SimDex: Exploiting Model Similarity in Exact Matrix Factorization Recommendations

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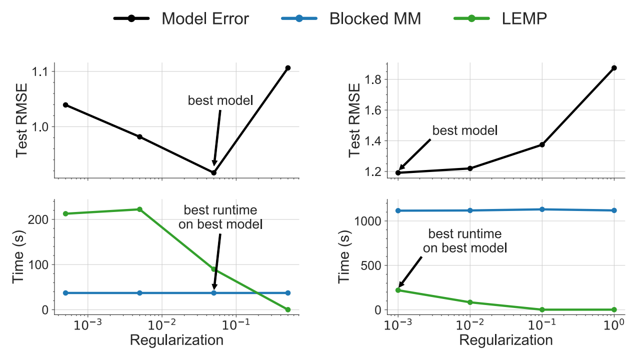
ABSTRACT

We present SIMDEX, a new technique for serving exact top-K recommendations on matrix factorization models that measures and optimizes for the similarity between users in the model. Previous serving techniques presume a high degree of similarity (e.g., L_2 or cosine distance) among users and/or items in MF models; however, as we demonstrate, the most accurate models are *not* guaranteed to exhibit high similarity. As a result, brute-force matrix multiply outperforms recent proposals for top-K serving on several collaborative filtering tasks. Based on this observation, we develop SIMDEX, a new technique for serving matrix factorization models that automatically optimizes serving based on the degree of similarity between users, and outperforms existing methods in both the high-similarity and low-similarity regimes. SIMDEX first measures the degree of similarity among users via clustering and uses a cost-based optimizer to either construct an index on the model or defer to blocked matrix multiply. It leverages highly efficient linear algebra primitives in both cases to deliver predictions either from its index or from brute-force multiply. Overall, SIMDEX runs an average of 2× and up to 6× faster than highly optimized baselines for the most accurate models on several popular collaborative filtering datasets.



(a) Netflix **(b)** Yahoo R2

Figure 1: An example of the relationship between regularization and top-K prediction runtime. We trained MF models on the popular Netflix Prize [7] and the Yahoo R2 [42] datasets using NOMAD [44] with four different regularization settings (λ). For each dataset, the top graph shows the root-mean-square error (RMSE) on the test set for each value of λ, while the bottom graph shows the corresponding top-K runtime for LEMP [37] and blocked matrix multiply for $K = 1$. For Netflix, blocked matrix multiply is 2× faster than LEMP for the *most accurate model*, whereas for Yahoo R2, LEMP outperforms matrix multiply by over two orders of magnitude. Note that, unlike LEMP, matrix multiply's runtime is unaffected by λ, since it does not attempt to index the MF model to speed up computation. In this paper, we develop MF serving techniques that optimize for the resulting degree of similarity in a target model. We also revisit this experimental configuration in Section 4.

1. INTRODUCTION

Recommender systems have attracted broad interest across a range of application domains, including e-commerce [27, 34], social networks [20], media [13, 23], and online advertising [31]. In particular, matrix factorization (MF) models have proven both accurate and practical for these recommendation tasks [32, 39, 40] and enjoy popularity both in research and in industry. As a result, efficiently *serving* the results of MF models to make predictions is a critical task in large-scale applications. For example, when users log in to Netflix (a service with over 86 million users [1]), they are greeted with a variety of different movie recommendations that Netflix has predicted for them. Predicted ratings for movies are subject to change whenever a user interacts with the system (e.g., watches a new movie, or rates a movie she has already watched) and whenever a new movie is added to the catalog, so these recommendations must be recomputed on a regular basis. Similarly, Facebook computes content recommendations using matrix factorization for over 1 billion users [20], and Amazon applies matrix factorization to a catalog of several million items [27].

The literature contains many solutions for fast top-K serving of MF recommendations, including locality-sensitive hashing (LSH) [35], and tree-based strategies [4,22,29], and other indexing techniques [25, 37]. These techniques all rely on a key assumption: that the user and/or item vectors in the model are sufficiently "similar"—they have similar L_2 norms, lie close together in Euclidean metric space, or have small pairwise cosine distances. This assumption motivates several of the key optimizations in LEMP [37] and FEXIPRO [25], the current state of the art for top-K serving: LEMP bucketizes the item vectors by their L_2 norms, ensuring each bucket fits in a processor's L3 cache, while FEXIPRO applies a singular value decomposition to the user and item matrices to prune its search for top-K items.

