Efficient Retrieval with Learned Similarities

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Abstract

Retrieval plays a fundamental role in recommendation systems, search, and natural language processing by efficiently finding relevant items from a large corpus given a query. Dot products have been widely used as the similarity function in such retrieval tasks, thanks to Maximum Inner Product Search (MIPS) that enabled efficient retrieval based on dot products. However, state-of-the-art retrieval algorithms have migrated to learned similarities. Such algorithms vary in form; the queries can be represented with multiple embeddings, complex neural networks can be deployed, the item ids can be decoded directly from queries using beam search, and multiple approaches can be combined in hybrid solutions. Unfortunately, we lack efficient solutions for retrieval in these state-of-the-art setups. Our work investigates techniques for approximate nearest neighbor search with learned similarity functions. We first prove that Mixture-of-Logits (MoL) is a universal approximator, and can express all learned similarity functions. We next propose techniques to retrieve the approximate top K results using MoL with a tight bound. We finally compare our techniques with existing approaches, showing that MoL sets new state-of-the-art results on recommendation retrieval tasks, and our approximate top-k retrieval with learned similarities outperforms baselines by up to $91\times$ in latency, while achieving $> .99$ recall rate of exact algorithms.

1 Introduction

Retrieval requires efficient storing, indexing, and querying relevant candidate items represented by high-dimensional vectors. Retrieval is widely used as the initial preprocessing stage for applications such as recommendations and natural language processing that operate over corpus with up to billions of items [5, 9, 26, 25, 2]. In many concrete use cases, such as vector databases [19], the query- and the item- embeddings are learned with deep neural networks in a dual-encoder setup, and dot products are applied on top of such embeddings as the similarity function for measuring relevance.

Despite the popularity of dot products and numerous work done to improve their efficiency [18, 35, 28, 4], state-of-the-art retrieval algorithms have long moved to various learned similarity functions. Their most basic versions preserve some dot product-related structures, but turn either the query or the item into multiple embeddings, and rely on a max operator to combine those similarity values [26, 22]. As another example, Probabilistic Label Trees (PLTs) [16] and Tree-based Deep Models (TDMs) [45, 46] map items to leaf nodes in a tree, and reduce retrieval to beam search by making decisions sequentially using learned classifiers while traversing trees from root to leaf. More recent work on generative retrieval in recommendations and natural language processing directly map the query to the item ids in sequence-to-sequence or decoder-only setups [38, 40]. Combinations of these approaches have also been studied, with some performing coarse-grained retrieval with generative approaches, followed by re-ranking using dot products [8]. Finally, the similarity function can be directly parameterized by carefully designed deep neural networks that take various forms [14, 41, 34, 42].

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Supporting efficient retrieval with these diverse learned similarities is challenging. Learned similarity functions are generally expensive to compute; with learned index structures, traversing a binary tree with 4 million items requires running beam search for 20 non-parallelizable steps [45, 42], while recommendation and NLP deployments commonly need to handle billions of items [6, 26, 3] with low end-to-end latency. When an arbitrary deep neural network is employed, it's no longer clear how to perform top-K retrieval other than through brute-force [14] or heuristics [42]. What is worse, these algorithms vary significantly in terms of their exact formulations, and the lack of a universal interface makes it even more difficult for designing a general solution for efficient retrieval.

Taking a step back, our key insight is that learned similarity approaches are but different ways to increase expressiveness of the retrieval stage. Formally, for a query q and an item x, the expressiveness of the similarity function boils down to deriving alternative parameterizations of $p(x|q)$ matrices, with full rank matrices being the most expressive among them. Dot products, on the other hand, induces a low-rank bottleneck due to the dimensionality of the embedding, i.e., $\ln p(x|q) \propto \langle f(q), g(x) \rangle$ ($f(q), g(x) \in \mathbb{R}^d$). This cannot be alleviated by simply increasing the embedding dimension d, due to memory bandwidth being the main bottleneck in modern dot-product based retrieval systems, such as vector databases [19, 4], and overfitting issues that come with larger embedding dimensions due to the need to co-train query- and item- encoders from data [5, 26, 8, 43].

This insight enables us to support efficient retrieval with learned similarity functions by approximating them with MoL. To the best of our knowledge, this is the first work that tackles the problem of efficient retrieval with universal learned similarities. We first show that Mixture-of-Logits (MoL) is a universal approximator as it can express $p(x|q)$ matrices of arbitrary high rank, and hence approximate all learned similarity functions. Compared with prior work on learned similarities [14, 38] which often fail to outperform dot product baselines in large-scale settings [33, 36], our work lays theoretical foundations for MoL's empirical impressive performance gains of 20%-30% across Hit Rate@50-400 on corpus with hundreds of millions to billions of items [42, 3]. We next propose techniques to retrieve the approximate top-K results using MoL with a tight bound. Our solution leverages existing widely used APIs of vector databases like top-K queries, thus benefiting from prior work on efficient vector search like MIPS [18, 35, 19, 12]. We empirically compare our techniques with existing approaches, showing that MoL sets new state-of-the-art results on recommendation retrieval tasks, and our approximate top-k retrieval with learned similarities outperforms baselines by up to $91\times$ in latency, while achieving $> .99$ recall rate of exact algorithms. Importantly, our approach with learned similarities efficiently utilizes modern accelerators due to MoL's higher arithmetic intensity [42], which results in MIPS-level inference latency and throughput. This concludes both theoretical and practical justifications to migrate away from the broadly adopted MIPS solution in vector databases to Retrieval with Learned Similarities (RAILS) on GPUs.

2   Expressiveness of Mixture of Logits

In this section, we describe Mixture of Logits (MoL) and show that MoL is expressive enough to represent any learned similarity function. Table 1 summarizes the notations in this paper.

We first describe the learned similarity function with Mixture of Logits (MoL).

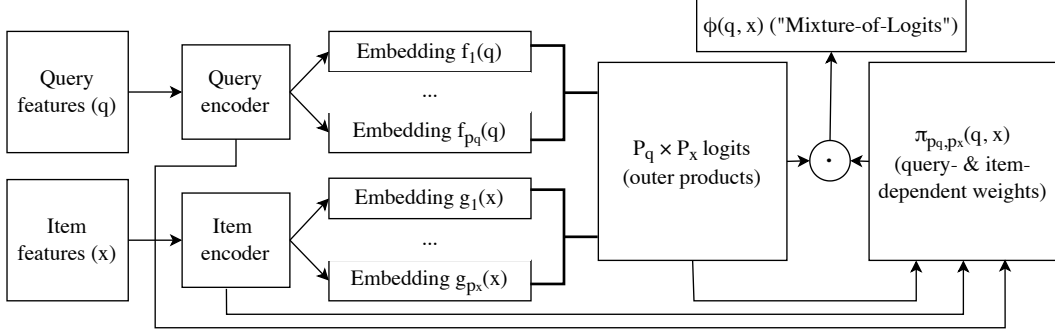| Notation	Description
$q\ (Q, |Q|)$	query (set of queries, number of queries)
$x\ (X, |X|)$	item (set of items, number of items)
$\phi(q, x)$	the learned similarity function, i.e., Mixture-of-Logits (MoL).
$P\ (P_q, P_x)$	MoL uses P low-rank embeddings ("component-level embeddings") to represent q and x. With the (batched) outer product form of MoL, P_q and P_x are the numbers of embeddings for q and x, respectively, and $P = P_q \times P_x$.
$\pi_p(q, x)\ (\pi_{p_q, p_x}(q, x))$	weight for the p-th (or p_q-th by p_x-th with outer product) embedding set for (q, x).
$f(q)\ (f_p(q))$	learned embedding for the query (p-th component-level query embedding)
$g(x)\ (g_p(x))$	learned embedding for the item (p-th component-level item embedding)
d_P	dimensionality of low-rank (component-level) embeddings. $f_p(q), g_p(q) \in \mathbb{R}^{d_P}$.
$\langle f(q), g(x) \rangle$	the dot product similarity function; $\langle f(q), g(x) \rangle = g(x)^T f(q)$.

