A Greedy Approach for Budgeted Maximum Inner Product Search

Hsiang-Fu Yu  
The University of Texas at Austin  
rofuyu@cs.utexas.edu

Cho-Jui Hsieh  
The University of California, Davis  
chohsieh@cs.ucdavis.edu

Qi Lei  
The University of Texas at Austin  
leiqi@ices.utexas.edu

Inderjit S. Dhillon  
The University of Texas at Austin  
derjit@cs.utexas.edu

Abstract

Maximum Inner Product Search (MIPS) is an important task in many machine learning applications such as the prediction phase of a low-rank matrix factorization model for a recommender system. There have been some works on how to perform MIPS in sub-linear time recently. However, most of them do not have the flexibility to control the trade-off between search efficient and search quality. In this paper, we study the MIPS problem with a computational budget. By carefully studying the problem structure of MIPS, we develop a novel Greedy-MIPS algorithm, which can handle budgeted MIPS by design. While simple and intuitive, Greedy-MIPS yields surprisingly superior performance compared to state-of-the-art approaches. As a specific example, on a candidate set containing half a million vectors of dimension 200, Greedy-MIPS runs 200x faster than the naive approach while yielding search results with the top-5 precision greater than 75%.

1 Introduction

In this paper, we study the computational issue in the prediction phase for many matrix factorization based latent embedding models in recommender systems, which can be mathematically formulated as a Maximum Inner Product Search (MIPS) problem. Specifically, given a large collection of $n$ candidate vectors

$$
\mathcal{H} = \{ h_j \in \mathbb{R}^k : 1, \ldots, n \}
$$

and a query vector $w \in \mathbb{R}^k$, MIPS aims to identify a subset of candidates that have top largest inner product values with $w$. We also denote $H = [h_1, \ldots, h_j, \ldots, h_n]^\top$ as the candidate matrix. A naive linear search procedure to solve MIPS for a given query $w$ requires $O(nk)$ operations to compute $n$ inner products and $O(n \log n)$ operations to obtain the sorted ordering of the $n$ candidates.\footnote{When only the largest $B$ elements are required, the sorting procedure can be reduced to $O(n + B \log B)$ on average using a selection algorithm \cite{hoare1962quicksort}.}

Recently, MIPS has drawn a lot of attention in the machine learning community. Matrix factorization (MF) based recommender system \cite{srivastava2015collaborative, koren2009matrix} is one of the most important applications. In an MF based recommender system, each user $i$ is associated with a vector $w_i$ of dimension $k$, while each item $j$ is associated with a vector $h_j$ of dimension $k$. The interaction (such as preference) between a user and an item is modeled by the value of the inner product between $w_i$ and $h_j$. It is clear that identifying top-ranked items in such a system for a user is exactly a MIPS problem. Because both the number of users (the number of queries) and the number of items (size of vector pool in MIPS) can easily grow to millions, a naive linear search is extremely expensive; for example, to compute the preference for all $m$ users over $n$ items with latent embeddings of dimension $k$ in a recommender system requires at least $O(mnk)$ operations. When both $m$ and $n$ are large, the prediction procedure is extremely time consuming; it is even slower than the training
procedure used to obtain the $m + n$ embeddings, which costs only $O(|\Omega|k)$ operations per iteration. Taking the yahoo-music dataset as an example, we have $m = 1M$, $n = 0.6M$, $|\Omega| = 250M$, and

$$mn = 600B \gg 250M = |\Omega|.$$ 

As a result, the development of efficient algorithms for MIPS is needed in large-scale recommender systems. In addition, MIPS can be found in many other machine learning applications, such as the prediction for a multi-class or multi-label classifier [15, 18], an object detector, a structure SVM predicator, and many others.

There is a recent line of research on accelerating MIPS for large $n$, such as [2, 3, 9, 11–13]. However, most of them do not have the flexibility to control the trade-off between search efficiency and search quality in the prediction phase. In this paper, we consider the budgeted MIPS problem, which is a generalized version of the standard MIPS with a computation budget: how to generate a set of top-ranked candidates under a given budget on the number of inner products one can perform. By carefully studying the problem structure of MIPS, we develop a novel Greedy-MIPS algorithm, which handles budgeted MIPS by design. While simple and intuitive, Greedy-MIPS yields surprisingly superior performance compared to existing state-of-the-art approaches.

**Contributions.** Our contributions can be summarized as follows:

- We carefully study the MIPS problem and develop Greedy-MIPS, which is a novel algorithm without any nearest neighbor search reduction that is essential in many state-of-the-art approaches [2, 11, 13].
- Greedy-MIPS is orders of magnitudes faster than many state-of-the-art MIPS approaches to obtain a desired search performance. As a specific example, on the yahoo-music data sets with $n = 624,961$ and $k = 200$, Greedy-MIPS runs 200x faster than the naive approach and yields search results with the top-5 precision more than 75%, while the search performance of other state-of-the-art approaches under the similar speedup drops to less than 3% precision.
- Greedy-MIPS supports MIPS with a budget, which brings the ability to control of the trade-off between computation efficiency and search quality in the prediction phase. To the best of our knowledge, among existing MIPS approaches, only the sampling approaches proposed in [3, 5] support the similar flexibility under a limited situation where all the candidates and query vectors are non-negative.

**Organization.** We first review existing fast MIPS approaches in Section 2 and introduce the budgeted MIPS problem in Section 3. In Section 4, we propose a novel greedy budgeted MIPS approach called Greedy-MIPS. We then show the empirical comparison in Section 5 and conclude this paper in Section 6.

## 2 Existing Approaches for Fast MIPS

Because of its wide applicability, several algorithms have been proposed to design efficient algorithms for MIPS. Most of existing approaches consider to reduce the MIPS problem to the nearest neighbor search problem (NNS), where the goal is to identify the nearest candidates of the given query, and apply an existing efficient NNS algorithm to solve the reduced problem [1, 2, 11, 13, 14]. [2] is the first MIPS work which adopts such a MIPS-to-NNS reduction. Variants MIPS-to-NNS reduction are also proposed in [13, 14]. Experimental results in [2] show the superiority of the NNS reduction over the traditional branch-and-bound search approaches for MIPS [9, 12].

Fast MIPS approaches with sampling schemes have become popular recently [3, 5]. Various sampling schemes have been proposed to handle MIPS problem with different constraints. We will briefly review two popular sampling schemes in Section 2.2.
Figure 1: MIPS-to-NN reduction. In 1(a), all the candidate vectors \{h_j\} and the query vector \(w\) are in \(\mathbb{R}^2\). \(h_2\) is the nearest neighbor of \(w\), while \(h_1\) is the vector yielding the maximum value of the inner product with \(w\). In 1(b), the reduction proposed in [2] is applied to \(w\) and \{\(h_j\)\}: \(\hat{w} = [w; 0]^\top\) and \(\hat{h}_j = [h_j; \sqrt{M - \|h_j\|^2}]^\top\), \(\forall j\), where \(M = \max_j \|h_j\|^2\). All the transformed vectors are in the 3-dimensional sphere with radius \(\sqrt{M}\). As a result, the nearest neighbor of \(\hat{w}\) in this transformed 3-dimensional NNS problem, \(\hat{h}_1\), corresponds to the vector \(h_1\) which yields the maximum inner product value with \(w\) in the original 2-dimensional MIPS problem.