However, not all models exhibit high similarity, and, in particular, many of the *most accurate* models are not guaranteed to benefit from these prior approaches that exploit similarity. Figure 1 illustrates this phenomena: on the popular Netflix Prize dataset, brute-force matrix multiply outperforms the LEMP index by a factor of three on the

ACM ISBN 123-4567-24-567/08/06. . . $15.00
DOI: 10.475/123_4

most accurate model. However, for the Yahoo R2 Music dataset, the LEMP index is over two orders of magnitude faster than brute-force matrix multiply. The difference between these two scenarios arises from the optimal choice of *regularization*, a hyperparameter that prevents model overfitting during the model's *training* phase. Training with high regularization leads to similar weights between users, increasing the efficiency of the LEMP index, while training with low regularization conversely decreases the LEMP index's efficiency. In contrast, matrix multiply is unaffected by regularization: brute force performs the same amount of computation for each model.

The key insight behind this example is that the best choice of regularization is *problem-dependent*: to achieve the best model accuracy, different datasets require different regularization parameters. As a result, the most efficient serving strategy is problem-dependent. To our knowledge, this observation has not been made or exploited in previous MF serving work, which has focused only on accelerating serving without considering the underlying test or training accuracy of the selected models.

In this paper, we present SIMDEX, the first top-K MF serving technique that directly measures and automatically optimizes for the amount of similarity in a target MF model. Given a model, SIMDEX *dynamically* determines the degree of similarity between users to decide the most efficient serving strategy. This requires a fast but accurate means of estimating runtime cost—if a model exhibits low degree of similarity and matrix multiply is in fact faster, SIMDEX should not add substantial overhead. To accomplish this goal, SIMDEX leverages a novel cost estimation routine that combines clustering and a new upper bound on MF predictions based on angular distance. First, inspired by Koenigstein et al. [22], SIMDEX computes clusters for the users. (In [22], the user clusters are used to compute approximate—not exact—top-K predictions.) Subsequently, SIMDEX estimates the cost of computing predictions both via the cluster centroids and via blocked matrix multiply; based on these estimates, SIMDEX then computes the actual predictions using the faster of the two techniques. This cost-based optimization is efficient and accurate, and, as an auxiliary benefit, SIMDEX uses the cluster centroids to construct an index, which is often as fast or faster than existing approaches to MF serving. As a result, SIMDEX computes the *exact* top-K for all users an average of $2\times$ (and up to $6\times$) faster than the state of the art in the batch query setting. In addition, SIMDEX can use its centroid index to achieve low latency in the online (i.e., point query) setting.

SIMDEX is designed to be highly efficient in both the high-similarity and low-similarity model regimes, and to incur a minimal overhead for its cost-based optimization. In particular, SIMDEX uses k-means clustering—a standard cluster algorithm with multiple efficient implementations in commodity software packages such as Armadillo [33] and Intel DAAL [2]—to determine the similarity of the data during its decision phase. This end-to-end decision process takes less than 2% of the total runtime on average. Subsequently, in both the index-based (high-similarity) and brute-force (low-similarity) serving methods, SIMDEX uses efficient BLAS (i.e., dense linear algebra) primitives to compute predictions. Designing SIMDEX to use these two highly optimized, commodity algorithms allows it to outperform previous methods in both the high-similarity and low-similarity regimes, and to improve performance on the *most accurate* models for several popular collaborative filtering tasks.

In summary, we make the following contributions in this paper:

1. We identify model *training* as a crucial factor in *serving* performance for the first time. In particular, we show that prior serving methods are optimized for models with a high degree of user and item similarity, but they perform worse than blocked matrix multiply for the *most accurate* (lowest error) models in several standard datasets.
2. We present SIMDEX, a new approach to quickly determine similarity between users in matrix factorization to either i) build and serve from a new index that exploits similarity or to ii) fall back to brute-force matrix multiply. SIMDEX exploits commodity clustering routines and a novel upper bound on predicted ratings to determine the optimal choice of serving strategy. This allows SIMDEX to serve MF models with either high or low degrees of structural similarity by choosing the more efficient approach with limited (< 2%) overhead.
3. We evaluate SIMDEX across several standard large-scale recommendation datasets. Our results show $2\times$ average (and up to $6\times$) speedups over highly optimized baselines including LEMP and FEXIPRO on the most accurate models for these datasets.

The remainder of this paper is organized as follows. In Section 2, we provide background on MF models and top-K serving and illustrate the effect of regularization on model serving. In Section 3, we describe the SIMDEX system in detail, explain each stage of its pipeline, and present its key optimizations for computing top-K queries. We evaluate SIMDEX experimentally in Section 4, we discuss related work in Section 5, and conclude in Section 6.