Table 1: Table of Notations.

Figure 1: Mixture-of-logits (MoL) learned similarity.

Mixture of Logits (MoL)   MoL [42, 3] assumes that the query q and the item x are already mapped to P groups of low-rank embeddings ("component-level embeddings"), $f_p(q), g_p(x) \in \mathbb{R}^{d_P}$, where $f_p(q), g_p(x)$ are parameterized with some neural networks based on query and item features, respectively. MoL then calculates the similarity between the query q and the item x by applying adaptive gating weights, $\pi_p(q, x) \in [0, 1]$, to the inner products of these P pairs of low-rank embeddings, or $\langle f_p(q), g_p(x) \rangle$s. Note that prior work assumes that $\sum_p \pi_p(q, x) = 1$ [42, 3], and parameterizes $\pi_p(q, x)$ utilizing some neural network with $f_p(q)$s, $g_p(x)$s, and $\langle f_p(q), g_p(x) \rangle$s as input features, but these details do not affect our analyses in this paper. Following [42]:

$$\phi(q, x) = \sum_{p=1}^{P} \pi_p(q, x) \langle f_p(q), g_p(x) \rangle \tag{1}$$

To extend this to large-scale datasets and to enable hardware-efficient implementations on accelerators like GPUs, Equation 1 was further modified by decomposing those P dot products as (batched) outer products of P_q query-side and P_x item-side embedding, where $P_q \times P_x = P$, and applying l2-norm to $f_p(q)$s and $g_p(x)$s:

$$\phi(q, x) = \sum_{p_q=1}^{P_q} \sum_{p_x=1}^{P_x} \pi_{p_q, p_x}(q, x) \left\langle \frac{f_{p_q}(q)}{||f_{p_q}(q)||_2}, \frac{g_{p_x}(x)}{||g_{p_x}(x)||_2} \right\rangle \tag{2}$$

We use Equation 1 and 2 interchangeably as the MoL form to analyze throughout the rest of this paper, given that the embedding normalization for $f_{p_q}(q)$s and $g_{p_x}(x)$s can be precomputed.

Now we show that any high rank matrix can be decomposed into a mixture of logits based on low rank matrices. Specifically, without loss of generality, we prove the following:

Theorem 1. *MoL decomposition: Let A be a matrix of $n \times m$, where $n \leq m$. There exists $\pi_1, B_1, \pi_2, B_2, \cdots, \pi_p, B_p$ such that $|A - \sum_{p=1}^{P} \pi_p \circ B_i| < \epsilon$, where ϵ is a small positive number. Here B_i is a matrix of $n \times m$ with rank equal to or less than d, and $\pi_1, \pi_2, \cdots, \pi_P$ are $n \times m$ matrices that together define a probability distribution over each (i, j) tuple, such that $\sum_{p=1}^{P} \pi_p(i, j) = 1, 0 \leq \pi_p(i, j) \leq 1$ for any $1 \leq i \leq n, 1 \leq j \leq m, 1 \leq p \leq P$.*

We can think about n as the number of queries and m the number of items (or vice versa). First, the theorem trivially holds if the rank of A is less than or equal to d ($d \leq n$):

Lemma 1. *MoL decomposition when $Rank(A) \leq d$: Let A be a matrix as defined in Theorem 1. If the rank of A is less than or equal to d, then we have $A = \pi \circ A$, where $\pi(i, j) = 1$ for any $1 \leq i \leq n, 1 \leq j \leq m$.*

Then we prove for the case where the rank of A is greater than d. Without loss of generality, we prove the case where the matrix has full rank, i.e., $Rank(A) = n$:

Lemma 2. *MoL decomposition when $Rank(A) = n$: Let A be a matrix as defined in Theorem 1. Then there exists π, B_1, B_2 such that $|A - (\pi \circ B_1 + (1 - \pi) \circ B_2)| < \epsilon$, where $Rank(B_1) \leq d$, $Rank(B_2) \leq d$, and $0 \leq \pi(i, j) \leq 1$ for $1 \leq i \leq n, 1 \leq j \leq m$.*

Proof. Because A is a matrix of rank n, it can be rewritten as $A = UI_nV$, where I_n is an identity matrix with rank n. Thus, $A_{ij} = \sum_{k=1}^{n} U_{ik}V_{kj}, 1 \leq i \leq n, 1 \leq j \leq m$. Let A' be a matrix of

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$n \times m$, where $A'_{ij} = \lambda_{ij} \cdot \sum_{k=1}^{d} U_{ik} V_{kj}$ for $1 \le i \le n, 1 \le j \le m$. Here, $\lambda_{ij} = 1 + \frac{\sum_{k=d+1}^{n} U_{ik} V_{kj}}{\sum_{k=1}^{d} U_{ik} V_{kj}}$ if $\sum_{k=1}^{d} U_{ik} V_{kj} \ne 0$, otherwise $\lambda_{ij} = 1 + \frac{\sum_{k=d+1}^{n} U_{ik} V_{kj}}{\epsilon}$. Thus, we have $|A - A'| \le \epsilon$.

Let $\lambda_{min} = \min \lambda_{ij}$, and $\lambda_{max} = \max \lambda_{ij}$. Let $B_1 = \lambda_{min} U D_{n,d} V$, $B_2 = \lambda_{max} U D_{n,d} V$, where $D_{n,d}$ denotes an n-by-n diagonal matrix with the first d elements of the diagonal being 1s and the rest being 0s. We have $A'_{ij} = \lambda_{ij} \sum_{k=1}^{d} U_{ik} V_{kj} = \pi(i,j) \cdot B_{1ij} + (1 - \pi(i,j)) \cdot B_{2ij}$, where $\pi(i,j) = \frac{\lambda_{max} - \lambda_{ij}}{\lambda_{max} - \lambda_{min}}$. Because $\lambda_{min} \le \lambda_{ij} \le \lambda_{max}$, we have $0 \le \pi(i,j) \le 1$.

Thus, we have constructed B_1, B_2, π such that $|A - (\pi \circ B_1 + (1 - \pi) \circ B_2)| = |A - A'| \le \epsilon$. $\quad\square$

Remark Here, we have shown that any high-rank matrix can be expressed as a mixture of logits of two low-rank matrices. Note that our decomposition is not intended to be used as a distillation of the original high-rank matrix. For instance, it is prohibitively expensive to populate the full matrix with a learned similarity function. In addition, the proof also does not indicate that having a sum of two mixture of logits is sufficient to train the embeddings and the learned similarity function. It is well-known that overparameterization is often necessary to enable efficient and performant training.