### 2.1 Approaches with Nearest Neighbor Search Reduction

We briefly introduce the concept of the reduction proposed in [2]. First, we consider the relationship between the Euclidean distance and the inner product:

\[
\|w - h_{j_1}\|^2 = \|w\|^2 + \|h_{j_1}\|^2 - 2w^\top h_{j_1},
\]

\[
\|w - h_{j_2}\|^2 = \|w\|^2 + \|h_{j_2}\|^2 - 2w^\top h_{j_2}.
\]

When all the candidate vectors \(h_j\) share the same length; that is,

\[
\|h_1\| = \|h_2\| = \cdots = \|h_n\|,
\]

the MIPS problem is exactly the same as the NNS problem because

\[
\|w - h_{j_1}\| > \|w - h_{j_2}\| \iff w^\top h_{j_1} < w^\top h_{j_2} \quad (1)
\]

when \(\|h_{j_1}\| = \|h_{j_2}\|\). However, when \(\|h_{j_1}\| \neq \|h_{j_2}\|\), (1) no longer holds. See Figure 1(a) for an example where not all the candidate vectors have the same length. We can see that \(h_1\) is the candidate vector yielding the maximum inner product with \(w\), while \(h_2\) is the nearest neighbor candidate.

To handle the situation where candidates have different lengths, [2] proposes the following transform to reduce the original MIPS problem with \(\mathcal{H}\) and \(w\) in a \(k\) dimensional space to a new NNS problem with...
\( \mathcal{H} = \{ \hat{h}_1, \ldots, \hat{h}_n \} \) and \( \hat{w} \) in a \( k + 1 \) dimensional space:

\[
\hat{w} = [w; 0]^\top, \\
\hat{h}_j = \left[ h_j; \sqrt{M - \|h_j\|^2} \right]^\top, \quad \forall j = 1, \ldots, n,
\]

(2)

where \( M \) is the maximum squared length over the entire candidate set \( \mathcal{H} \):

\[
M = \max_{j=1, \ldots, n} \|h_j\|^2.
\]

First, we can see that with the above transform, \( \|\hat{h}_j\|^2 = M \) for all \( j \):

\[
\|\hat{h}_j\|^2 = \|h_j\|^2 + M - \|h_j\|^2 = M, \quad \forall j.
\]

Then, for any \( j_1 \neq j_2 \), we have

\[
\|\hat{w} - \hat{h}_{j_1}\| < \|\hat{w} - \hat{h}_{j_2}\| \iff M + \|w\|^2 - 2w^\top h_{j_1} < M + \|w\|^2 - 2w^\top h_{j_2}
\]

\[
\iff w^\top h_{j_1} > w^\top h_{j_2}.
\]

With the above relationship, the original \( k \)-dimensional MIPS problem is equivalent to the transformed \( k + 1 \) dimensional NNS problem. In Figure 1(b), we show the transformed NNS problem for the original MIPS problem presented in Figure 1(a).

In [14], another MIPS-to-NNS reduction has been proposed. The high level idea is to apply a transformation to \( \mathcal{H} \) such that all the candidate vectors roughly have the same length by appending additional \( \bar{k} \) dimensions. In the procedure by [14], all the \( h_j \) vectors are assumed (or scaled) to have \( \|h_j\| \leq U, \forall j \), where \( U < 1 \) is a positive constant. Then the following transform is applied to reduce the original \( k \)-dimensional MIPS problem to a new NNS problem with \((k + \bar{k})\)-dimensional vectors \( \hat{h}_j \) and \( \hat{w} \) defined as:

\[
\hat{w} = [w; 0_{\bar{k}}]^\top, \\
\hat{h}_j = \left[ h_j; 1/2 - \|h_j\|^2; 1/2 - \|h_j\|^2; \ldots; 1/2 - \|h_j\|^2 \right]^\top,
\]

(3)

where \( 0_{\bar{k}} \) is a zero vector of dimension \( \bar{k} \). Because \( U < 1 \), [14] shows that with the transform (3), we have \( \|\hat{h}_j\|^2 = \bar{k}/4 + \|h_j\|^{2\bar{k} + 1} \), with the second term vanishing as \( \bar{k} \to \infty \). Thus, all the candidates \( \hat{h}_j \) approximately have the same length. We can see the idea behind (3) is similar to (2): transforming \( \mathcal{H} \) to \( \hat{\mathcal{H}} \) such that all the candidates have the same length. Note that (2) achieves this goal exactly while (3) achieves this goal approximately. Both transforms show a similar empirical performance in [11].

There are many choices to solve the transformed NNS problem after the MIPS-to-NN reduction has been applied. In [11, 13, 14], various locality sensitive hashing schemes have been considered. In [2], a PCA-tree based approach is proposed, and shows better performance than LSH-based approaches, which is consistent to the empirical observations in [1] and our experimental results shown in Section 5. In [1], a simple K-means clustering algorithm is proposed to handled the transformed NNS problem.

### 2.2 Sampling-based Approaches

The idea of the sampling-based MIPS approach is first proposed in [5] as an approach to perform approximate matrix-matrix multiplications. Its applicability on MIPS problems is studied very recently [3]. The idea
behind a sampling-based approach called Sample-MSIPS, is about to design an efficient sampling procedure such that the $j$-th candidate is selected with probability $p(j)$:

$$p(j) \sim h_j^\top w.$$ 

In particular, Sample-MSIPS is an efficient scheme to sample $(j,t) \in [n] \times [k]$ with the probability $p(j,t)$:

$$p(j,t) \sim h_{jt}w_t.$$ 

Each time a pair $(j,t)$ is sampled, we increase the count for the $j$-th item by one. By the end of the sampling process, the spectrum of the counts forms an estimation of $n$ inner product values. Due to the nature of the sampling approach, it can only handle the situation where all the candidate vectors and query vectors are nonnegative.

Diamond-MSIPS, a diamond sampling scheme proposed in [3], is an extension of Sample-MSIPS to handle the maximum squared inner product search problem (MSIPS) where the goal is to identify candidate vectors with largest values of $(h_j^\top w)^2$. If both $w$ and $H$ are nonnegative or $h_j^\top w \geq 0$, $\forall j$, MSIPS can be used to generate the solutions for MIPS. However, the solutions to MSIPS can be very different from the solutions to MIPS in general. For example, if all the inner product values are negative, the ordering for MSIPS is the exactly reverse ordering induced by MIPS. Here we can see that the applicability of both Sample-MSIPS and Diamond-MSIPS to MIPS is very limited.

3 Budgeted Maximum Inner Product Search

The core idea behind the fast approximate MIPS approaches is to trade the search quality for the shorter query latency: the shorter the search latency, the lower the search quality. In most existing fast MIPS approaches, the trade-off depends on the approach-specific parameters such as the depth of the PCA tree in [2] or the number of hash functions in [11, 13, 14]. Such approach-specific parameters are usually required to construct approach-specific data structures before any query is given, which means that the trade-off is somewhat fixed for all the queries. Particularly, the computation cost for all the query requests is fixed. However, in many real-world scenarios, each query request might have a different computational budget, which raises the question: Can we design a fast MIPS approach which supports the dynamic adjustment of the trade-off in the query phase?

In this section, we formally define the budgeted MIPS problem which is an extension of the standard MIPS problem with a computational budget as a parameter given in the query phase. We first summarize the essential components for fast MIPS approaches in Section 3.1 and give the problem definition of budgeted MIPS in Section 3.2.