2. PRELIMINARIES

In this section, we provide additional background regarding collaborative filtering and matrix factorization, the top-K retrieval problem, and the effect of model regularization on efficient serving.

2.1 Matrix Factorization

Collaborative filtering (CF) methods are an extremely popular method for building recommender systems. They utilize user feedback on items (either explicit or implicit) to infer relations between users and between items, and ultimately relate users to items they like. Since the advent of the Netflix Prize [6], the KDD-Cup 2011 [21], and other similar contests, CF models have become widely popular in recommender systems, largely due to their high accuracy across a variety of datasets.

One of the most common examples of collaborative filtering is the matrix factorization (MF) model [47]. Given a partially filled rating matrix $\mathcal{D} \in \mathbb{R}^{|U| \times |I|}$, where U is a set of users and I is a set of items for which we wish to compute recommendations, an MF model will factorize $\mathcal{D}$ into two matrices of low rank: $\mathcal{U} \in \mathbb{R}^{|U| \times f}$ for users, and $\mathcal{I} \in \mathbb{R}^{|I| \times f}$ for items, where $f \ll \min(|U|, |I|)$. The rank of each matrix f is called the number of *latent factors* of the model. Once factorized, the model predicts the unknown entries in $\mathcal{D}$ by computing the matrix product $\mathcal{U}\mathcal{I}^T$. There are various techniques for training MF models: typically, an objective function is defined on the prediction error on the known ratings in $\mathcal{D}$. This function is then minimized by an optimization algorithm, such as Stochastic Gradient Descent (SGD) or Alternating Least Squares (ALS). Both of these algorithms are highly parallelizable [17, 23, 30, 44, 47] and generally linear in cost with the number of *known* ratings in the matrix $\mathcal{D}$.

In the trained model, each individual user is modeled by a vector $\mathbf{u} \in \mathbb{R}^f$ and each item as a vector $\mathbf{i} \in \mathbb{R}^f$. A user u's predicted rating for an item i can be computed by taking the inner product between these vectors:

$$r_{ui} = \mathbf{u} \cdot \mathbf{i}$$

Unfortunately, naïvely computing r_{ui} for each user-item pair to find the top-K predictions is expensive—it takes time proportional to

$|U| \times |I|$. In contrast, the training process is only proportional to the number of known ratings, which is typically multiple order of magnitude smaller than the full matrix product $\mathcal{U}\mathcal{I}^T$. As we discuss in the next section, we focus on optimizing this rating computation.

2.2 Problem Statement: Top-K Retrieval

Given our definition for a predicted rating, we can formally define the inner-product top-K problem: for a given user $\mathbf{u}$, find the user's K highest rated items, the K largest inner products $\mathbf{u} \cdot \mathbf{i}$ among all $\mathbf{i} \in I$. For K=1, the top-K problem can be expressed as:

$$\mathbf{i}^* = \arg\max_{\mathbf{i} \in I} \mathbf{u} \cdot \mathbf{i}$$

This top-K retrieval is an instance of the *Maximum Inner Product Search (MIPS)* problem [29, 35, 37].

At first glance, the exact MIPS problem is similar to many standard problems in the literature, such as nearest-neighbor search (NNS) and cosine similarity search. However, classic approaches to NNS do not directly solve exact MIPS. In particular, exact MIPS requires accounting for both the *magnitude* of item vectors and their angular *orientation*: items with a similar orientation to a user will have a high inner product, but so will items large a high magnitude but a different orientation. In particular, standard spatial indexing methods pose significant challenges for exact MIPS. Our goal here is to provide intuition; we describe related work that proposes modifications to each strategy in detail in Section 5. We conclude this discussion with an overview of the empirically best-performing prior methods, LEMP and FEXIPRO:

Nearest-Neighbor Search in Metric Space (NNS). The exact top-K problem can be expressed as a nearest-neighbor search:

$$\mathbf{i}^* = \arg\max_{\mathbf{i} \in I} \mathbf{u} \cdot \mathbf{i} = \arg\min_{\mathbf{i} \in I} \|\mathbf{u} - \mathbf{i}\|^2 - \frac{\|\mathbf{i}\|^2}{2}$$

The second term, $\frac{\|\mathbf{i}\|^2}{2}$ is problematic: unless all item vectors $\mathbf{i} \in I$ have the same magnitude, it is difficult to apply these techniques. Moreover, in practice, the item vector norms in I can have significant variations [22], meaning NNS must be modified (e.g., [4]) to deliver the correct answer.

