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Breaking the Top-K Barrier: Advancing Top-K Ranking Metrics Optimization in Recommender Systems

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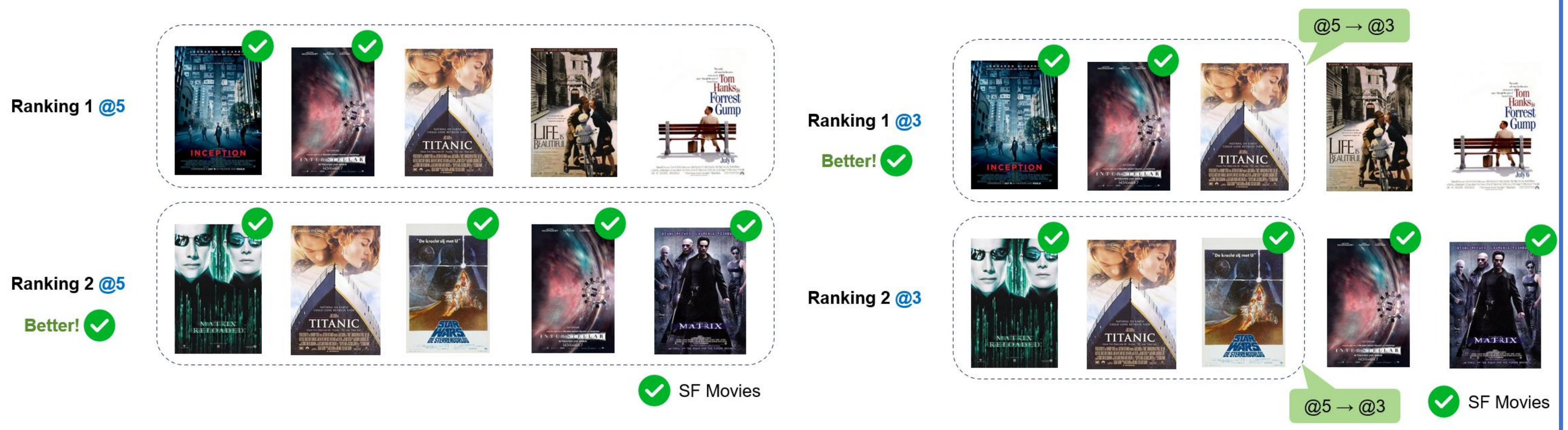
Top-K Recommendation

In Top-K recommendation, even for the same ranking list, different values of K may lead to different recommendation performance!



NDCG vs. NDCG@K Metrics

NDCG (Normalized Discounted Cumulative Gain):

- The most representative **ranking metrics** in recommender systems (RS).
- Evaluates performance over the **entire** ranked list.

$$\mathrm{NDCG}(u) = \frac{\mathrm{DCG}(u)}{\mathrm{IDCG}(u)}, \quad \mathrm{DCG}(u) = \sum_{i \in \mathcal{P}_u} \frac{1}{\log_2(\pi_{ui}+1)}$$

NDCG@K (NDCG with Top-K Truncation):

- **Truncated** version of NDCG, which is used to evaluate the real-world RS.
- Only the **top K ranked items** are taken into account.
- NDCG is equivalent to NDCG@∞.

Top-K truncated

$$\mathrm{NDCG@}K(u) = \frac{\mathrm{DCG@}K(u)}{\mathrm{IDCG@}K(u)}, \quad \mathrm{DCG@}K(u) = \sum_{i \in \mathcal{P}_u} \frac{\mathbb{I}(\pi_{ui} \le K)}{\log_2(\pi_{ui}+1)}$$

π_{ui} : ranking position of interaction (u, i) ; $\mathcal{P}_u$: positive items; IDCG : ideal DCG.

How to optimize for NDCG: Softmax Loss (SL)

Softmax Loss (SL, a.k.a. Cross Entropy Loss in RS):

- **SOTA** recommendation loss, initially derived from the MLE objective [1].
- Later proven to be **an upper bound of –log NDCG** [2].
- Minimizing SL leads to improved NDCG (**theoretical guarantees**).

$$\mathcal{L}_{\mathrm{SL}}(u) = -\sum_{i \in \mathcal{P}_u} \log \left(\frac{\exp(s_{ui}/\tau)}{\sum_{j \in \mathcal{I}} \exp(s_{uj}/\tau)} \right)$$

s_{ui} : predicted score of user u on item i ; τ : temperature parameter.