3.1 Essential Components for Fast MIPS Approaches

Before diving into the details of budgeted MIPS, we first review the essential components in fast MIPS algorithms:

- **Before any query request:**
  - **Query-Independent Data Structure Construction:** A pre-processing procedure is performed on the entire candidate sets to construct an approach-specific data structure $D$ to store information about $H$, such as the LSH hash tables [11, 13, 14], space partition trees (e.g., KD-tree or PCA-tree [2]), or cluster centroids [1].

- **For each query request:**
  - **Query-dependent Pre-processing:** In some approaches, a query dependent pre-processing is needed. For example, a vector augmentation is required in all approaches with the MIPS-to-NNS reduction [1, 2, 11, 13]. In addition, [2] also requires another normalization. $T_P$ is used to denote the time complexity of this stage.
– **Candidate Screening**: In this stage, based on the pre-constructed data structure \( D \), an efficient procedure is performed to filter candidates such that only a subset of candidates \( C(w) \subset \mathcal{H} \) is selected. In a naive linear approach, no screening procedure is performed, so \( C(w) \) simply contains all the \( n \) candidates. For a tree-based structure, \( C(w) \) contains all the candidates stored in the leaf node of the query vector. In a sampling-based MIPS approach, an efficient sampling scheme is designed to generate highly possible candidates to form \( C(w) \). \( T_S \) denotes the computational cost of the screening stage.

– **Candidate Ranking**: An exact ranking is performed on the selected candidates in \( C(w) \) obtained from the screening stage. This involves the computation of \(|C(w)| \) inner products and the sorting procedure among these \(|C(w)| \) values. The overall time complexity \( T_R \) is

\[
T_R = O(|C(w)|k + |C(w)| \log |C(w)|).
\]

The per-query computational cost \( T_Q \) is

\[
T_Q = T_P + T_S + T_R.
\]

It is clear that the candidate screening stage is the key component for a fast MIPS approach. In terms of the search quality, the performance highly depends on whether the screening procedure can identify highly possible candidates. In terms of the query latency, the efficiency highly depends on the size of \( C(w) \) and how fast to generate \( C(w) \). The major difference between various fast MIPS approaches is the choice of the data structure \( D \) and the corresponding screening procedure.

### 3.2 Budgeted MIPS: Problem Definition

Budgeted maximum inner product search is an extension of the standard approximate MIPS problem with a computation budget: how to generate top-ranked candidates under a given budget on the number of inner product operations one can perform. Budgeted MIPS has a wide applicability. For example, a real-time recommender system must provide a list of recommended items for its users in a very short response time.

Note that the cost for the candidate ranking \( (T_R) \) is inevitable in the per-query cost: \( T_Q = T_P + T_S + T_R \). A viable approach to support budgeted MIPS must include a screening procedure which satisfies the following requirements:

- the flexibility to control the size of \( C(w) \) in the candidate screening stage such that \(|C(w)| \leq B \), where \( B \) is a given budget, and
- an efficient screening procedure to obtain \( C(w) \) in \( O(Bk) \) time such that the overall per-query cost is

\[
T_Q = O(Bk + B \log B).
\]

As mentioned earlier, most recently proposed efficient algorithms such as PCA-MIPS [2] and LSH-MIPS [11, 13, 14] adopt the approach to reduce the MIPS problem to an instance of NNS problem, and apply various search space partition data structures or techniques (e.g., LSH, KD-tree, or PCA-tree) designed for NNS to index the candidates \( \mathcal{H} \) in the query-independent pre-processing stage. As the construction of \( D \) is query independent, both the search performance and the computation cost are fixed when the construction is done. For example, the performance of a PCA-MIPS depends on the depth of the PCA-tree. Given a query vector \( w \), there is no control to the size of \( C(w) \) in the candidate generating phase. LSH-based approaches also have the similar issue. As a result, it is not clear how to generalize PCA-MIPS and LSH-MIPS in a principled way to handle the situation with a computational budget: how to reduce the size of \( C(w) \) under a limited budget and how to improve the performance when a larger budget is given.

Unlike other NNS-based algorithms, the design of Sample-MSIPS naturally enables it to support budgeted MIPS for a nonnegative candidate matrix \( H \) and a nonnegative query \( w \). Recall that the core idea behind Sample-MSIPS is to draw a sample candidate \( j \) among \( n \) candidates such that

\[
p(j) \propto h_j^T w.
\]
The more the number of samples, the lower the variance of the estimated frequency spectrum. Clearly, Sample-MSIPS has the flexibility to control the size of $C(w)$, and thus is a viable approach for the budgeted MIPS problem. However, Sample-MSIPS works only on the situation where the entire $H$ and $w$ are non-negative. Diamond-MSIPS has the similar issue.

4 Greedy-MIPS: A Novel Approach for Budgeted MIPS

In this section, we carefully study the problem structure of MIPS and develop a simple but novel algorithm called Greedy-MIPS, which handles budgeted MIPS by design. Unlike the most recent approaches [1, 2, 11, 13, 14], Greedy-MIPS is an approach without any reduction to a NNS problem. Moreover, Greedy-MIPS is a viable approach for the budgeted MIPS problem without the non-negativity limitation inherited in the sampling approaches.

As mentioned earlier that the key component for a fast MIPS approach is the algorithm used in the candidate screening phase. In budgeted MIPS, for any given budget $B$ and query $w$, an ideal procedure for the candidate screening phase costs $O(Bk)$ time to generate $C(w)$ which contains the $B$ items with the largest $B$ inner product values over the $n$ candidates in $H$. The requirement on the time complexity $O(Bk)$ implies that the procedure is independent from $n = |H|$, the number of candidates in $H$. One might wonder whether such an ideal procedure exists or not. In fact, designing such an ideal procedure with the requirement to generate the largest $B$ items in $O(Bk)$ time is even more challenging than the original budgeted MIPS problem.

4.1 A Motivating Example for Greedy-MIPS

Although the existence of an ideal procedure for a general budgeted MIPS problem seems to be impossible, we demonstrate that an ideal approach exists for budgeted MIPS when $k = 1$. It is not hard to observe that Property 1 holds for any given $H = \{h_1, \ldots, h_n \mid h_j \in \mathbb{R} \}$:

**Property 1.** For any nonzero query $w \in \mathbb{R}$ and any budget $B > 0$, there are only two possible results for that top $B$ inner products between $w$ and $H$:

- $w > 0 \Rightarrow$ Largest $B$ elements in $H$,
- $w < 0 \Rightarrow$ Smallest $B$ elements in $H$.

This property leads to the following simple approach, which is an ideal procedure for the budgeted MIPS problem when $k = 1$:

- **Query-independent data structure:** a sorted list of indices of $H$: $s[\cdot]$, $r = 1, \ldots, n$ such that $s[r]$ stores the index to the $r$-th largest candidate. That is
  \[ h_{s[1]} \geq h_{s[2]} \geq \cdots \geq h_{s[n]} \],
- **Candidate screening phase:** for any given $w \neq 0$ and $B > 0$,

  \[
  \text{return } \begin{cases} 
  \{s[1], \ldots, s[B]\} & \text{if } w > 0, \\
  \{s[n], \ldots, s[n - B + 1]\} & \text{if } w < 0
  \end{cases}
  \]

as the indices of the exact largest-$B$ candidates.