Cosine Similarity. We can also cast the top-K in terms of maximizing the cosine similarity between $\mathbf{u}$ and $\mathbf{i}$:

$$\begin{aligned} \mathbf{i}^* &= \arg\max \frac{\mathbf{u} \cdot \mathbf{i}}{\|\mathbf{u}\| \, \|\mathbf{i}\|} \\ &= \arg\max \frac{\mathbf{u} \cdot \mathbf{i}}{\|\mathbf{i}\|} \end{aligned}$$

Once again, a challenge here is that the items in I do not share the same magnitude. We can approximate MIPS using this approach, but exact computation is challenging [37].

Locality-Sensitive Hashing (LSH). The LSH technique involves constructing a set of hash functions h which satisfy the following for any pair of points $\mathbf{u}, \mathbf{i} \in \mathbb{R}^f$:

$$\Pr[h(\mathbf{u}) = h(\mathbf{i})] = \mathrm{sim}(\mathbf{u}, \mathbf{i})$$

where $\mathrm{sim}(\mathbf{u}, \mathbf{i}) \in [0, 1]$ is a similarity function of our own choosing; for MIPS, the similarity function would be $\mathrm{sim}(\mathbf{u}, \mathbf{i}) = \mathbf{u} \cdot \mathbf{i}$. Classic approaches to LSH are not suitable for MIPS [28, 35]: for any similarity function to admit an LSH function family, its distance function $(1 - \mathrm{sim}(\mathbf{u}, \mathbf{i}))$ must satisfy the triangle inequality [10]. However, for MIPS, the distance function $1 - \mathbf{u} \cdot \mathbf{i}$ does not satisfy the triangle inequality. (See [35] for a detailed proof.) Thus, LSH cannot be directly applied to finding the exact maximum inner product, but can be used in approximate MIPS [4, 35, 45].

State-of-the-Art: LEMP and FEXIPRO. The state of the art in terms of reported empirical performance on MIPS are LEMP [37] and FEXIPRO [25]. LEMP maps users into a smaller set of buckets, then uses the Cauchy-Schwarz inequality and incremental pruning to accelerate the search. FEXIPRO uses singular value decomposition, integer quantization, and a novel monotonicity transformation on the user and item matrices to further prune computation. We find that, when properly blocked and vectorized, blocked matrix multiply is competitive with LEMP and FEXIPRO for many models; for other models, SIMDEX's novel bound more selectively prunes the candidate set of items. End-to-end, SIMDEX improves performance by up to 6×, while also maintaining efficient performance for single-user queries.

2.3 Impact of Model Training

As we discussed in Section 1, the role of model training has a large effect on top-K computation for MF models. The MF model training procedure—and, in particular, how its hyperparameters, such as regularization, are chosen during training—has a direct impact on the ability to index and serve predictions for the resulting model. The hyperparameters have a significant impact on accuracy—both on the training set and the test set. As a result, hyperparameter tuning has been studied extensively in the ML learning community, with much ongoing work [26]. SIMDEX does not attempt to address hyperparameter tuning; instead, our goal is to find ways to efficiently index and serve top-K queries on the most accurate MF model for a dataset (or any MF model provided to the system), independent of the hyperparameters used during training.

To illustrate mathematically, consider the following objective function, which is typically used to train MF models:

$$\min_{\mathcal{U},\mathcal{I}} \sum_{r_{ui} \text{observed} \in \mathcal{D}} (r_{ui} - \mathbf{u}^T \mathbf{i})^2 + \lambda \Big(\sum_{\mathbf{u}} \|\mathbf{u}\|^2 + \sum_{\mathbf{i}} \|\mathbf{i}\|^2 \Big)$$

For this objective function, λ acts as a penalty on the L_2 norms of the individual user and item vectors $\mathbf{u}$ and $\mathbf{i}$; the larger λ is, the smaller the L_2 norms for $\mathbf{u} \in \mathcal{U}$ and $\mathbf{i} \in \mathcal{I}$ will be. Therefore, as λ increases, the factorized matrices are easier to index—their component vectors have smaller L_2 norms and fit inside a smaller L_2 "ball" in R^f.

However, a highly indexable model does not translate to a highly accurate one, and there is no clear relationship between the two. Therefore, we cannot rely solely on indexing MF models for fast top-K serving; multiple methods—including blocked matrix multiply—are necessary to serve a wide variety of accurate models as efficiently as possible. If we want to serve top-K queries on *accurate* models efficiently, then deciding between these techniques and choosing the appropriate one is paramount. We explain our approach to this problem in the following section.