[1] Wu, Jiancan, et al. On the Effectiveness of Sampled Softmax Loss for Item Recommendation. TOIS 2024.
[2] Yang, Weiqin, et al. PSL: Rethinking and Improving Softmax Loss from Pairwise Perspective for Recommendation. NIPS 2024

How to optimize for NDCG@K: SL@K

Challenge 1: Top-K Truncation
How to handle the Top-K truncation term $\mathbb{I}(\pi_{ui} \le K)$?

This term involves **estimating the ranking position** for each interaction, which is **intractable** for large scale RS with complexity: $O(|U| \log I|)$.

U/I is the size of user/item set.

Solution: Quantile Technique

Given the **Top-K quantile** defined as $\beta_u^K := \inf\{s_{ui} : \pi_{ui} \le K\}$ for each user u, then the Top-K truncation term can be rewritten as $\mathbb{I}(\pi_{ui} \le K) = \mathbb{I}(s_{ui} \ge \beta_u^K)$

No need for global ranking: it only needs to estimate the Top-K quantile β_u^K.

Efficient Quantile Estimation

Sample Quantile Estimation

Complexity: $O(UN \log N)$

Sample N scores and sort them, then estimate the original Top-K quantile by the Top-$\left(\frac{K}{I}\right) * N$ quantile of the sampled scores. The estimation error decreases **exponentially** w.r.t. the sample size N.

Quantile Regression

Complexity: $O(UNT)$
T: interaction steps

Minimizing the following (convex) quantile regression loss:

$$\beta_u^K = \arg\min_{\beta} \mathcal{L}_{\mathrm{QR}}(\beta; u) := \sum_{i \in \mathcal{I}} \left(1 - \frac{K}{I}\right)(s_{ui} - \beta)_+ + \frac{K}{I}(\beta - s_{ui})_+$$

The optimal solution is precisely the Top-K quantile.

Challenge 2: Discontinuity

We derive an upper bound of –log DCG@K:

$$-\log \mathrm{DCG@}K(u) \le \sum_{i \in \mathcal{P}_u} \delta(s_{ui} - \beta_u^K) \cdot \log \left(\sum_{j \in \mathcal{I}} \delta(d_{uij}) \right)$$

where $d_{uij} = s_{uj} - s_{ui}$, and $\delta(\cdot)$ is the Heaviside step function.

However, this bound is still **non-smooth**! We can smooth the two Heaviside functions with **sigmoid** and **exp** functions, respectively.

NDCG@K Surrogate Loss: SL@K

$$\mathcal{L}_{\mathrm{SL@}K}(u) = \sum_{i \in \mathcal{P}_u} \underbrace{\sigma_w(s_{ui} - \beta_u^K)}_{\text{weight: } w_{ui}} \cdot \underbrace{\log \left(\sum_{j \in \mathcal{I}} \sigma_d(d_{uij}) \right)}_{\text{SL term: } \mathcal{L}_{\mathrm{SL}}(u,i)}$$

$d_{uij} = s_{uj} - s_{ui}$

$\sigma_w(x) = 1/(1 + e^{-x/\tau_w})$ is the sigmoid function.

$\sigma_d(x) = e^{x/\tau_d}$ is the exponential function.

Theoretical Guarantees	SL@K serves as an **upper bound of –log NDCG@K**.
Ease of Implementation	SL@K is a **weighted SL**, introducing only a quantile-based weight.
Computational Efficiency	SL@K has **similar computational complexity** compared with SL.
Gradient Stability	SL@K is more **stable** in training compared to other surrogate losses.
Noise Robustness	SL@K is **robust to false positive noise**.

Empirical Results in Top-K Recommendation

Table 2: Top-20 recommendation performance comparison of SL@K with existing losses. The best results are highlighted in bold, and the best baselines are underlined. "Imp." denotes the improvement of SL@K over the best baseline.