Note that for this simple scenario ($k = 1$), neither the query dependent pre-processing nor the candidate ranking is needed. Thus, the overall time complexity per query is $T_Q = O(B)$. We can see that Property 1 is the key to the correctness of the above procedure. Nevertheless, it is not clear how to generalize Property 1 for MIPS problems with $k \geq 2$. Fortunately, we can directly utilize the fact that Property 1 holds for $k = 1$ to design an efficient greedy procedure for the candidate screening when $k \geq 2$. 

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4.2 A Greedy Procedure to Candidate Screening

To better describe the idea of the proposed algorithm Greedy-MIPS, we consider the following definition (4):

**Definition 1.** The rank of an item \( x \) among a set of items \( \mathcal{X} = \{x_1, \ldots, x_{|\mathcal{X}|}\} \) is defined as

\[
\text{rank}(x \mid \mathcal{X}) := \sum_{j=1}^{|\mathcal{X}|} \mathbb{1}[x_j \geq x],
\]

where \( \mathbb{1}[\cdot] \) is the indicator function. A ranking induced by \( \mathcal{X} \) is a function \( \pi(\cdot) : \mathcal{X} \rightarrow \{1, \ldots, |\mathcal{X}|\} \) such that \( \pi(x_j) = \text{rank}(x_j \mid \mathcal{X}) \forall x_j \in \mathcal{X} \).

One way to store a ranking \( \pi(\cdot) \) induced by \( \mathcal{X} \) is by a sorted index array \( s[x] \) of size \( |\mathcal{X}| \) such that

\[
\pi(x_{s[1]}) \leq \pi(x_{s[2]}) \leq \cdots \leq \pi(x_{s[|\mathcal{X}|]}).
\]

We can see that \( s[x] \) stores the index to the item \( x \) with \( \pi(x) = r \).

In order to design an efficient candidate screening procedure, we carefully study the operations required for MIPS. In the naive linear MIPS approach, \( nk \) multiplication operations are required to obtain \( n \) inner product values \( \{h_1^\top w, \ldots, h_n^\top w\} \). To understand and analyze the computation required for MIPS, we define an implicit matrix \( Z \in \mathbb{R}^{n \times k} \):

\[
Z = H \text{diag}(w),
\]

where \( \text{diag}(w) \in \mathbb{R}^{k \times k} \) is a matrix with \( w \) as its diagonal. The \((j,t)\) entry of \( Z \) denotes the multiplication operation \( z_{jt} = h_{jt} w_t \) and \( z_j = \text{diag}(w) h_j \) denotes the \( j\)-th row of \( Z \). In Figure 2, we use \( Z^\top \) to demonstrate the implicit matrix. The implicit matrix \( Z \) is query dependent, that is, the values of \( Z \) depend on the query vector \( w \). Note that \( n \) inner product values can be obtained by taking the column-wise summation of \( Z^\top \).

In particular, we have

\[
h_j^\top w = \sum_{t=1}^k z_{jt}, \quad j = 1, \ldots, n.
\]

Thus, the ranking induced by the \( n \) inner product values can be characterized by the marginal ranking \( \pi(j\mid w) \) defined on the implicit matrix \( Z \) as follows:

\[
\pi(j\mid w) := \text{rank} \left( \sum_{t=1}^k z_{jt} \mid \sum_{t=1}^k z_{1t}, \ldots, \sum_{t=1}^k z_{nt} \right)
\]

\[
= \text{rank}(h_j^\top w \mid \{h_1^\top w, \ldots, h_n^\top w\}).
\]

As mentioned earlier, it is hard to design an ideal candidate screening procedure which generates \( C(w) \) based on the marginal ranking. Because the main goal for the candidate screening phase is to quickly
identify candidates which are highly possible to be top-ranked items, it suffices to have an efficient procedure generating \( \mathcal{C}(\mathbf{w}) \) by an approximation ranking. Here we propose a greedy heuristic ranking:

\[
\bar{\pi}(j|\mathbf{w}) := \operatorname{rank}\left( \max_{t=1}^{k} z_{jt} \bigg| \left\{ \max_{t=1}^{k} z_{1t}, \ldots, \max_{t=1}^{k} z_{nt} \right\} \right), \tag{6}
\]

which is obtained by replacing the summation terms in (5) by max operators. The intuition behind this heuristic is that the largest element of \( z_j \) multiplied by \( k \) is an upper bound of \( \mathbf{h}_j^T \mathbf{w} \):

\[
\mathbf{h}_j^T \mathbf{w} = \sum_{t=1}^{k} z_{jt} \leq k \left( \max_{t=1}^{k} z_{jt} \right).
\]

Thus, \( \bar{\pi}(j|\mathbf{w}) \), which is induced by such an upper bound of \( \mathbf{h}_j^T \mathbf{w} \), could be a reasonable approximation ranking for the marginal ranking \( \pi(j|\mathbf{w}) \).

Next we design an efficient procedure which generates \( \mathcal{C}(\mathbf{w}) \) according to the ranking \( \bar{\pi}(j|\mathbf{w}) \) defined in (6). First, based on the relative orderings of \( \{z_{jt}\} \), we consider the joint ranking and the conditional ranking defined as follows:

- Joint ranking: \( \pi(j,t|\mathbf{w}) \) is the exact ranking over the \( nk \) entries of \( \mathbf{Z} \).
  \[
  \pi(j,t|\mathbf{w}) := \operatorname{rank}(z_{jt} \mid \{z_{1t}, \ldots, z_{nt}\}).
  \]

- Conditional ranking: \( \pi_t(j|\mathbf{w}) \) is the exact ranking over the \( n \) entries of the \( t \)-th row of \( \mathbf{Z}^T \).
  \[
  \pi_t(j|\mathbf{w}) := \operatorname{rank}(z_{jt} \mid \{z_{1t}, \ldots, z_{nt}\}).
  \]

See Figure 2 for an illustration for both rankings. Similar to the marginal ranking, both joint and conditional rankings are query dependent.

Observe that, in (6), for each \( j \), only a single maximum entry of \( \mathbf{Z} \), \( \max_{t=1}^{k} z_{jt} \), is considered to obtain the ranking \( \bar{\pi}(j|\mathbf{w}) \). To generate \( \mathcal{C}(\mathbf{w}) \) based on \( \bar{\pi}(j|\mathbf{w}) \), we can iterate \( (j,t) \) entries of \( \mathbf{Z} \) in a greedy sequence such that \( (j_1,t_1) \) is visited before \( (j_2,t_2) \), if \( z_{j_1t_1} > z_{j_2t_2} \), which is exactly the sequence corresponding to the joint ranking \( \pi(j,t|\mathbf{w}) \). Each time an entry \( (j,t) \) is visited, we can include the index \( j \) into \( \mathcal{C}(\mathbf{w}) \) if \( j \notin \mathcal{C}(\mathbf{w}) \).

**Theorem 1.** For all \( j_1 \) and \( j_2 \) such that \( \bar{\pi}(j_1|\mathbf{w}) < \bar{\pi}(j_2|\mathbf{w}) \), \( j_1 \) will be included into \( \mathcal{C}(\mathbf{w}) \) before \( j_2 \) if we iterate \( (j,t) \) pairs following the sequence induced by the joint ranking \( \pi(j,t|\mathbf{w}) \).