In summary, we make several observations in this section. First, the regularization parameter used during MF training affects both the accuracy of the model and the ability to index the model efficiently for top-K serving. Second, these two relationships—regularization vs. accuracy, and regularization vs. top-K runtime—do not behave similarly. As regularization increases, the running time of many MIPS top-K algorithms decreases proportionally, but this relationship is not the case for model accuracy. Third, since the regularization vs. accuracy relationship is not monotonic, MF models that are easy to index and serve efficiently are not necessarily more accurate than other models that are difficult to index. Fourth, we show in Section 4 that the model training procedure can also affect this trade-off.

3. SIMDEX

In this section, we present SIMDEX, a technique for automatically optimizing top-K queries over MF models based on their degree of similarity. SIMDEX proceeds in three stages, depicted in Figure 2:

1. **Cluster Users**: SIMDEX clusters users into representative clusters with similar feature vectors.

2. **Optimizer: Choose Index vs. Blocked Matrix Multiply**: We perform cost-based optimization to determine whether the top-K should be computed using the cluster centers or blocked matrix multiply. If SIMDEX estimates that blocked matrix multiply will be faster, SIMDEX abandons the remaining steps and calls optimized matrix multiply routines; otherwise, SIMDEX proceeds to construct the index for top-K querying.

3. **Construct and Query Index**: Using the clustering from Step 1, SIMDEX computes a conservative estimate of the maximum distortion between each cluster's predicted rating and the predicted ratings for users in the cluster. SIMDEX subsequently applies this conservative upper bound to the inner product between each cluster centroid and each item and, for each cluster, stores a list of items in descending order of the computed upper bounds. Subsequently, to compute a user's top-K items, SIMDEX walks the item list of the user's corresponding cluster, using the upper bound to terminate when there are guaranteed to be no more items with higher ratings than those that the user has previously seen.

We next describe each of these steps in detail. We first describe SIMDEX's clustering strategy and means of relating user predictions to cluster centroid predictions (Section 3.1). We show that, provided SIMDEX decides to use the cluster centroids as a prediction index, SIMDEX can short-circuit computation during exact top-K computation (Section 3.2). Subsequently, we combine the two prior steps to describe SIMDEX's cost-based optimizer, which selects between SIMDEX's index and matrix multiply prediction strategies (Section 3.3). We conclude with a recap, discussion of optimizations for performance, and correctness and runtime analysis of the SIMDEX index (Section 3.4).

Before continuing, we wish to highlight that the idea to cluster users based on similarities is explicitly *not* new and was first suggested by Koenigstein et al. [22], who use centroids of clustered users to build an approximate top-K index (see also Section 5). In contrast, SIMDEX's key innovation is in the combination of clustering with a new, conservative upper bound that allows SIMDEX to recover the *exact* top-K efficiently, while also using the same clusters in an optimizer that determines whether to instead perform blocked matrix multiply.

3.1 Clustering Users

SIMDEX first partitions the set of users $U \in \mathbb{R}^f$ into a set of C clusters, with $C \ll |U|$. We will use a user $\mathbf{u}$'s assigned cluster centroid $\mathbf{c}$ as a means of finding an initial approximation of $\mathbf{u}$'s top-K items, which we then can iteratively refine per user to find the exact top-K.

Choosing Clusters. Ideally, our clustering algorithm should minimize the angular distance between any user vector $\mathbf{u}$ and its assigned centroid $\mathbf{c}$. We wish to minimize the angle between $\mathbf{u}$ and $\mathbf{c}$:

$$\theta_{uc} = \cos^{-1}\left(\frac{\mathbf{u}\cdot\mathbf{c}}{\|\mathbf{u}\|\,\|\mathbf{c}\|}\right)$$

for all user vectors and their respective centroids. This is because the relative *ordering* of a given user's top-K items is unchanged if we scale the user's vector $\mathbf{u}$ by some constant; that is, the centroid's ability to accurately represent the user's preferences is only dependent on the angle between centroid and the user. This implies that the magnitude of each centroid $\|\mathbf{c}\|$ does not have an effect on the quality of our clusters.

In selecting a clustering algorithm, a natural choice for our given criteria is spherical clustering [46]; by design, the algorithm minimizes angular distance between inputs and centroids, thus directly achieving our stated objective of minimizing θ_{uc}. However, for the purpose of SIMDEX, we find that spherical clustering offers poor runtime performance for two reasons: i) cosine similarity, rather than Euclidean distance, is used as the distance metric in spherical clustering, requiring expensive materialization of the pairwise similarity matrix, a superset of the work required to compute the top-K using brute-force; and ii) after each iteration, all centroids must be projected onto the unit hypersphere. Instead, we use standard k-means for our clustering; minimizing the L_2 distance between user vectors provides an empirically good approximation of the angular differences between different user vectors.

