(r_{s_i})p_i \). Note that all differences \( S_{i}^{up} - S_{j}^{low} \) take into account all documents on positions from \( j + 1 \) up to \( i \) inclusively.

Note that \( S_{n}^{mid} = L(z + \epsilon, \xi) \), indeed
\[
\sum_{i=1}^{n} w_i g(r_{s_i})p_i = \sum_{i=1}^{n} w_i g(r_{s_i}) \prod_{j=1}^{i-1} d_{s_j} = L(z + \epsilon, \xi).
\]

Therefore, we obtain:
\[
L(z', z_{\epsilon_{s_i}} + \sigma \epsilon_{s_i}, \xi) = g(r_{s_i})(w - w') - (T^{up} - T^{low}) + S_{n}^{mid}.
\]

(9)

E. Global Optimization by Diffusion

E.1. Overview of SGLB idea

Global convergence of SGLB is guaranteed by Predictions’ Space Langevin Dynamics Stochastic Differential Equation
\[
dF(t) = -\gamma F(t)dt - P\nabla F L_N^\sigma(F(t), \sigma)dt + \sqrt{2\beta^{-1}} PdW(t),
\]
where \( F(t) := \Phi(\theta(t)) = (\Phi_{\xi_1}(\theta(t)), \ldots, \Phi_{\xi_N}(\theta(t))) \in \mathbb{R}^{N'} \) denotes the predictions Markov Process on the train set \( D_N \), \( \Gamma = \sqrt{P^{-1}} \) is an implicitly defined regularization matrix, \( W(t) \) denotes a standard Wiener process with values in \( \mathbb{R}^{N'} \), where \( N' := \sum_{i=1}^{N} n_i \). \( P = P^T \) is an implicit preconditioner matrix of the boosting algorithm, and \( \beta > 0 \) is a temperature parameter that controls exploration/exploitation trade-off. Note that here we override the notation \( L_N(F) \equiv L_N(\theta) \) since \( F = \Phi(\theta) \).

The global convergence is implied by the fact that the stationary distribution \( p_\beta(F) \) of \( F(t) \) as \( t \to \infty \) concentrates around the global optima of the implicitly regularized loss
\[
L_N^\gamma(F, \sigma, \gamma) = L_N^\sigma(F, \sigma) + \frac{\gamma}{2} \| \Gamma F \|^2_2.
\]

More formally, the distribution is given by \( p_\beta(F) \propto \exp(-\beta L_N^\gamma(F, \sigma, \gamma)) \). According to Ustimenko & Prokhorenkova (2020), the optimization is performed within a linear space \( V := \text{im} \Phi \) that encodes all possible predictions \( F \) of all possible finite ensembles formed by the weak learners associated with the boosting algorithm. We refer interested readers to (Ustimenko & Prokhorenkova, 2020) for the details.

E.2. Proof of Theorem 5

Let us first prove the following lemma.

**Lemma 6.** The function \( L_N^\gamma(F, \sigma) \) is uniformly bounded, Lipshitz continuous with constant \( L_0 = O(\sigma^{-1}) \), and Lipshitz smooth with constant \( L_1 = O(\sigma^{-2}) \).

**Proof.** The proof of Lipshitz continuity is a direct consequence of the uniform boundedness by \( O(\sigma^{-1}) \) of CCS. If we differentiate CCS estimate one more time, we obtain the estimates for the Hessian that due to the uniform boundedness of \( \nabla \pi \) must be uniformly bounded by \( O(\sigma^{-2}) \), thus giving Lipschitz smoothness.

In addition to Lipshitz smoothness, continuity and boundedness from above, we also need \( \| \nabla \pi L_N^\sigma(F, \sigma) \|_2 = O(1) \) (Ustimenko & Prokhorenkova, 2020), but that condition is satisfied since both terms are uniformly bounded by \( O(\sigma^{-1}) \). Thus, the algorithm has limiting stationary measure \( p_\beta(F) \propto \exp(-\beta L_N^\gamma(F, \sigma, \gamma)) \).

Then, consistency of the smoothing ensures that as \( \sigma \to 0_+ \), \( p_\beta(F) \to p_\beta^*(F) \), where \( p_\beta^*(F) \propto \exp(-\beta (L_N(F) + \frac{1}{2} \| \Gamma F \|^2_2)) \) and thus for \( \beta \gg 1 \) the measures \( p_\beta^* \) and \( p_\beta \) for \( \sigma \approx 0 \) concentrate around the global optima of \( L_N(F) \).

E.3. Proof of Theorem 6

Following Raginsky et al. (2017); Ustimenko & Prokhorenkova (2020) we immediately obtain that \( \| E_{\theta \sim p_\beta(\theta)} L_N^\gamma(\theta, \sigma) - E_{\theta \sim p_\beta(\theta)} L_N^\gamma(\theta, \sigma) \| = \)
\(O\left(\frac{(\beta+d)^2}{N\lambda}\right)\) with \(\lambda_* > 0\) and \(d = V_\beta\). In general non-convex case \(\frac{1}{\lambda_*}\) can be of order \(\exp(O(d))\) (Raginsky et al., 2017) but for smoothed SF losses we can give a better estimate without exponential dependence on the dimension.

Observe that our measure is the sum of uniformly bounded Lipschitz smooth with constant \(O(\sigma^{-2})\) and a Gaussian \(\frac{\gamma}{2}\|\Gamma \phi \|_2^2\), then the more appropriate bound from the logarithmic Sobolev inequality applies according to Lemma 2.1 (Bardet et al., 2015) \(\frac{1}{\lambda_*} = O\left(\frac{\exp(O(\frac{1}{\gamma\beta})))}{\gamma\beta}\right)\) being dimension-free. Note that Miclo’s trick in the proof of the lemma should be skipped since \(\mathcal{L}_\gamma(\theta, \sigma)\) is already fine enough. Coupling the spectral gap bound with the generalization gap, we obtain the theorem.

F. Experiments

F.1. Parameter tuning

For tuning, we use the random search (500 samples) with the following distributions:

- For **learning-rate** log-uniform distribution over \([10^{-3}, 1]\).
- For **l2-leaf-reg** log-uniform distribution over \([10^{-1}, 10^{3}]\) for baselines and **l2-leaf-reg=0** for StochasticRank.
- For **depth** uniform distribution over \([6, 7, 8, 9, 10]\).
- For **model-shrink-rate** log-uniform distribution over \([10^{-5}, 10^{-2}]\) for StochasticRank.
- For **diffusion-temperature** log-uniform distribution over \([10^{2}, 10^{14}]\) for StochasticRank.
- For **resolution-strength** log-uniform distribution over \([10^{-2}, 10]\) for StochasticRank-R_1.

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