**Proof.** Let \( t_1 = \arg\max_{t=1}^{k} z_{j_1t} \) and \( t_2 = \arg\max_{t=1}^{k} z_{j_2t} \). By the definition of \( t_1 \), we have \( \pi(j_1,t_1|\mathbf{w}) < \pi(j_1,t|\mathbf{w}) \), \( \forall t \neq t_1 \). Thus, \( (j_1,t_1) \) will be first entry among \( \{(j_1,1), \ldots, (j_1,k)\} \) to be visited in the sequence corresponding to the joint ranking \( \pi(j,t|\mathbf{w}) \). Similarly, \( (j_2,t_2) \) will be the first visited entry among \( \{(j_2,1), \ldots, (j_2,k)\} \). We also have

\[
\bar{\pi}(j_1|\mathbf{w}) < \bar{\pi}(j_2|\mathbf{w}) \Rightarrow z_{j_1t_1} > z_{j_2t_2} \Rightarrow \pi(j_1,t_1|\mathbf{w}) < \pi(j_2,t_2|\mathbf{w}).
\]

Thus, \( j_1 \) will be included into \( \mathcal{C}(\mathbf{w}) \) before \( j_2 \). \hfill \Box

At first glance, generating \( (j,t) \) in the sequence according to the joint ranking \( \pi(j,t|\mathbf{w}) \) might require the access to all the \( nk \) entries of \( \mathbf{Z} \) and cost \( O(nk) \) time. In fact, based on Property 2 of conditional rankings, we can design an efficient variant of the \( k \)-way merge algorithm [8, Chapter 5.4.1] to generate \( (j,t) \) pairs in the desired sequence iteratively.

**Property 2.** Given a fixed candidate matrix \( \mathbf{H} \), for any possible \( \mathbf{w} \) with \( w_t \neq 0 \), the conditional ranking \( \pi_t(j|\mathbf{w}) \) is either \( \pi_{t+}(j) \) or \( \pi_{t-}(j) \):

- \( \pi_{t+}(j) = \operatorname{rank}(h_{jt} \mid \{h_{1t}, \ldots, h_{nt}\}) \),
- \( \pi_{t-}(j) = \operatorname{rank}(-h_{jt} \mid \{-h_{1t}, \ldots, -h_{nt}\}) \).
**Algorithm 1** ConditionalIterator: an iterator iterates \( j \in \{1, \ldots, n\} \) based on the conditional ranking \( \pi_t(j|w) \). This pseudo code assumes that the \( k \) sorted index arrays \( s_t[r] \), \( r = 1, \ldots, n \), \( t = 1, \ldots, k \) are available.

```python
class ConditionalIterator:
    def __init__(dim_idx, query_val):
        t, w, ptr ← dim_idx, query_val, 1
    def current(): return \( s_t[\text{ptr}] \) if \( w > 0 \), \( s_t[n - \text{ptr} + 1] \) otherwise.
    def hasNext(): return (ptr < n)
    def getNext(): ptr ← ptr + 1 and return current()
```

In particular, we have

\[
\pi_t(j|w) = \begin{cases} 
\pi_{t+}(j) & \text{if } w_t > 0, \\
\pi_{t-}(j) & \text{if } w_t < 0.
\end{cases}
\]

Similar to Property 1, Property 2 enables us to characterize a *query dependent* conditional ranking \( \pi_t(j|w) \) by two *query independent* rankings \( \pi_{t+}(j) \) and \( \pi_{t-}(j) \). As a result, similar to the motivating example in Section 4.1, for each \( t \), we can construct and store a **sorted** index array \( s_t[r] \), \( r = 1, \ldots, n \) such that

\[
\pi_{t+}(s_t[1]) \leq \pi_{t+}(s_t[2]) \leq \cdots \leq \pi_{t+}(s_t[n]),
\]

or equivalently

\[
\pi_{t-}(s_t[1]) \geq \pi_{t-}(s_t[2]) \geq \cdots \geq \pi_{t-}(s_t[n]).
\]

Thus, in the phase of *query-independent data structure construction* of Greedy-MIPS, we compute and store *query-independent* rankings \( \pi_{t+}(\cdot) \), \( t = 1, \ldots, k \) by \( k \) sorted index arrays of length \( n \): \( s_t[r] \), \( r = 1, \ldots, n \), \( t = 1, \ldots, k \) such that (7) holds. The entire construction costs \( O(kn \log n) \) time and \( O(kn) \) space.

Next we describe the details of the proposed Greedy-MIPS algorithm when a query \( w \) and the budget \( B \) are given. As mentioned earlier, Greedy-MIPS utilizes the idea of the \( k \)-way merge algorithm to visit \( (j, t) \) entries of \( Z \) according to the joint ranking \( \pi(j, t|w) \). Designed to merge \( k \) **sorted** sublists into a single sorted list, the \( k \)-way merge algorithm uses 1) \( k \) pointers, one for each sorted sublist, and 2) a binary tree structure (either a heap or a selection tree) containing the elements pointed by these \( k \) pointers to obtain the next element to be appended into the sorted list [8, Chapter 5.4.1].

### 4.2.1 Query-dependent Pre-processing

In Greedy-MIPS, we divide \( nk \) entries of \( (j, t) \) into \( k \) groups. The \( t \)-th group contains \( n \) entries:

\[
\{(j,t): j = 1, \ldots, n\}.
\]

Here we need an *iterator* playing a similar role as the pointer which can iterate index \( j \in \{1, \ldots, n\} \) in the **sorted** sequence induced by the conditional ranking \( \pi_t(\cdot|w) \). Utilizing Property 2, the \( t \)-th pre-computed sorted arrays \( s_t[r] \), \( r = 1, \ldots, n \) can be used to construct such an iterator, called ConditionalIterator, which iterates an index \( j \) one by one in the desired sorted sequence. ConditionalIterator needs to support current() to access the currently pointed index \( j \) and getNext() to advance the iterator. In Algorithm 1, we describe a pseudo code for ConditionalIterator, which utilizes the facts (7) and (8) such that both the construction and the index access cost \( O(1) \) space and \( O(1) \) time. For each \( t \), we use iters[t] to denote the ConditionalIterator for the \( t \)-th conditional ranking \( \pi_t(j|w) \).
Algorithm 2 Query-dependent pre-processing procedure in Greedy-MIPS.

- **Input:** query \( w \in \mathbb{R}^k \)
- For \( t = 1, \ldots, k \)
  - \( \text{iters}[t] \leftarrow \text{ConditionalIterator}(t, w_t) \)
  - \( j \leftarrow \text{iters}[t].\text{current}() \)
  - \( z \leftarrow h_{jt} w_t \)
  - \( Q.\text{push}((z, t)) \)

- **Output:**
  - \( \text{iters}[t], t = 1, \ldots, k \): iterators for conditional ranking \( \pi_t(:|w) \).
  - \( Q \): a max-heap containing \( \{(z, t) \mid z = \max_{j=1}^{n} z_{jt}, \ t = 1, \ldots, k \} \).

Regarding the binary tree structure used in Greedy-MIPS, we consider a max-heap \( Q \) of \((z, t)\) pairs. \( z \in \mathbb{R} \) is the compared key used to maintain the heap property of \( Q \), and \( t \in \{1, \ldots, k\} \) is an integer to denote the index to a entry group. Each \((z, t) \in Q \) denotes the \((j, t)\) entry of \( Z \) where

\[
j = \text{iters}[t].\text{current}() \quad \text{and} \quad z = z_{jt} = h_{jt} w_t.
\]

Note that there are most \( k \) elements in the max-heap at any time. Thus, we can implement \( Q \) by a binary heap such that it supports
- \( Q.\text{top}() \): returns the maximum pair \((z, t)\) of \( Q \) in \( O(1) \) time,
- \( Q.\text{pop}() \): deletes the maximum pair of \( Q \) in \( O(\log k) \) time, and
- \( Q.\text{push}((z, t)) \): inserts a new pair in \( O(\log k) \) time.