Using cluster centroids as a proxy for true ratings. Before continuing, we introduce a novel upper bound that allows us to use the centroid $\mathbf{c}$ in place of the user vector $\mathbf{u}$ to quickly estimate $\mathbf{u}$'s top-K items. We use this in both cost estimation and index walking. By computing a conservative correction based on the maximum distortion among the users in the cluster, we can generate an approximation of $\mathbf{u}$'s true preference ordering and use this approximation to prune items that cannot belong in $\mathbf{u}$'s top-K.

To begin, let θ_{ui} be the angle between $\mathbf{u}$ and $\mathbf{i}$, θ_{ic} be the angle between $\mathbf{i}$ and $\mathbf{c}$ and θ_{uc} be the angle between $\mathbf{u}$ and $\mathbf{c}$. (Figure 3 illustrates these relationships.) Finally, let r_{ui} be the rating for the user-item pair $\mathbf{u}, \mathbf{i}$.

By the triangle inequality on angular distances, we know that

$$|\theta_{ic} - \theta_{uc}| \leq \theta_{ui} \leq \theta_{ic} + \theta_{uc}$$

Thus, we can compute an upper bound on r_{ui}:

$$\begin{aligned} r_{ui} &= \mathbf{u}\cdot\mathbf{i} \\ &= \|\mathbf{u}\|\,\|\mathbf{i}\|\cos\theta_{ui} \\ &\leq \|\mathbf{u}\|\,\|\mathbf{i}\|\max_{\theta\in[\theta_{ic}\pm\theta_{uc}]}\cos\theta \end{aligned}$$

For top-K, each user's ranking of predicted ratings is invariant (i.e., are preserved) under linear scaling. Thus, we can omit $\|u\|$ to preserve the *relative* ordering of items for a single user and obtain a linear scaling of r_{ui}, denoted r^*_{ui} such that $r^*_{ui}\,\|\mathbf{u}\| = r_{ui}$:

$$r^*_{ui} \leq \|\mathbf{i}\|\max_{\theta\in[\theta_{ic}\pm\theta_{uc}]}\cos\theta$$

Now, note that θ_{ic} and θ_{uc} lie in $[0,\pi]$: that is, we have $\mathbf{i}\cdot\mathbf{c} = \|i\|\,\|c\|\cos(\theta_{uc})$, and, solving for θ_{uc} with unit $\mathbf{i}$ and $\mathbf{c}$, we have $\theta_{ic} = \arccos(\mathbf{i}\cdot\mathbf{c}) \in [0,\pi]$ (similarly for θ_{uc}). Therefore, if $\theta_{uc} \geq \theta_{ic}$, then $0 \in [\theta_{ic} \pm \theta_{uc}]$ and so $r_{ui} \leq \|i\|$. Otherwise, because $\cos(\theta)$ monotonically decreases from 0 to π, if $\theta_{uc} < \theta_{ic}$, we have $\cos(\theta_{ic} - \theta_{uc}) > \cos(\theta_{ic} + \theta_{uc})$. Plugging in, we have:

$$r^*_{ui} \leq \begin{cases} \|\mathbf{i}\|\cos(\theta_{ic} - \theta_{uc}) & \text{if } \theta_{uc} < \theta_{ic} \\ \|\mathbf{i}\| & \text{otherwise} \end{cases} \tag{1}$$

Equation 1 provides a means of monotonically ranking items according to their angular distance from the cluster center. However, θ_{uc} still appears in this bound, so computing this bound for every user-item pair would require time proportional to $O(|U||I|)$, a

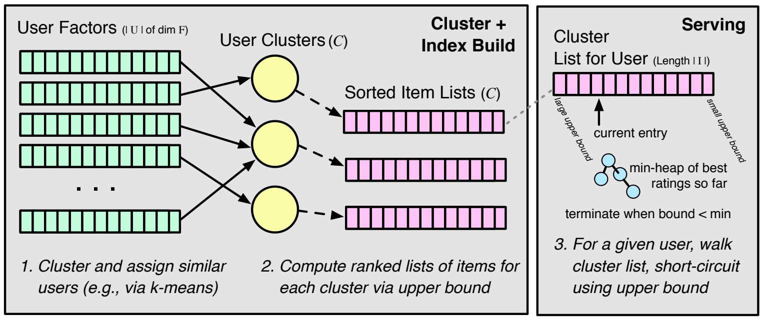


Figure 2: Overview of SIMDEX index construction and querying (Sections 3.1 and 3.2). SIMDEX's optimizer constructs the index (steps one and two), then probes the index using a sample of users to quickly estimate the benefit of index-based serving compared to matrix-multiply routines (Section 3.3).