3 Retrieval Algorithms

In this section, we describe the problem of retrieving the top K items with *MoL* and both exact and approximate algorithms for retrieval. Formally, we define the top K retrieval problem as follows:

Definition 1. *Top K with MoL: Let q be a query and X be a set of items, where both the query q and each item $x \in X$ are associated with P embeddings. Together we have P pairs of embeddings, $(f_p(q), g_p(x)), 1 \le p \le P$. Let $\phi(q,x) = \sum_{p=1}^{P} \pi_p(q,x) \langle f_p(q), g_p(x) \rangle$ be the similarity score of q, x, where $x \in X$. The top K query with MoL returns the K items from X with the highest $\phi(q,x)s$.*

For approximate top K retrieval with *MoL*, we define the gap of the approximate and exact top K results as follows:

Definition 2. *Gap of approximate top K: Let q be a query and X_K be the set of exact top K items for the query q from a set of items X. Let X^* be the approximate top K results, where $X^* \subseteq X$. Let $S = \min\{\phi(q,x), x \in X^*\}$ and $S' = \max\{\phi(q,x), x \in X_K \setminus X^*\}$. We call $S_\Delta = S' - S$ the gap of the top K with X^*.*

3.1 Exact algorithm

The brute-force algorithm to retrieve the exact top K with *MoL* is to evaluate $\phi(q,x)$ for each query q and item x. This algorithm can be prohibitively expensive if the number of items is large. Instead, we describe a more efficient two-pass algorithm to retrieve the exact top K items as shown in Algorithm 1.

Algorithm 1 Exact top K algorithm.

Input: query q, a set of items X, $f_p(\cdot)$, $g_p(\cdot)$ for constructing the component-level embeddings $f_p(q), g_p(x)$
Output: exact top K items
 1: $G \leftarrow \emptyset$
 2: **for** $p \in P$ **do**
 3:     $X_p \leftarrow \{g_p(x), x \in X\}$ $\triangleright$ Can be preprocessed and materialized.
 4:     $G \leftarrow G \cup TopKDotProduct(f_p(q), X_p)$ $\triangleright$ Retrieve top K items for each pair of embeddings
 5: $S_{min} \leftarrow \infty$
 6: **for** $x \in G$ **do**
 7:     $s \leftarrow MoL(q,x)$
 8:     **if** $s < S_{min}$ **then** $S_{min} \leftarrow s$
 9: $G' \leftarrow \emptyset$
10: **for** $p \in P$ **do**
11:     $G' \leftarrow G' \cup RangeDotProduct(f_p(q), S_{min}, X_p)$ $\triangleright$ Retrieve all items with a dot product higher than or equal to S_{min} for $f_p(q)$ from X_p
12: **return** $BruteForceTopKMoL(q, G')$ $\triangleright$ Retrieve the top K items from G' with *MoL*

We start by retrieving the top K items with the highest dot product scores for each group of embeddings as the initial candidate set G (line 1-4). Then we evaluate the *MoL* scores of the items in G and find the minimal learned similarity score S_{min} (line 5-8). Next we retrieve all items within a distance of S_{min} with the query q as the candidate set G' (line 9-11). Finally, we evaluate the *MoL* scores of the items in G', and return the top K items with the highest scores (line 12).

We argue that Algorithm 1 retrieves the exact top K items with *MoL*. Let X_K be the set of the exact top K items and X' be the result of Algorithm 1. Let $x \in X_K$ and $\phi(q, x)$ be the *MoL* score of x and q. Since x has the highest top K score with *MoL*, $\phi(q, x) \geq S_{min}$. Since the *MoL* score is a weighted score over the dot product scores, we have $\max\{\langle f_p(q), g_p(x)\rangle, 1 \leq p \leq P\} \geq \phi(q, x) \geq S_{min}$. Since Algorithm 1 retrieves all the items with a dot product higher than or equal to S_{min} of q for each embedding q_p (line 9-11), we have $x \in G'$. Thus, $x \in X'$. So we have shown that $X_K = X'$.

3.2 Approximate algorithms

In the exact algorithm shown in Algorithm 1, we need to retrieve all the items with a dot product higher than or equal to a threshold. When the threshold is a loose filter of the item set, which may happen when the dot product scores are skewed, G' can be large, and the evaluation of *MoL* over a large set of candidate items can still be expensive. Here, we describe two heuristics to approximately retrieve the top K items and analyze their gap against the exact top K algorithm.

In both heuristics, we perform a two-stage retrieval as shown in Algorithm 2. In the first stage, we retrieve a set of K' candidate items that are potentially high in *MoL* score by using dot products (line 2). Note that K' can be larger than K, e.g., due to oversampling. In the second stage, we evaluate the *MoL* scores of the candidate items and return the top K items (line 3).

Algorithm 2 Approximate top K algorithms.

Input: a query q, a set of items X
Output: approximate top K items
1: **function** APPROXTOPK(q, X, K, K')
2:     $G \leftarrow TopKCandidate(q, X, K')$ ▷ Retrieve the top K' candidate items
3:     **return** $BruteForceTopKMoL(q, G, K)$ ▷ Retrieve the top K items with *MoL*

Input: a query q, a set of items X, $f_p(\cdot)$, $g_p(\cdot)$ for constructing the component-level embeddings $f_p(q), g_p(x)$
Output: union of top K items over P component-level embeddings by dot product
4: **function** TOPKPEREMBEDDING(q, X, K)
5:     $G \leftarrow \emptyset$
6:     **for** $p \in P$ **do**
7:         $X_p \leftarrow \{g_p(x), x \in X\}$ ▷ Can be preprocessed and materialized.
8:         $G \leftarrow G \cup TopKDotProduct(f_p(q), X_p, K)$ ▷ Retrieve the top K items by dot product
9:     **return** G

Input: a query q, a set of items X, $f_p(\cdot)$, $g_p(\cdot)$ for constructing the component-level embedding $f_p(q), g_p(x)$
Output: top K items based on the averaged dot product, $\sum_p \langle f_p(q), g_p(x)\rangle / P$.
10: **function** TOPKAVG(q, X, K)
11:     $q' \leftarrow \sum_{p=1}^{P} f_p(q)$
12:     $X' \leftarrow \{\sum_{p=1}^{P} g_p(x)/P, x \in X\}$ ▷ Can be preprocessed and materialized.
13:     **return** $TopKDotProduct(q', X', K)$

Here, we describe two heuristics to retrieve the candidate item set:

Top K per embedding. Given a query q and a set of items X, for each embedding set p, retrieve top K items $X_{K,p}$ based on dot product ($\langle f_p(q), g_p(x)\rangle$). Return the union across P queries.

The top K per embedding heuristic returns the union of the top K items for each embedding by dot product. We analyze the gap of this heuristic as follows:

Theorem 2. *Upper bound of the gap of top K per embedding: Let $X_{K,p}$ be the top K items of the embedding set p and $S = \max\{\phi(q, x), x \in X_{K+1,p}\}$. Let S_{min} be the top K^{th} MoL score of the items in $\cup_p X_{K,p}$, then the gap of $S_\Delta \leq S' - S_{min}$.*

Remark Note that there exists an *MoL* such that $S_\Delta = S - S_{min}$, i.e., when $\pi_p(q, x) = 1$ for $x_p = \arg\max_{x,p}\{\langle f_p(q), g_p(x)\rangle, x \in X_{K+1,p} \setminus X_{K,p}\}$. Thus, the upper bound of S_Δ is tight.

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Top K average. Given a query q and a set of items X, return the top K items with the highest average dot product $\sum_p \langle f_p(q), g_p(x) \rangle / P$.

Note that the top K average heuristic returns the exact top K items when the gating weight distribution in *MoL*, π, is uniform.