Note that the entire Greedy-MIPS can also be implemented using a selection tree among the \( k \) entries pointed by the \( k \) iterators. For the simplicity of presentation, we use a max-heap to describe the idea of Greedy-MIPS first and describe the details of Greedy-MIPS with a selection tree in the end of Section 4.2.2.

In the query-dependent pre-processing phase of Greedy-MIPS, we need to construct \( \text{iters}[t], \ t = 1, \ldots, k \), one for each conditional ranking \( \pi_t(j|w) \), and a max-heap \( Q \) which is initialized to contain

\[
\left\{(z, t) \mid z = \max_{j=1}^{n} z_{jt}, \ t = 1, \ldots, k \right\}.
\]

A detailed procedure is described in Algorithm 2, which costs \( O(k \log k) \) time and \( O(k) \) space.

### 4.2.2 Candidate Screening

Recall the requirements for a viable candidate screening procedure to support budgeted MIPS: 1) the flexibility to control the size \( |C(w)| \leq B \); and 2) an efficient procedure runs in \( O(Bk) \). The core idea of Greedy-MIPS is to iteratively traverse \((j, t)\) entries of \( Z \) in a greedy sequence and collect newly observed indices \( j \) into \( C(w) \) until \( |C(w)| = B \). In particular, if \( r = \pi(j, t|w) \), then \((j, t)\) entry is visited at the \( r \)-th iterate. Utilizing the max-heap \( Q \) and the \( k \) iterators: \( \text{iters}[t] \), we can design an iterator, called \( \text{JointIterator} \), which iterates \((j, t)\) pairs one by one in the desired greedy sequence induced by joint ranking \( \pi(j, t|w) \). Following the \( k \)-way merge algorithm, in Algorithm 3, we describe a detailed pseudo code for such an iterator. \( \text{JointIterator} \) costs \( O(k \log k) \) time to run Algorithm 2 to construct and initialize \( Q \) and \( \text{iters}[t] \), and costs \( O(\log k) \) time to advance to the next entry. In Algorithm 4, we describe our first candidate screening procedure with a budget \( B \) for Greedy-MIPS, which is a simple while-loop to iterate \((j, t)\) entries using the \( \text{JointIterator} \) with \( w \) until \( |C(w)| = B \).

To analyze the time complexity of Algorithm 4, we need to know the number of the iterations of the while-loop before the stop condition is satisfied. The following Theorem 2 gives an upper bound on this number of iterations.
Algorithm 3 JointIterator: an iterator generates \((j,t)\) pairs one by one based on the joint ranking \(\pi(j,t|w)\). The constructor costs \(O(k \log k)\) time to build a max-heap \(Q\). The time complexity to generate a pair is \(O(\log k)\).

```python
class JointIterator:
    def constructor(w):
        # Run Algorithm 2 with w to initialize Q and iters[t], t = 1,...,k
        ptr ← 1.
    def current():
        (z,t) ← Q.top()
        j ← iters[t].current()
        return (j,t)
    def hasNext(): return (ptr < nk)
    def getNext():
        (z,t) ← Q.pop()
        if iters[t].hasNext():
            j ← iters[t].getNext()
            z ← hjw
            Q.push((z,t))
        ptr ← ptr + 1
        return current()
```

Algorithm 4 Candidate screening procedure in Greedy-MIPS.

- **Input:** \(w\) and an empty \(C(w)\)
- \(\text{jointIter} ← \text{JointIterator}(w)\) \(\cdots O(k \log k)\)
- \((j,t) ← \text{jointIter}.current()\)
- while \(|C(w)| < B\):
  - if \(j \notin C(w)\): append \(j\) to \(C(w)\)
  - \((j,t) ← \text{jointIter}.getNext()\) \(\cdots O(\log k)\)
- **Output:** \(C(w) = \{j | \bar{\pi}(j|w) \leq B\}\)
As a result, at the beginning of the entire screening procedure. To budgeted MIPS approach. Here we propose an improved candidate screening procedure which reduces the array will be modified during the screening procedure. Furthermore, the auxiliary array can be reset to zero.

\[ \pi(j, t) \text{ defined in (6).} \]

Theorem 2. There are at least \( B \) distinct indices \( j \) in the first \( Bk \) entries \((j, t)\) in terms of the joint ranking \( \pi(j, t|w) \) for any \( w \); that is,

\[
|\{j \mid \forall (j, t) \text{ such that } \pi(j, t|w) \leq Bk\}| \geq B. 
\]

Proof. By grouping these first \( Bk \) entries by the index \( t \) and applying the pigeonhole principle, we know that there exists a group \( G \) such that it contains at least \( B \) entries. Because each entry in the same group has a distinct \( j \) index, we know that the group \( G \) contains at least \( B \) distinct indices \( j \).

Theorem 1 guarantees the correctness of Algorithm 4 to generate \( C(w) \) based on \( \bar{\pi}(j|w) \) defined in (6). By Theorem 2, the overall time complexity of Algorithm 4 is \( O(Bk \log k) \) as each iteration of the while-loop costs \( O(\log k) \) time.

The \( O(Bk \log k) \) time complexity of Algorithm 4 does not satisfy the efficiency requirement of a viable budgeted MIPS approach. Here we propose an improved candidate screening procedure which reduces the overall time complexity to \( O(Bk) \). Observe that the \( \log k \) term comes from the \( Q.push((z_{jt}, t)) \) and \( Q.pop() \) operations of the max-heap for each visited \((j, t)\) entry. As the goal of the screening procedure is to identify \( j \) indices only, we can skip the \( Q.push((z_{jt}, t)) \) for an entry \((j, t)\) with the \( j \) having been included in \( C(w) \). As a result, \( Q.pop() \) is executed at most \( B + k - 1 \) times when \(|C(w)| = B\). The extra \( k - 1 \) times occurs in the situation that

\[ \text{iters[1].current() = iters[2].current() = \cdots = iters[k].current()} \]

at the beginning of the entire screening procedure.

In Algorithm 5, we give a detailed description for this improved candidate screening procedure for Greedy-MIPS. See Figure 3 for a detailed illustration of this algorithm on a toy example. Note that in Algorithm 5, we use an auxiliary zero-initialized array of length \( n \): \( \text{visited}[j], j = 1, \ldots, n \) to denote whether an index \( j \) has been included in \( C(w) \) or not. As \( C(w) \) contains at most \( B \) indices, only \( B \) elements of this auxiliary array will be modified during the screening procedure. Furthermore, the auxiliary array can be reset to zero.