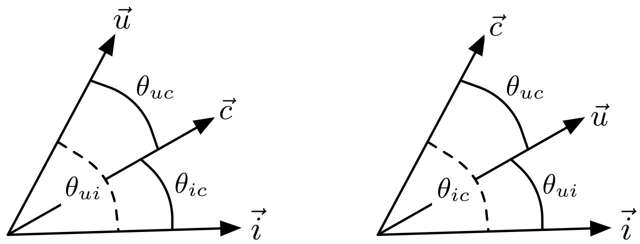


Figure 3: Illustration of the angular relationships between $\mathbf{u}$, $\mathbf{i}$, and $\mathbf{c}$. SIMDEX leverages the triangle inequality to bound the distance between users and their corresponding centroids.

computational overhead we seek to avoid.

Instead, imagine we were to substitute a pessimistic upper bound on θ_{uc} in Equation 1, say some $\theta_b \in [0, \pi]$ such that $\theta_b \geq \theta_{uc}$. This θ_b is likely to cause the upper bound to loosen, but it still serves as an upper bound. For each centroid $\mathbf{c}$, SIMDEX picks a set of θ_b's by computing the angles between $\mathbf{c}$ and each of the users assigned to the centroid, which we denote Θ_c. Then, we set θ_b to be the *maximum* θ_{uc} in Θ_c. Subsequently, we have:

$$r^*_{ci} \leq \begin{cases} \|\mathbf{i}\| \cos(\theta_{ic} - \theta_b) & \text{if } \theta_b < \theta_{ic} \\ \|\mathbf{i}\| & \text{otherwise} \end{cases} \tag{2}$$

Recap. We used the triangle inequality to derive a bound that relates the user-cluster angular distance (θ_{uc}) and cluster-item angular distance (θ_{ic}) to the user-item angular distance (θ_{ui}) for each item (Equation 1). However, this bound only held for a given θ_{uc}, and there are many users per cluster. Therefore, we relaxed this bound (Equation 2) and, within each cluster, SIMDEX computes an over-approximation θ_b such that $\theta_b \geq \theta_{uc}$ for all users $\mathbf{u}$. Using Equation 2, SIMDEX will compute a sorted list of items for each cluster used for both cost estimation and indexing.

3.2 Computing Queries Using Centroid Index

Before describing how SIMDEX decides whether to serve predictions using its cluster centroids or to use matrix multiply, we first illustrate how to use Equation 2 to serve predictions used based on the centroids. We will use this procedure in our cost-based optimizer in the next section.

Index construction. Using Equation 2, SIMDEX first computes r^*_{ci} for each centroid $\mathbf{c}$ and item $\mathbf{i}$ and, for each centroid $\mathbf{c}$, produces a list of items sorted by r^*_{ci}, which we denote L_c. We call the set of such L_c the SIMDEX index.

Given the SIMDEX index, we can perform top-K queries for each user. Informally, we walk the user's corresponding centroid list and apply our conservative correction from the previous step, r^*_{ci}. Once we encounter at least K items with (actual) predicted rating higher than the current item's r^*_{ci}, we can return the current top-K, which is guaranteed to be exact. The larger the angular distance between a user and its centroid, the more index entries the user will consult.

Algorithm 1 True Top K using Indexed Upper Bound

Require: K, $\mathbf{u}$: user, upperBounds: sorted list of $\mathbf{i}$, r^*_{ci} for $\mathbf{u}$'s respective cluster as constructed in Section 3.2

```
minHeap ← []
j ← 0
while j ≤ K do
    (upperBound, i) ← upperBounds[j]
    r_ui ← u · i
    minHeap.push((r_ui, i))
end while
while j ≤ upperBounds.length() do
    (upperBound, i) ← upperBounds[j]
    if minHeap.min() > upperBound then
        break
    end if
    r_ui ← u · i
    if minHeap.min() < r_ui then
        minHeap.pop()
        minHeap.push((r_ui, i))
    end if
end while
```

Computing the top-K items for each user consists of walking the corresponding centroid list, computing the true inner product $\mathbf{u} \cdot \mathbf{i}$, and stopping once we have evaluated at least K items and encounter an item that has predicted rating less than Equation 2. The entire pseudocode can be found in Algorithm 1.