This heuristic is interesting for two reasons. First, the items retrieved by this heuristic are likely to be the top K items of *MoL* when the weight distribution is more balanced. This complements the heuristic that retrieves top K per embedding. Second, in the setup where the set of embedding pairs is constructed as the outer product of the embeddings of a query and those of an item (Equation 2), the average dot product can be efficiently preprocessed and materialized for the items, and the computation of the top K average is then *agnostic* to the number of embedding sets $P = P_q \times P_x$.

Formally, let $P = P_q \cdot P_x$ be the number of embedding pairs, where P_q is the number of embeddings of a query q and P_x is that of an item x. The average dot product can be computed as

$$\frac{1}{P} \cdot \sum_{p=1}^{P} \langle f_p(q), g_p(x) \rangle = \frac{1}{P} \cdot \sum_{p_q=1}^{P_q} \sum_{p_x=1}^{P_x} \langle f_{p_q}(q), g_{p_x}(x) \rangle = \frac{1}{P} \cdot \left\langle \sum_{p_q=1}^{P_q} f_{p_q}(q), \sum_{p_x=1}^{P_x} g_{p_x}(x) \right\rangle \quad (3)$$

Thus, we can preprocess the embeddings of the items and the query, so the number of embeddings accessed is 1 per item for a given query, regardless of the overall number of component-level embeddings used by *MoL*, i.e., P.

Finally, we can combine the candidates retrieved from top K per embedding group and the top K average as the following:

Combined top K. Given a query q, a set of items X, and K, return the union of the items from the top K per embedding group across the P groups and the top K items from the top K average.

Theorem 3. *Upper bound of the gap of combined top K. Let $X_{K,p}$ be the top K items of the embedding set p and S_{min} as defined in Theorem 2. Let X'_K be the top K items from top K average. Let $S' = \max\{\phi(q,x), x \in X \setminus (\cup_p X_{K,p} \cup X'_K)\}$. Then the gap of $S_\Delta \leq S' - S_{min}$.*

Remark Similar to Theorem 2, the upper bound of the gap is tight. In practice, we can configure the K to be different for the two heuristics, i.e., K_1 and K_2. For example, when the weight distribution π is more balanced, K_2 can be configured to be larger as the top K average approach approximates *MoL* well while being more computationally efficient.

4 Evaluation

In this section, we evaluate the performance of the *MoL* based learned similarity and the efficiency of our retrieval algorithms discussed in Section 3.

4.1 Setup

Workloads. We consider a classical retrieval task (next-item prediction) in recommendation systems [5, 45, 26, 42]. We employ three widely used datasets, the 1M and 20M subsets of MovieLens [13], and the largest Books subset of Amazon Reviews [29]. We utilize sequential user encoders, as they have been shown to achieve state-of-the-art results on these datasets [20, 42]. In the next-item prediction setting in sequential recommendations, the query q corresponds to the user representation at a particular time step, which is then mapped to P_q embeddings using an multi-layer perceptron (MLP) when using the MoL learned similarity, consistent with prior work. We discuss detailed hyperparameter settings in Appendix A. Table 2 shows the statistics of these three workloads.

Workload	$|Q|$	$|X|$	$|P_q|$	$|P_x|$	d_P
ML-1M	6,040	3,649	8	4	64
ML-20M	138,493	24,186	8	4	128
Books	694,897	674,044	8	8	32

Table 2: Workload statistics.

	Method	HR@1	HR@10	HR@50	HR@200	MRR
ML-1M	SASRec	.0610	.2818	.5470	.7540	.1352
	SASRec + MoL	.0710	.3034	.5655	.7680	.1448
	HSTU	.0750	.3332	.5956	.7824	.1579
	HSTU + MoL	**.0837**	**.3460**	**.6048**	**.7874**	**.1673**
ML-20M	SASRec	.0653	.2883	.5484	.7658	.1375
	SASRec + MoL	.0790	.3124	.5685	.7784	.1551
	HSTU	.0962	.3557	.6146	.8080	.1800
	HSTU + MoL	**.1008**	**.3697**	**.6244**	**.8124**	**.1880**
Books	SASRec	.0058	.0306	.0754	.1431	.0153
	SASRec + MoL	.0083	.0402	.0970	.1813	.0203
	HSTU	.0101	.0469	.1066	.1876	.0233
	HSTU + MoL	**.0150**	**.0613**	**.1292**	**.2167**	**.0315**

Table 3: Evaluation of recommendation retrieval performance, utilizing the next-item prediction task.

Model. We implemented MoL on top of two popular sequential architectures, SASRec [20] and HSTU [43], with cosine similarity as the default similarity function (SASRec / HSTU rows in Table 3). The models are are implemented in PyTorch and trained with 2x NVIDIA RTX 6000 Ada GPUs.

Metrics. We use Recall (Hit Rate) as the main metric. It's worth noting that HSTU + MoL sets new state-of-the-art results on MovieLens and Amazon Reviews (Table 3). Mixture-of-Logits (+ MoL rows) also consistently outperform dot products by an average of 24.2% in HR@1, 14.3% in HR@10, and 16.3% in MRR across the six scenarios, validating that learned similarities, in particular MoL, are not only theoretically expressive but also practically learnable. We evaluate our proposed retrieval algorithms relative to the best performing rows, "HSTU + MoL", which exhaustively evaluates $\phi(q, x)$ over all xs and corresponds to *BruteForce* rows in the next section.

4.2 Top K retrieval performance

We evaluate the following methods on their top K retrieval performance:

- Brute-force top K (*BruteForce*): Evaluate the *MoL* scores for all items and return the top K items. This is the ground truth in our top K evaluation [2].

- Per embedding top K (*TopKPerEmbd*(N)): This algorithm is described in Section 3.2. N is the number of candidate items retrieved from each embedding set, where $N \times P \geq K$.

- Average top K (*TopKAvg*(N)): This algorithm is described in Section 3.2. N is the number of the candidate items retrieved by average dot products, where $N \geq K$.

- Combined top K from per embedding top K and average top K (*CombTopKN_1_N_2*): This is described in Section 3.2. N_1 is the number of candidate items retrieved from per embedding top K and N_2 is the number of candidate items retrieved from average top K, where $N_1 \times P + N_2 \geq K$.

Table 4 shows the hit rate (HR) and latency of all the methods. The hit rate is normalized by the ground truth, i.e., the hit rate achieved with brute-force top K. We measure latency by evaluating a batch of retrieval queries, in order to achieve high accelerator utilization; this is consistent with prior work on GPU/TPU-based retrieval algorithms [19, 4, 42]. We set batch size to 32 for *ML-1M*, *ML-20M*, and *Books*. We perform evaluation on a single NVIDIA RTX 6000 Ada GPU. We report latency averaged over 20 warm runs.

We observe that our approximate heuristics achieve high HR with oversampling. For example, *TopKAvg*500 is $> .99$ in relative HR across the board for *ML-1M* and *ML-20M*, and *TopKAvg*4000 is $> .99$ in relative HR across the board for *Books*. In addition, the combined top K algorithm can outperform both *TopKPerEmbd* and *TopKAvg* of the corresponding configurations, sometimes significantly, e.g., *CombTopK*5_200 vs. *TopKPerEmbd*5 and *TopKAvg*200 on *Books*. This indicates

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[2]We omit the baseline with the two-pass exact algorithm (Section 3.1) because the range-based item retrieval can still be expensive when the range threshold is loose. Empirically, the brute-force top K is more efficient on our datasets. We leave the efficient implementation of the two-pass exact algorithm as future work.