**Algorithm 5** An improved candidate screening procedure in Greedy-MIPS. The overall time complexity is \( O(Bk) \).

- **Input:**
  - \( H, w \), and the computational budget \( B \)
  - \( Q \) and \( \text{iters}[t] \): output of Algorithm 2
  - \( C(w) \): an empty list
  - \( \text{visited}[j] = 0, j = 1, \ldots, n \): a zero-initialized array of length \( n \)

- **while** \(|C(w)| < B:\)
  - \((z, t) \leftarrow Q.pop() \)
  - \( j \leftarrow \text{iters}[t]\cdot current() \)
  - \( \text{if} \ \text{visited}[j] = 0:\)
    - \* append \( j \) into \( C(w) \)
    - \* \( \text{visited}[j] \leftarrow 1 \)
  - \( \text{while} \ \text{iters}[t]\cdot hasNext():\)
    - \* \( j \leftarrow \text{iters}[t]\cdot getNext() \)
    - \* \( \text{if} \ \text{visited}[j] = 0:\)
      - \* \( z \leftarrow h_{jt}w_t \)
      - \* \( Q.push((z, t)) \)
      - \* \( \text{break} \)

- \( \text{visited}[j] \leftarrow 0, \forall j \in C(w) \)

- **Output:** \( C(w) = \{j \mid \bar{\pi}(j|w) \leq B\} \)

**Theorem 2.** There are at least \( B \) distinct indices \( j \) in the first \( Bk \) entries \((j, t)\) in terms of the joint ranking \( \pi(j, t|w) \) for any \( w \); that is,
Figure 3: Illustration of Algorithm 5 with $\mathbf{w} = [1, 1, 0.1]^\top$ and $B = 3$. The left plot for each sub-figure shows the heap structure in the max-heap $Q$: the value in each rectangle denotes $z$, and each index $t$ is shown in a different color (red for 1, green for 2, and blue for 3). The sorted index arrays are shown in the upper part of circles on the right plot for each sub-figure; for example, $s_1[4] = 7$, $s_2[1] = 6$, and $s_3[5] = 5$. The value in lower part of circles is the corresponding $h_{jt}$; for example, $h_{t1} = -4$, $h_{62} = 7$, and $h_{53} = 29$. Three downward triangles denote the current position of $\text{iter}_t$, $t = 1, 2, 3$. Figure 3(a) shows the status for each data data structure at the beginning of Algorithm 5. Three pairs are pushed into $Q$: $(-1 = h_{41}w_{11}, 1)$, $(7 = h_{71}w_{22}, 2)$, and $(6.9 = h_{13}w_{33}, 3)$. Figures 3(b)-3(c) show the status in the end of the first and the second iterations of the outer $\text{while}$-loop in Algorithm 5. In Figure 3(c), we show that at the third iteration, after $(z, t) = (6, 2) \leftarrow Q.\text{pop}()$ is executed and $7 = \text{iter}_2.\text{current}()$ is appended into $C(\mathbf{w})$, we need to advance $\text{iter}_2$ twice because the index $j = 1$ has been included in $C(\mathbf{w})$. Note that for this example $h_1$ is the candidate with the largest inner product value with $\mathbf{w}$.

using $O(B)$ time in the end of Algorithm 5, so this auxiliary array can be utilized again for a different query vector $\mathbf{w}$.

Notice that Algorithm 5 still iterates $Bk$ entries of $Z$ but at most $B + k - 1$ entries will be pushed into or pop from the max-heap. Thus, the overall time complexity of Algorithm 5 is $O(Bk + B\log k) = O(Bk)$, which satisfies the efficiency requirement for a viable approach for budgeted MIPS.

Greedy-MIPS with a Selection Tree. As there are at most $k$ pairs in the max-heap $Q$, one from each $\text{iter}_t$, the max-heap can be replaced by a selection tree to achieve a slightly faster implementation as suggested in [8, Chapter 5.4.1]. In Algorithm 6, we give a pseudo code for the selection tree with a $O(k)$ time constructor, a $O(1)$ time maximum element look-up, and a $O(\log k)$ time updata. To apply the selection tree for our Greedy-MIPS, we only need to the following modifications:

- In Algorithm 2, remove $Q.\text{push}((z, t))$ from the for-loop and construct $Q$ by $Q \leftarrow \text{SelectionTree}(\mathbf{w}, k, \text{iter})$.
- In Algorithm 3 and Algorithm 5, replace $Q.\text{pop}()$ by $Q.\text{top}()$ and replace $Q.\text{push}((z, t))$ by $Q.\text{updateValue}(t, z)$.

4.2.3 Connection to Sampling-based MIPS Approaches

Sample-MSIPS, as mentioned earlier, is essentially a sampling algorithm with replacement scheme to draw entries of $Z$ such that $(j, t)$ is sampled with the probability proportional to $z_{jt}$. Thus, Sample-MSIPS can be thought as a traversal of $(j, t)$ entries using in a stratified random sequence determined by a distribution of the values of $\{z_{jt}\}$, while the core idea of Greedy-MIPS is to iterate $(j, t)$ entries of $Z$ in a greedy sequence induced by the ordering of $\{z_{jt}\}$. Next, we discuss the differences between Greedy-MIPS and Sample-MSIPS in a few perspectives:

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Algorithm 6 A pseudo code of a selection tree used for Greedy-MIPS.

```python
class SelectionTree:
    def __init__(w, k, iters):
        K ← min{2^i | 2^i ≥ k}
        for i = 1, ..., 2K:
            buf[i] ← (−∞, 0)
        for t = 1, ..., k:
            j ← iters[t].current()
            buf[K + t] ← (h_j^T w, t)
        for i = K, ..., 1:
            if buf[2i].first > buf[2i + 1].first:
                buf[i] ← buf[2i]
            else:
                buf[i] ← buf[2i + 1]
    def top():
        return buf[1]
    def updateValue(t, z):
        i ← K + t
        buf[i] ← (z, t)
        while i > 1:
            i ← ⌊i/2⌋
            if buf[2i].first > buf[2i + 1].first:
                buf[i] ← buf[2i]
            else:
                buf[i] ← buf[2i + 1]
```

**Applicability:** Sample-MSIPS can be applied to the situation where both \( \mathcal{H} \) and \( \mathbf{w} \) are nonnegative because of the nature of sampling scheme. In contrast, Greedy-MIPS can work on any MIPS problems as only the ordering of \( \{z_{jt}\} \) matters in Greedy-MIPS. Instead of \( \mathbf{h}_j^\top \mathbf{w} \), Diamond-MSIPS is designed for the MSIPS problem which is to identify candidates with largest \( (\mathbf{h}_j^\top \mathbf{w})^2 \) or \( |\mathbf{h}_j^\top \mathbf{w}| \) values \[3\]. In fact, for nonnegative MIPS problems, the diamond sampling is equivalent to Sample-MSIPS. Moreover, for MSIPS problems with negative entries, when the number of samples is set to be the budget \( B \), the Diamond-MSIPS is equivalent to apply Sample-MSIPS to sample \((j, t)\) entries with the probability \( p(j, t) \propto |z_{jt}| \). Thus, the applicability of the existing sampling-based approaches is still very limited for general MIPS problems.

**Flexibility to Control** \( |C(\mathbf{w})| \): By Theorem 2, we know that Greedy-MIPS can guarantee both the time complexity of the candidate screening procedure and the size of output \( |C(\mathbf{w})| \) for any \( \mathcal{H}, \mathbf{w}, \) and \( B \). For a sampling-based approach, one can easily control either the time complexity of the sampling procedure or the size of \( C(\mathbf{w}) \), but not both. Because all the existing sampling-based approaches are a sampling scheme with replacement, the same entry \((j, t)\) could be sampled repeatedly. Thus, the time complexity to guarantee that \( C(\mathbf{w}) = B \) depends on the distribution of values of \( \mathbf{w} \) and \( \mathcal{H} \). Hence, Greedy-MIPS is more flexible than sampling-based approaches in terms of the controllability of \( C(\mathbf{w}) \).