Backbone	Loss	Health		Electronic		Gowalla		Book	
		Recall@20	NDCG@20	Recall@20	NDCG@20	Recall@20	NDCG@20	Recall@20	NDCG@20
MF	BPR	0.1627	0.1234	0.0816	0.0527	0.1355	0.1111	0.0665	0.0453
	GuidedRec	0.1568	0.1093	0.0644	0.0385	0.1135	0.0863	0.0518	0.0361
	SONG@20	0.0874	0.0650	0.0708	0.0444	0.1237	0.0970	0.0747	0.0542
	LLPAUC	0.1644	0.1209	0.0821	0.0499	0.1610	0.1189	0.1150	0.0811
	SL	<u>0.1719</u>	0.1261	0.0821	0.0529	0.2064	0.1624	0.1559	0.1210
	AdvInfoNCE	0.1659	0.1237	0.0829	0.0527	0.2067	0.1627	0.1557	0.1172
	BSL	<u>0.1719</u>	0.1261	0.0834	0.0530	0.2071	0.1630	0.1563	0.1212
	PSL	0.1718	<u>0.1268</u>	<u>0.0838</u>	<u>0.0541</u>	<u>0.2089</u>	<u>0.1647</u>	<u>0.1569</u>	<u>0.1227</u>
	SL@20 (Ours)	**0.1823**	**0.1390**	**0.0901**	**0.0590**	**0.2121**	**0.1709**	**0.1612**	**0.1269**
	Imp. %	+6.05%	+9.62%	+7.52%	+9.06%	+1.53%	+3.76%	+2.74%	+3.42%
LightGCN	BPR	0.1618	0.1203	0.0813	0.0524	0.1745	0.1402	0.0984	0.0678
	GuidedRec	0.1550	0.1073	0.0657	0.0393	0.0921	0.0686	0.0468	0.0310
	SONG@20	0.1353	0.0960	0.0816	0.0511	0.1261	0.0968	0.0820	0.0573
	LLPAUC	0.1685	0.1207	<u>0.0831</u>	0.0507	0.1616	0.1192	0.1147	0.0810
	SL	0.1691	0.1235	0.0823	0.0526	0.2068	0.1628	0.1567	0.1220
	AdvInfoNCE	<u>0.1706</u>	0.1264	0.0823	0.0528	0.2066	0.1625	0.1568	0.1177
	BSL	0.1691	0.1236	0.0823	0.0526	0.2069	0.1628	0.1568	0.1220
	PSL	0.1701	<u>0.1270</u>	0.0830	<u>0.0536</u>	<u>0.2086</u>	<u>0.1648</u>	<u>0.1575</u>	<u>0.1233</u>
	SL@20 (Ours)	**0.1783**	**0.1371**	**0.0903**	**0.0591**	**0.2128**	**0.1729**	**0.1625**	**0.1280**
	Imp. %	+4.51%	+7.95%	+8.66%	+10.26%	+2.01%	+4.92%	+3.17%	+3.81%
XSimGCL	BPR	0.1496	0.1108	0.0777	<u>0.0508</u>	0.1966	0.1570	0.1269	0.0905
	GuidedRec	0.1539	0.1088	0.0760	0.0473	0.1685	0.1277	0.1275	0.0951
	SONG@20	0.1378	0.0948	0.0525	0.0320	0.1367	0.0985	0.1281	0.0964
	LLPAUC	0.1519	0.1083	0.0781	0.0481	0.1632	0.1200	0.1363	0.1008
	SL	0.1534	0.1113	0.0772	0.0490	0.2005	0.1570	0.1549	0.1207
	AdvInfoNCE	0.1499	0.1072	0.0776	0.0489	0.2010	0.1564	0.1568	0.1179
	BSL	<u>0.1649</u>	<u>0.1201</u>	0.0800	0.0507	<u>0.2037</u>	<u>0.1597</u>	0.1550	0.1207
	PSL	0.1579	0.1143	<u>0.0801</u>	0.0507	<u>0.2037</u>	0.1593	<u>0.1571</u>	<u>0.1228</u>
	SL@20 (Ours)	**0.1753**	**0.1332**	**0.0869**	**0.0571**	**0.2095**	**0.1717**	**0.1624**	**0.1277**
	Imp. %	+6.31%	+10.91%	+8.49%	+12.40%	+2.85%	+7.51%	+3.37%	+3.99%

Table 3: NDCG@K (D@K) comparisons with varying K on Health and Electronic datasets and MF backbone. The best results are highlighted in bold, and the best baselines are underlined. "Imp." denotes the improvement of SL@K over the best baseline.