	Method	HR@1	HR@5	HR@10	HR@50	HR@100	Latency / ms
ML-1M	*BruteForce*	1.00	1.00	1.00	1.00	1.00	.64±.03
	*TopKPerEmbd*5	.838	.768	.681	.499	.437	.95±.03
	*TopKPerEmbd*10	.932	.905	.842	.678	.618	.94±.05
	*TopKPerEmbd*50	**1.00**	**.997**	**.999**	.977	.954	.95±.05
	*TopKPerEmbd*100	**1.00**	**1.00**	**1.00**	**.995**	**.990**	1.24±.04
	*TopKAvg*200	.980	.970	.967	.958	.948	.74±.06
	*TopKAvg*500	**.992**	**.986**	**.989**	**.990**	**.990**	.71±.04
	*TopKAvg*1000	**.996**	**.994**	**.998**	**.997**	**.999**	.72±.03
	*CombTopK*5_200	**1.00**	**.997**	**.988**	.975	.960	1.09±.08
	*CombTopK*50_500	**1.00**	**.999**	**.999**	**.998**	**.997**	1.13±.04
ML-20M	*BruteForce*	1.00	1.00	1.00	1.00	1.00	3.08±.02
	*TopKPerEmbd*5	.755	.702	.645	.467	.402	1.19±.05
	*TopKPerEmbd*10	.946	.876	.817	.645	.564	1.17±.05
	*TopKPerEmbd*50	**.993**	**.986**	.977	.931	.900	1.55±.03
	*TopKPerEmbd*100	**.998**	**.997**	**.994**	.979	.966	2.26±.03
	*TopKAvg*200	**.992**	**.992**	**.992**	.980	.958	.76±.04
	*TopKAvg*500	**.992**	**.993**	**.995**	**.995**	**.993**	.77±.04
	*TopKAvg*1000	**.992**	**.994**	**.996**	**.998**	**.997**	.75±.03
	*CombTopK*5_200	**1.00**	**.998**	**.998**	.983	.962	1.32±.06
	*CombTopK*50_500	**1.00**	**1.00**	**1.00**	**.999**	**.996**	1.85±.03
Books	*BruteForce*	1.00	1.00	1.00	1.00	1.00	149.02±.49
	*TopKPerEmbd*5	.907	.915	.809	.509	.396	20.17±.06
	*TopKPerEmbd*10	.936	**.986**	.914	.698	.561	20.33±.06
	*TopKPerEmbd*50	**.993**	**.992**	**.994**	.956	.902	21.09±.04
	*TopKPerEmbd*100	**1.00**	**.995**	**.996**	**.985**	.959	22.53±.06
	*TopKAvg*200	**1.00**	.978	.948	.845	.767	.68±.03
	*TopKAvg*500	**1.00**	**.992**	**.996**	.919	.875	.68±.03
	*TopKAvg*1000	**1.00**	**1.00**	**.996**	.963	.939	.84±.01
	*TopKAvg*2000	**1.00**	**1.00**	**1.00**	.980	.968	1.04±.02
	*TopKAvg*4000	**1.00**	**1.00**	**1.00**	**.996**	**.987**	1.64±.04
	*CombTopK*5_200	.979	.984	.981	.892	.818	20.29±.05
	*CombTopK*50_500	**.993**	**.989**	**.994**	.975	.961	21.57±.06
	*CombTopK*100_1000	**1.00**	**.997**	**.996**	**.993**	**.992**	23.00±.08

Table 4: Evaluation of top K retrieval performance, with hit rate (HR) normalized by the brute-force top K method and latency with standard deviation measured over the evaluation of retrieval for a batch of queries (where the batch size is 32). (Relative) hit rate higher than .99 is marked in **bold**.

that the set of candidate items retrieved by each individual approximate algorithm indeed complements each other when the weight distributions vary in *MoL*.

In terms of efficiency, we observe that our approximate heuristics are significantly lower in latency than the exact baseline, especially as the number of items in the dataset becomes large. For example, compared to *BruteForce*, *TopKAvg* achieves $> .99$ relative HR@100 with a speedup of $4\times$ and $91\times$ in latency for *ML-20M* and *Books*, respectively. While the latency of the retrieval grows with the size of the dataset in the brute-force baseline, it grows much slower with the approximate methods. For example, the latency of retrieval increases by $4.8\times$ from *ML-1M* to *ML-20M* in *BruteForce*, while the growth rate is $1.8\times$ and $1.1\times$ for *TopKPerEmbd*100 and *TopKAvg*1000 respectively. Thus, we expect that the speedup of the approximate methods to become even more prominent as the size of the dataset further increases.

We also notice that *TopKAvg* tends to be more efficient than *TopKPerEmbd* with comparable HR, e.g., *TopKAvg*2000 vs. *TopKPerEmbd*100 on *Books* with $22\times$ speedup in latency. We believe that this is mainly due to two reasons. First, when the HR is comparable, the maximal number of candidate items from *TopKPerEmbd* is larger than that of *TopKAvg*. Second, compared to *TopKPerEmbd*, the computation of *TopKAvg* is agnostic to the number of embedding sets because of the materialization optimization described in Section 3.2. Interestingly, we also see that the combined top K is more efficient than the summation of the latency of its individual components, e.g., *CombTopK*5_200 is $1.5\times$ faster than the sum of the latency from *TopKPerEmbd*5 and *TopKAvg*200 on *ML-20M*. This is

because our implementation reduces the overhead of the combined method by consolidating some shared processing of the two components.

Overall, empirically *TopKAvg* strikes a good balance between high HR and low latency, and the combined top K can be used if the target HR is extremely stringent.

5 Related work

Similarity Functions in Retrieval. Most information retrieval models in recommendations and natural language processing follow a classical two-stage paradigm [5], where up to billions of items [6, 26, 3] are first filtered down to hundreds in the *retrieval* stage, followed by the *ranking* stage that produces the final top 1-10 candidates. Earlier work on large-scale neural retrieval models primarily utilize dual-encoder (dense retrieval, etc.) setups, with dot products as the similarity function [5, 21]. Researchers quickly realized that dot products limited retrieval stage's performance, and explored various learned similarity-based approaches. Prominent variants include maximum similarity based on multiple embeddings [26, 22, 34], specialized neural networks, often based on Hadamard products [14, 37, 39, 3], and representing item ids as token sequences ("learned index structures"), either implicitly defined during tree traversal [16, 45, 46] or explicitly in the "generative retrieval" setups [8, 38, 40, 36]. It has been shown, however, that learned neural distances often fail to outperform dot products, e.g., Hadamard MLPs in recommendations [33] and DSI in NLP [36]. Learned index structures further introduce stability and latency challenges as both NLP and recommendation systems need to support billion-scale realtime updated set of items [3]. Despite these challenges, significant gains (17% gains at Hit Rate@100 [42] to 24% gains at Hit Rate@400 [3]) with learned similarities have been reported in recent years; these can be attributed to careful construction of learned similarity functions [34, 42], implicit diversification done as part of beam search [8, 36], explicit representation of side-information using special neural architectures [3], and hardware-aware similarity function and inference algorithm design on GPUs [4, 42, 3].