5 Experimental Results

In this section, we perform extensive empirical comparisons to compare Greedy-MIPS with other state-of-the-art fast MIPS approaches on both real-world and synthetic datasets.

---

\[2\] This setting is used in the experiments in [3]
We use Netflix and Yahoo-Music as our real-world recommender system datasets. There are 17,770 and 624,961 items in Netflix and Yahoo-Music, respectively. In particular, we obtain the low rank model $(W, H)$ by the standard low-rank matrix factorization:

$$
\min_{W,H} \sum_{(i,j) \in \Omega} (A_{ij} - w_i^T h_j)^2 + \lambda \left( \frac{1}{n} \sum_{i=1}^{m} |\Omega_i| \|w_i\|^2 + \frac{1}{m} \sum_{j=1}^{n} |\Omega_j| \|h_j\|^2 \right),
$$

where $A_{ij}$ is the rating of the $j$-th item given by the $i$-th user, $\Omega$ is the set of observed ratings, $\Omega_i = \{ j \mid (i,j) \in \Omega \}$, and $\Omega_j = \{ i \mid (i,j) \in \Omega \}$, and $\lambda$ is a regularization parameter. We use the CCD++ [16] algorithm implemented in LIBPMF\(^3\) to solve the above optimization problem and obtain the user embeddings $\{w_i\}$ and item embeddings $\{h_j\}$. We use the same $\lambda$ used in [4]. We also obtain $(W, H)$ with a different $k$: 50, 100, and $k = 200$.

We also generate synthetic datasets with various $n = 2^{17,18,19,20}$ and $k = 2^{2,5,7,10}$. For each synthetic dataset, both candidate vector $h_j$ and query $w$ vector are drawn from the normal distribution.

\(^3\)http://www.cs.utexas.edu/~rofuyu/libpmf
5.1 Experimental Settings and Evaluation Criteria

All the experiments are performed on a Linux machine with 20 cores and 256 GB memory. We ensure that only single core/thread is used for our experiments. To have a fair comparison, all the compared approaches are implemented in C++:

- Greedy-MIPS: our proposed approach in Section 4. We compare the following variants in Section 5.2:
Figure 6: MIPS Comparison on synthetic datasets with $n \in \{2^{17}, 2^{18}, 2^{19}, 2^{20}\}$ and $k = 128$. The datasets used to generate results are created with each entry drawn from a normal distribution.

- The improved Greedy-MIPS in Algorithm 5 with the selection tree in Algorithm 6.
- The improved Greedy-MIPS in Algorithm 5 with a max-heap.
- The original Greedy-MIPS in Algorithm 4 with the selection tree in Algorithm 6.

**NNS-based MIPS approaches:**

- PCA-MIPS: the approach proposed in [2], which is shown to be the state-of-the-art among tree-based approaches [2]. We implement a complete PCA-Tree with the neighborhood boosting techniques described in [2]. We vary the depth of PCA tree to control the trade-off between the search quality and the search efficiency.
- LSH-MIPS: the approach proposed in [11, 13]. We use the nearest neighbor transform function proposed in [2, 11] and use the random projection scheme as the LSH function as suggested in [11]. We also implement the standard amplification procedure with an OR-construction of $b$ hyper LSH hash functions. Each hyper LSH function is a result of an AND-construction of $a$ random projections. We vary the values $(a, b)$ to control the trade-off between the search quality and the search efficiency.

- Diamond-MSIPS: the sampling scheme proposed in [3] for the maximum squared inner product search. As it shows better performance than LSH-MIPS in [3] in terms of MIPS problems, we also include Diamond-MSIPS into our comparison. F+Tree [17] is implemented as the multinomial sampling procedure.
- Naive-MIPS: the baseline approach which applies a linear search to identify the exact top-$K$ candidates.
**Evaluation Criteria.** For each dataset, the actual top-20 items for each query are regarded as the ground truth. We report the average performance on a randomly selected 2,000 query vectors. To evaluate the search quality, we use the precision on the top-$K$ prediction (prec@$K$), obtained by selecting top-$K$ items from $C(w)$ returned by the candidate screening procedure of a compared MIPS approach. $K = 5$ and $K = 10$ are used in our experiments. To evaluate the search efficiency, we report the relative speedups over the Naive-MIPS approach as follows:

$$\text{speedup} = \frac{\text{prediction time required by Naive-MIPS}}{\text{prediction time by a compared approach}}.$$  

**Remarks on Budgeted MIPS versus Non-Budgeted MIPS.** As mentioned in Section 3, PCA-MIPS and LSH-MIPS cannot handle MIPS with a budget. Both the search computation cost and the search quality are fixed when the corresponding data structure is constructed. As a result, to understand the trade-off between search efficiency and search quality for these two approaches, we can only try various values for its parameters (such as the depth for PCA tree and the amplification parameters $(a, b)$ for LSH). For each combination of parameters, we need to re-run the entire query-independent pre-processing procedure to construct a new data structure.

Figure 7: MIPS Comparison on synthetic datasets with $n = 2^{18}$ and $k \in \{2, 5, 7, 10\}$. The datasets used to generate results on are created with each entry drawn from a normal distribution.

5.2 Experimental Results

**Results on Variants of Greedy-MIPS.** In Figure 4, we shows the comparison between the three variants of Greedy-MIPS on netflix and yahoo-music. We can see that the difference between the use of a selection-tree
and a max-heap is small, while the different between the use of Algorithm 4 and the use of Algorithm 5 is more significant. For the comparison to other MIPS approaches, we use Greedy-MIPS to denote the results obtained from the version with the combination of Algorithm 5 and Algorithm 6.

**Results on Real-World Data sets.** Comparison results for netflix and yahoo-music are shown in Figure 5. The first, second, and third columns present the results with $k = 50$, $k = 100$, and $k = 200$, respectively. It is clearly observed that given a fixed speedup, Greedy-MIPS yields predictions with much higher search quality. In particular, on the yahoo-music data set with $k = 200$, Greedy-MIPS runs 200x faster than Naive-MIPS and yields search results with $p_5 = 70\%$, while none of PCA-MIPS, LSH-MIPS, and Diamond-MSIPS can achieve a $p_5 > 10\%$ while maintaining the similar 200x speedups.

**Results on Synthetic Data Sets.** We also perform comparisons on synthetic datasets. The comparison with various $n \in 2^{\{17,18,19,20\}}$ is shown in Figure 6, while the comparison with various $k \in 2^{\{2,5,7,10\}}$ is shown in Figure 7. We observe that the performance gap between Greedy-MIPS over other approaches remains when $n$ increases, while the gap becomes smaller when $k$ increases. However, Greedy-MIPS still outperforms other approaches significantly.

6 Conclusions

In this paper, we study the computational issue in the prediction phase for many MF-based models: a maximum inner product search problem (MIPS) with a very large number of candidate embeddings. By carefully studying the problem structure of MIPS, we develop a novel Greedy-MIPS algorithm, which can handle budgeted MIPS by design. While simple and intuitive, Greedy-MIPS yields surprisingly superior performance compared to state-of-the-art approaches. As a specific example, on a candidate set containing half a million vectors of dimension 200, Greedy-MIPS runs 200x faster than the naive approach while yielding search results with the top-5 precision greater than 75%.

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