Method	Health						Electronic					
	D@5	D@10	D@20	D@50	D@75	D@100	D@5	D@10	D@20	D@50	D@75	D@100
BPR	<u>0.0940</u>	0.1037	0.1234	<u>0.1621</u>	<u>0.1804</u>	<u>0.1925</u>	0.0345	0.0419	0.0527	0.0690	0.0777	0.0845
GuidedRec	0.0769	0.0881	0.1093	0.1484	0.1671	0.1811	0.0228	0.0294	0.0385	0.0551	0.0635	0.0703
SONG	0.0353	0.0392	0.0488	0.0709	0.0834	0.0930	0.0316	0.0393	0.0493	0.0661	0.0744	0.0803
SONG@K	0.0503	0.0535	0.0650	0.0896	0.1037	0.1135	0.0276	0.0349	0.0444	0.0581	0.0651	0.0706
LLPAUC	0.0887	0.0996	0.1209	0.1592	0.1765	0.1892	0.0305	0.0388	0.0499	0.0686	0.0778	<u>0.0848</u>
SL	0.0922	0.1037	0.1261	0.1620	0.1791	0.1924	0.0353	0.0430	0.0529	0.0696	0.0783	0.0845
AdvInfoNCE	0.0926	0.1038	0.1237	0.1608	0.1789	0.1920	0.0341	0.0423	0.0527	0.0697	0.0782	0.0843
BSL	0.0922	0.1037	0.1261	0.1620	0.1791	0.1924	0.0344	0.0425	0.0530	0.0691	0.0776	0.0843
PSL	<u>0.0940</u>	<u>0.1048</u>	<u>0.1268</u>	0.1613	0.1789	0.1912	<u>0.0356</u>	<u>0.0434</u>	<u>0.0541</u>	<u>0.0700</u>	<u>0.0784</u>	0.0845
SL@K (Ours)	**0.1080**	**0.1190**	**0.1390**	**0.1736**	**0.1916**	**0.2035**	**0.0402**	**0.0484**	**0.0590**	**0.0760**	**0.0844**	**0.0908**
Imp. %	+14.89%	+13.55%	+9.62%	+7.09%	+6.21%	+5.71%	+12.92%	+11.52%	+9.06%	+8.57%	+7.65%	+7.08%

Table 4: Performance exploration of SL@K on NDCG@K' with varying K and K'. The best results are highlighted in bold.

SL@K	Health						Electronic					
	D@5	D@10	D@20	D@50	D@75	D@100	D@5	D@10	D@20	D@50	D@75	D@100
SL@5	**0.1080**	0.1180	0.1379	0.1724	0.1906	0.2032	**0.0402**	0.0480	0.0583	0.0753	0.0839	0.0900
SL@10	0.1077	**0.1190**	0.1377	0.1734	0.1909	0.2028	0.0400	**0.0484**	0.0583	0.0755	0.0839	0.0901
SL@20	0.1076	0.1188	**0.1390**	0.1733	0.1909	0.2029	0.0400	0.0483	**0.0590**	0.0759	0.0837	0.0900
SL@50	0.1062	0.1167	0.1364	**0.1736**	0.1901	0.2020	0.0398	0.0481	0.0587	**0.0760**	0.0842	0.0907
SL@75	0.1073	0.1179	0.1387	0.1734	**0.1916**	0.2031	0.0397	0.0481	0.0587	0.0759	**0.0844**	0.0907
SL@100	0.1071	0.1177	0.1375	0.1727	0.1904	**0.2035**	0.0399	0.0481	0.0587	0.0759	0.0843	**0.0908**
SL (@∞)	0.0922	0.1037	0.1261	0.1620	0.1791	0.1924	0.0353	0.0430	0.0529	0.0696	0.0783	0.0845

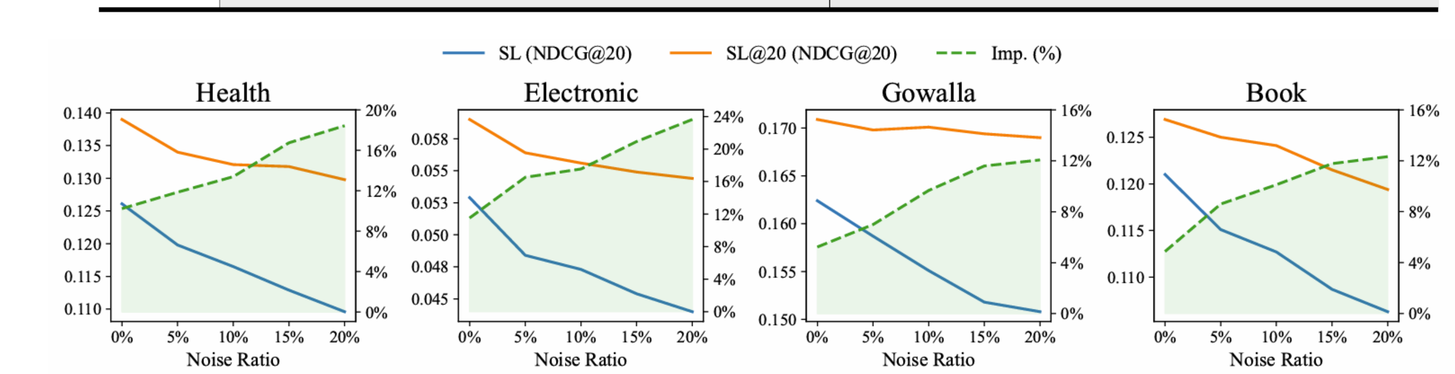


Figure 8: NDCG@20 performance of SL@K compared with SL under varying ratios of imposed false positive instances. "Noise Ratio" denotes the ratio of false positive instances. "Imp." indicates the improvement of SL@K over SL.