Efficient Nearest Neighbor Search (NNS). Nearest neighbor search has been a popular topic of research due to their critical role in large-scale retrieval and vector databases. Most studies focus on the dot product case, also known as Maximum Inner Product Search (MIPS). Various techniques were proposed and analyzed, including tree structures [1, 32], locality sensitive hashing [10, 35], production quantization [18, 11], data partitioning [27, 44], graph-based methods [28, 17], and so on. The general case for NNS utilizing learned similarities remains less studied; for learned index structures, techniques to construct trees have been proposed to ensure beam search result in globally optimal top-K results [46]. Algorithms based on implicit [28, 17, 39, 31] or explicit graphs [39] have been proposed to obtain a tractable candidate set in multi-stage retrieval setups; however, such approaches' performance can degrade when the similarity function is not a metric, and constructing appropriate graph indices for non-metric similarity functions can remain challenging even for the inner product case [30]. Due to GPUs and other accelerators having orders of magnitude higher arithmetic intensity vs CPUs, traditional quantization techniques [35, 11] no longer fully utilize GPUs; accelerator-specific nearest neighbor algorithms that benefit from increased compute have been proposed and analyzed in recent work [4, 42, 31, 3].

6 Conclusion

We have analyzed techniques for efficient retrieval with learned similarities in this work. We begin by showing Mixture-of-Logits (*MoL*) is a universal approximator of learned similarity functions, and further empirically learnable – *MoL* consistently outperforms dot products in HR across 6 scenarios by an average of 24.2% in HR@1 and 14.3% in HR@10, setting new state-of-the-art on recommendation datasets. We next propose both exact and approximate algorithms to enable efficient retrieval using learned similarity functions, and show their correctness and bounds. Across all datasets evaluated, we demonstrate that our approximate top K algorithms can reach .99 of Hit Rate relative to exact algorithms, while achieving up to $91\times$ reduction in end-to-end latency and with minimal indexing overheads. We expect the speedups to be further amplified with larger-scale datasets and GPU kernel optimizations. Given MoL's empirical impressive performance gains of 20%-30% across Hit Rate@50-400 over hundreds of millions to billions of items [42, 3], our work concludes both theoretical and practical justifications for migrating vector databases away from dense retrieval and MIPS to Retrieval with Learned Similarities (RAILS) on GPUs.

Limitations

While we have performed evaluations on top of one of the largest recommendation datasets publicly available with 674,044 items, we expect potentially different algorithmic behaviors as we scale our approximate top-K algorithms to handle hundreds to millions to billions of items. Additional low-level GPU kernel optimizations, one of which being an efficient grouped top-K query kernel that fetches top-K for multiple query embeddings (e.g., $f_1(q), \ldots, f_{P_q}(q)$), could also change the relative efficiency of approximate methods we discussed, in particular *TopKAvg*(N) and *CombTopK*$N_1\_N_2$. We also leave more efficient implementations of the two-pass exact algorithm as future work.

References

[1] Jon Louis Bentley. Multidimensional binary search trees used for associative searching. *Commun. ACM*, 18(9):509–517, sep 1975.

[2] Sebastian Borgeaud, Arthur Mensch, Jordan Hoffmann, Trevor Cai, Eliza Rutherford, Katie Millican, George van den Driessche, Jean-Baptiste Lespiau, Bogdan Damoc, Aidan Clark, Diego de Las Casas, Aurelia Guy, Jacob Menick, Roman Ring, Tom Hennigan, Saffron Huang, Loren Maggiore, Chris Jones, Albin Cassirer, Andy Brock, Michela Paganini, Geoffrey Irving, Oriol Vinyals, Simon Osindero, Karen Simonyan, Jack W. Rae, Erich Elsen, and Laurent Sifre. Improving language models by retrieving from trillions of tokens. In Kamalika Chaudhuri, Stefanie Jegelka, Le Song, Csaba Szepesvári, Gang Niu, and Sivan Sabato, editors, *International Conference on Machine Learning, ICML 2022, 17-23 July 2022, Baltimore, Maryland, USA*, volume 162 of *Proceedings of Machine Learning Research*, pages 2206–2240. PMLR, 2022.

[3] Fedor Borisyuk, Qingquan Song, Mingzhou Zhou, Ganesh Parameswaran, Madhu Arun, Siva Popuri, Tugrul Bingol, Zhuotao Pei, Kuang-Hsuan Lee, Lu Zheng, Qizhan Shao, Ali Naqvi, Sen Zhou, and Aman Gupta. Linr: Model based neural retrieval on gpus at linkedin, 2024.

[4] Felix Chern, Blake Hechtman, Andy Davis, Ruiqi Guo, David Majnemer, and Sanjiv Kumar. TPU-KNN: K nearest neighbor search at peak FLOP/s. In *Advances in Neural Information Processing Systems*, 2022.

[5] Paul Covington, Jay Adams, and Emre Sargin. Deep neural networks for youtube recommendations. In *Proceedings of the 10th ACM Conference on Recommender Systems*, RecSys '16, page 191–198, 2016.

[6] Chantat Eksombatchai, Pranav Jindal, Jerry Zitao Liu, Yuchen Liu, Rahul Sharma, Charles Sugnet, Mark Ulrich, and Jure Leskovec. Pixie: A system for recommending 3+ billion items to 200+ million users in real-time. In *Proceedings of the 2018 World Wide Web Conference*, WWW '18, page 1775–1784, 2018.

[7] Stefan Elfwing, Eiji Uchibe, and Kenji Doya. Sigmoid-weighted linear units for neural network function approximation in reinforcement learning. *CoRR*, abs/1702.03118, 2017.

[8] Weihao Gao, Xiangjun Fan, Chong Wang, Jiankai Sun, Kai Jia, Wenzi Xiao, Ruofan Ding, Xingyan Bin, Hui Yang, and Xiaobing Liu. Learning an end-to-end structure for retrieval in large-scale recommendations. In *Proceedings of the 30th ACM International Conference on Information and Knowledge Management*, CIKM '21, page 524–533, 2021.

[9] Daniel Gillick, Alessandro Presta, and Gaurav Singh Tomar. End-to-end retrieval in continuous space, 2018.

[10] Aristides Gionis, Piotr Indyk, and Rajeev Motwani. Similarity search in high dimensions via hashing. In *Proceedings of the 25th International Conference on Very Large Data Bases*, VLDB '99, page 518–529, San Francisco, CA, USA, 1999. Morgan Kaufmann Publishers Inc.

[11] Ruiqi Guo, Sanjiv Kumar, Krzysztof Choromanski, and David Simcha. Quantization based fast inner product search. In *Proceedings of the 19th International Conference on Artificial Intelligence and Statistics, AISTATS 2016*, volume 51, pages 482–490, 2016.

[12] Ruiqi Guo, Philip Sun, Erik Lindgren, Quan Geng, David Simcha, Felix Chern, and Sanjiv Kumar. Accelerating large-scale inference with anisotropic vector quantization. In *Proceedings of the 37th International Conference on Machine Learning*, ICML'20. JMLR.org, 2020.

[13] F. Maxwell Harper and Joseph A. Konstan. The movielens datasets: History and context. *ACM Trans. Interact. Intell. Syst.*, 5(4), dec 2015.

[14] Xiangnan He, Lizi Liao, Hanwang Zhang, Liqiang Nie, Xia Hu, and Tat-Seng Chua. Neural collaborative filtering. In *Proceedings of the 26th International Conference on World Wide Web*, WWW '17, page 173–182, 2017.

[15] Balázs Hidasi, Alexandros Karatzoglou, Linas Baltrunas, and Domonkos Tikk. Session-based recommendations with recurrent neural networks. In Yoshua Bengio and Yann LeCun, editors, *4th International Conference on Learning Representations, ICLR 2016, San Juan, Puerto Rico, May 2-4, 2016, Conference Track Proceedings*, 2016.

[16] Kalina Jasinska, Krzysztof Dembczynski, Robert Busa-Fekete, Karlson Pfannschmidt, Timo Klerx, and Eyke Hullermeier. Extreme f-measure maximization using sparse probability estimates. In Maria Florina Balcan and Kilian Q. Weinberger, editors, *Proceedings of The 33rd International Conference on Machine Learning*, volume 48 of *Proceedings of Machine Learning Research*, pages 1435–1444, New York, New York, USA, 20–22 Jun 2016. PMLR.

[17] Suhas Jayaram Subramanya, Fnu Devvrit, Harsha Vardhan Simhadri, Ravishankar Krishnawamy, and Rohan Kadekodi. Diskann: Fast accurate billion-point nearest neighbor search on a single node. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019.

[18] Herve Jegou, Matthijs Douze, and Cordelia Schmid. Product quantization for nearest neighbor search. *IEEE Trans. Pattern Anal. Mach. Intell.*, 33(1):117–128, jan 2011.

[19] J. Johnson, M. Douze, and H. Jegou. Billion-scale similarity search with gpus. *IEEE Transactions on Big Data*, 7(03):535–547, Jul 2021.

[20] Wang-Cheng Kang and Julian McAuley. Self-attentive sequential recommendation. In *2018 International Conference on Data Mining (ICDM)*, pages 197–206, 2018.

[21] Vladimir Karpukhin, Barlas Oguz, Sewon Min, Patrick Lewis, Ledell Wu, Sergey Edunov, Danqi Chen, and Wen-tau Yih. Dense passage retrieval for open-domain question answering. In Bonnie Webber, Trevor Cohn, Yulan He, and Yang Liu, editors, *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, pages 6769–6781, Online, November 2020. Association for Computational Linguistics.

[22] Omar Khattab and Matei Zaharia. Colbert: Efficient and effective passage search via contextualized late interaction over bert. In *Proceedings of the 43rd International ACM SIGIR Conference on Research and Development in Information Retrieval*, SIGIR '20, page 39–48, New York, NY, USA, 2020. Association for Computing Machinery.

[23] Anton Klenitskiy and Alexey Vasilev. Turning dross into gold loss: is bert4rec really better than sasrec? In *Proceedings of the 17th ACM Conference on Recommender Systems*, RecSys '23, page 1120–1125, New York, NY, USA, 2023. Association for Computing Machinery.

[24] Yehuda Koren, Robert Bell, and Chris Volinsky. Matrix factorization techniques for recommender systems. *Computer*, 42(8):30–37, 2009.

[25] Patrick Lewis, Ethan Perez, Aleksandra Piktus, Fabio Petroni, Vladimir Karpukhin, Naman Goyal, Heinrich Küttler, Mike Lewis, Wen-tau Yih, Tim Rocktäschel, Sebastian Riedel, and Douwe Kiela. Retrieval-augmented generation for knowledge-intensive nlp tasks. In *Proceedings of the 34th International Conference on Neural Information Processing Systems*, NIPS '20, Red Hook, NY, USA, 2020. Curran Associates Inc.

[26] Chao Li, Zhiyuan Liu, Mengmeng Wu, Yuchi Xu, Huan Zhao, Pipei Huang, Guoliang Kang, Qiwei Chen, Wei Li, and Dik Lun Lee. Multi-interest network with dynamic routing for recommendation at tmall. In *Proceedings of the 28th ACM International Conference on Information and Knowledge Management*, CIKM '19, page 2615–2623, 2019.

[27] Chen Li, E. Chang, H. Garcia-Molina, and G. Wiederhold. Clustering for approximate similarity search in high-dimensional spaces. *IEEE Transactions on Knowledge and Data Engineering*, 14(4):792–808, 2002.

[28] Yu A. Malkov and D. A. Yashunin. Efficient and robust approximate nearest neighbor search using hierarchical navigable small world graphs. *IEEE Trans. Pattern Anal. Mach. Intell.*, 42(4):824–836, apr 2020.

[29] Julian McAuley, Christopher Targett, Qinfeng Shi, and Anton van den Hengel. Image-based recommendations on styles and substitutes. In *Proceedings of the 38th International ACM SIGIR Conference on Research and Development in Information Retrieval*, SIGIR '15, page 43–52, New York, NY, USA, 2015. Association for Computing Machinery.

[30] Stanislav Morozov and Artem Babenko. Non-metric similarity graphs for maximum inner product search. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 31. Curran Associates, Inc., 2018.

[31] Hiroyuki Ootomo, Akira Naruse, Corey Nolet, Ray Wang, Tamas Feher, and Yong Wang. Cagra: Highly parallel graph construction and approximate nearest neighbor search for gpus, 2024.

[32] Parikshit Ram and Alexander G. Gray. Maximum inner-product search using cone trees. In *Proceedings of the 18th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, KDD '12, page 931–939, 2012.

[33] Steffen Rendle, Walid Krichene, Li Zhang, and John Anderson. Neural collaborative filtering vs. matrix factorization revisited. In *Fourteenth ACM Conference on Recommender Systems (RecSys'20)*, page 240–248, 2020.

[34] Keshav Santhanam, Omar Khattab, Jon Saad-Falcon, Christopher Potts, and Matei Zaharia. ColBERTv2: Effective and efficient retrieval via lightweight late interaction. In Marine Carpuat, Marie-Catherine de Marneffe, and Ivan Vladimir Meza Ruiz, editors, *Proceedings of the 2022 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies*, pages 3715–3734, Seattle, United States, July 2022. Association for Computational Linguistics.

[35] Anshumali Shrivastava and Ping Li. Asymmetric lsh (alsh) for sublinear time maximum inner product search (mips). In *Advances in Neural Information Processing Systems*, volume 27, 2014.

[36] Weiwei Sun, Lingyong Yan, Zheng Chen, Shuaiqiang Wang, Haichao Zhu, Pengjie Ren, Zhumin Chen, Dawei Yin, Maarten Rijke, and Zhaochun Ren. Learning to tokenize for generative retrieval. In A. Oh, T. Naumann, A. Globerson, K. Saenko, M. Hardt, and S. Levine, editors, *Advances in Neural Information Processing Systems*, volume 36, pages 46345–46361. Curran Associates, Inc., 2023.

[37] Shulong Tan, Zhixin Zhou, Zhaozhuo Xu, and Ping Li. Fast item ranking under neural network based measures. In *Proceedings of the 13th International Conference on Web Search and Data Mining*, WSDM '20, page 591–599, New York, NY, USA, 2020. Association for Computing Machinery.

[38] Yi Tay, Vinh Q. Tran, Mostafa Dehghani, Jianmo Ni, Dara Bahri, Harsh Mehta, Zhen Qin, Kai Hui, Zhe Zhao, Jai Gupta, Tal Schuster, William W. Cohen, and Donald Metzler. Transformer memory as a differentiable search index. In Alice H. Oh, Alekh Agarwal, Danielle Belgrave, and Kyunghyun Cho, editors, *Advances in Neural Information Processing Systems*, 2022.

[39] Yiwei Wang, Bryan Hooi, Yozen Liu, Tong Zhao, Zhichun Guo, and Neil Shah. Flashlight: Scalable link prediction with effective decoders. In Bastian Rieck and Razvan Pascanu, editors, *Proceedings of the First Learning on Graphs Conference*, volume 198 of *Proceedings of Machine Learning Research*, pages 14:1–14:17. PMLR, 09–12 Dec 2022.

[40] Yujing Wang, Yingyan Hou, Haonan Wang, Ziming Miao, Shibin Wu, Qi Chen, Yuqing Xia, Chengmin Chi, Guoshuai Zhao, Zheng Liu, Xing Xie, Hao Sun, Weiwei Deng, Qi Zhang, and Mao Yang. A neural corpus indexer for document retrieval. In S. Koyejo, S. Mohamed, A. Agarwal, D. Belgrave, K. Cho, and A. Oh, editors, *Advances in Neural Information Processing Systems*, volume 35, pages 25600–25614. Curran Associates, Inc., 2022.

[41] Zhilin Yang, Zihang Dai, Ruslan Salakhutdinov, and William W. Cohen. Breaking the softmax bottleneck: A high-rank RNN language model. In *International Conference on Learning Representations (ICLR'18)*, 2018.

[42] Jiaqi Zhai, Zhaojie Gong, Yueming Wang, Xiao Sun, Zheng Yan, Fu Li, and Xing Liu. Revisiting neural retrieval on accelerators. In *Proceedings of the 29th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, KDD '23, page 5520–5531, New York, NY, USA, 2023. Association for Computing Machinery.

[43] Jiaqi Zhai, Lucy Liao, Xing Liu, Yueming Wang, Rui Li, Xuan Cao, Leon Gao, Zhaojie Gong, Fangda Gu, Jiayuan He, Yinghai Lu, and Yu Shi. Actions speak louder than words: Trillion-parameter sequential transducers for generative recommendations. In Ruslan Salakhutdinov, Zico Kolter, Katherine Heller, Adrian Weller, Nuria Oliver, Jonathan Scarlett, and Felix Berkenkamp, editors, *Proceedings of the 41st International Conference on Machine Learning*, volume 235 of *Proceedings of Machine Learning Research*, pages 58484–58509. PMLR, 21–27 Jul 2024.

[44] Jiaqi Zhai, Yin Lou, and Johannes Gehrke. Atlas: A probabilistic algorithm for high dimensional similarity search. In *Proceedings of the 2011 ACM SIGMOD International Conference on Management of Data*, SIGMOD '11, page 997–1008, 2011.

[45] Han Zhu, Xiang Li, Pengye Zhang, Guozheng Li, Jie He, Han Li, and Kun Gai. Learning tree-based deep model for recommender systems. In *Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, KDD '18, page 1079–1088, 2018.

[46] Jingwei Zhuo, Ziru Xu, Wei Dai, Han Zhu, Han Li, Jian Xu, and Kun Gai. Learning optimal tree models under beam search. In *Proceedings of the 37th International Conference on Machine Learning*, ICML'20. JMLR.org, 2020.

A   Experiment Setups

Reproducibility.   Our code is publicly available online, and detailed implementations and hyperparameter settings for reproducing our experiment results can be found at the following url: `https://github.com/bailuding/rails`. We discuss key settings below.

Parameterization of low-rank ("component-level") embeddings, $f_p(q)$ **and** $g_p(x)$**s for** $1 \leq p \leq P$**.** We note that embedding parameterization was not explicitly discussed in the original Mixture-of-Logits paper [42]. A specific implementation utilizing cluster id information has been proposed and discussed in a follow up work [3], where in the context of large-scale recommendation systems, the authors suggested cluster information based on interests of cohorts of members and topics of posts by themselves can lead to 10% recall gain at $K = 400$. However, we cannot easily access similar information in the publicly available MovieLens and Amazon Reviews datasets. We therefore follow implementation provided by the authors [42] and additionally optionally utilizes a User ID keyed one-hot embedding as one query-side low-rank ("component-level") embeddings $f_p(q)$, which is a widely used technique in recommendation systems [24]. All other $f_p(q)$s and $g_p(x)$s are obtained by applying an MLP on top of query-side/item-side representations in standard sequential recommendation setups [15, 20].

Parameterization of $\pi_p(q, x)$ matrices. We follow the implementation provided by the authors [42], which parameterizes $\pi_p(q, x)$ as a two-layer multi-layer perceptron (MLP) with SiLU [7] non-linearity. The inputs to this MLP consist of user-side features, item-side features, and the P dot products $\langle f_p(q), g_p(x) \rangle$s between the learned low-rank embeddings.

Hyperparameter settings. We use an identical number of sampled negatives for dot product baselines (cosine similarity, "SASRec", "HSTU" rows in Table 3) and Mixture-of-logits ("SASRec + MoL", "HSTU + MoL" rows in Table 3) to ensure a fair comparison, which is 128 for ML-1M and ML-20M and 512 for Amazon Books following prior work. For "+ MoL" rows, we additionally grid searched $|P_x|$ in $\{2, 4, 8, 16\}$, d_P in $\{32, 64, 128\}$), whether to enable user-id based learned embeddings, and the dropout rate to apply to user-id based embeddings in $\{0.2, 0.5, 0.8\}$ for the smaller MovieLens datasets. Due to resource constraints, we followed initial hyperparameters provided by the authors [42] for all other parameters.

A.1 Efficiency

	Method	HR@10	HR@50	MRR	Time/Epoch
ML-1M	SASRec	.2818	.5470	.1352	37s
	SASRec + MoL	.3034 (+7.7%)	.5655 (+3.4%)	.1448 (+7.1%)	44s (+18.9%)
	HSTU	.3332	.5956	.1579	41s
	HSTU + MoL	**.3460 (+3.8%)**	**.6048 (+1.5%)**	**.1673 (+6.0%)**	46s (+12.2%)
ML-20M	SASRec	.2883	.5484	.1375	197s
	SASRec + MoL	.3124 (+8.4%)	.5685 (+3.7%)	.1551 (+12.8%)	449s (+127.9%)
	HSTU	.3557	.6146	.1800	526s
	HSTU + MoL	**.3697 (+3.9%)**	**.6244 (+1.6%)**	**.1880 (+4.4%)**	773s (+47.0%)
Books	SASRec	.0306	.0754	.0153	506s
	SASRec + MoL	.0402 (+31.4%)	.0970 (+28.6%)	.0203 (+32.7%)	964s (+90.5%)
	HSTU	.0469	.1066	.0233	1883s
	HSTU + MoL	**.0613 (+30.7%)**	**.1292 (+21.2%)**	**.0315 (+35.2%)**	2236s (+18.7%)

Table 5: Evaluation of recommendation retrieval performance, utilizing the next-item prediction task. Note that these results are identical to those reported in Table 3 but with relative gains (MoL vs dot product) and training cost changes illustrated under different sequential encoder backbones.

Training efficiency. We measure the training efficiency of the setups in Section 4 over one epoch of data, utilizing a single RTX 6000 Ada GPU and with a constant batch size of 128 for ML-1M and ML-20M, and 64 for Amazon Books in Table 5. Consistent with prior findings [42, 3], MoL's model quality increases do not generally come with a large increase in training time, thanks to MoL's higher arithmetic intensity on GPUs, with an average increase of 53% across the six scenarios. To contextualize this 1.53x training cost, prior work on sequential recommenders, such as self-supervised bidirectional models, came with a 5.9x training time increase on ML-20M and 4.5x training time increase on Amazon Reviews (BERT4Rec vs SASRec rows) [23]. We expect additional GPU kernel-level optimizations, such as kernel fusions, to further improve efficiency of the "+ MoL" rows.

Inference efficiency. Given the number of items (3K, 24K, and 674K) in these datasets, as discussed in Table 2, these public benchmark datasets are not good candidates for measuring inference latency. We note that prior work have reported batched inference latency between 5ms and 20ms on datasets with hundreds of millions to billions of items [42, 3], which is inline with optimized MIPS baselines.