More precisely, to compute the top-K for a user $\mathbf{u}$ assigned to cluster $\mathbf{c}$, initialize a min-heap and begin to walk L_c. For the first K items in L_c, compute the *true* rating $r_{ui} = \mathbf{u} \cdot \mathbf{i}$ and add them to the min-heap. Continue iterating through the remaining items $\mathbf{i}_{K+1}, \ldots, \mathbf{i}_{|I|}$, and, for each item $\mathbf{i}_j$, check if its upper bound $r^*_{ci_j}$ is less than the smallest value in the min-heap. If $r^*_{ci_j}$ is less than the smallest value in our min-heap, we can terminate: our list is sorted in descending order by upper bound, so the remaining items $\mathbf{i}_{j+1}, \ldots, \mathbf{i}_{|I|}$ cannot, by construction, appear in the true top-K. Thus, we can safely terminate our traversal and return the current contents of the min-heap, which represent the true top-K. Otherwise, we compute the true user rating r_{ui_j} for this item; if r_{ui_j} is greater than the current minimum value in the heap, then we replace the min-heap's minimum element with $\mathbf{i}_j$. Otherwise, if r_{ui_j} is less than the current minimum, we ignore $\mathbf{i}_j$ and move on to $\mathbf{i}_{j+1}$, the next element in the list.

Recap. Given a user, we walk its centroids' corresponding sorted list and compute the true top-K. The sorted list is monotonically decreasing with respect to the upper bound on each r_{ui}, so, once we find K items with rating greater than the current upper bound, we can safely stop. We may visit more items than needed (and the exact number will depend on both the size of θ_b and the distribution of rating, but, because each L_c is monotonically decreasing in the upper bound given by Equation 2, we will not "miss" any items for each user $\mathbf{u}$.

3.3 Optimizing: Choosing Between Index and Blocked Matrix Multiply

Given this overview of the SIMDEX index, we finally present the SIMDEX optimizer. Recall that the SIMDEX index can be constructed quickly: fast k-means followed by bound and index list calculations for each cluster is inexpensive, typically taking takes less than 1% of all execution time in practice. Thus, SIMDEX *always* performs clustering and sorts item lists for each cluster; however, SIMDEX must decide whether it should use these item lists to serve predictions or to resort to matrix multiply.

The most efficient solution depends on how many items SIMDEX's index is able to prune during index walk time. Given an estimate $\hat{w}$ of the average number of items that SIMDEX will visit during index walk, where $\hat{w} \leq |I|$, we can estimate the overall runtime of predicting using SIMDEX's index. Specifically, predicting using SIMDEX's index will require an expected $|U|\hat{w}$ evaluations of Equation 2. In contrast, blocked matrix multiply will require $|U||I|$ inner products. Given that $\hat{w} \leq |I|$, one might be tempted to determine that SIMDEX's index will always be faster. However, each inner product in blocked matrix multiply is in fact much cheaper than in SIMDEX: blocked matrix multiply routines take advantage of memory locality and are often hardware-optimized, in the form of vectorized and highly specialized libraries and routines.

Thus, to determine whether SIMDEX's index is faster than blocked matrix multiply, we must correct for the *hardware efficiency* of blocked matrix multiply. We capture this machine- and library-dependent factor via a constant h, which we empirically fit and validate in Section 4. Given this corrective factor, we say that we should choose SIMDEX when $|U|\hat{w} < |U||I|h$, or when:

$$\frac{\hat{w}}{|I|} < h. \tag{3}$$

In our evaluation environment, we find that for top-1 queries, $h \approx 0.05$, meaning blocked matrix multiply delivers an order of magnitude speedup. For larger K in top-K, matrix multiply must perform additional post-processing in the form of top-K selection sort; when implemented with a heap, this empirically (and perhaps unsurprisingly) results in an approximately $\log_2(K)$ performance penalty to matrix multiply's hardware efficiency.

The above discussion presumes that $\hat{w}$ is known in advance; in practice, how should we compute it? We exploit the fact that, due to the central limit theorem, we can obtain an estimate of the population average in time that is independent of the population size. By sampling a small number of users from the set of users to be predicted, we can perform Algorithm 1 for those users, directly compute the number of items visited, and obtain an estimate of $\hat{w}$ with confidence by applying well known confidence intervals for approximation [9]. Empirically, we find that sampling 0.1% of the users results in accurate estimates of $\hat{w}$.

Recap. SIMDEX uses a decision rule to determine whether the top-K should be computed using our index or blocked matrix multiply. After clustering the users, SIMDEX samples a small number and performs a simple arithmetic calculation that accounts for hardware efficiency of blocked matrix multiply to decide whether to perform further index lookups or matrix multiply.

Algorithm 2 SIMDEX Overview

Require: I: items, U: users, C: # clusters, M: cluster index size
1: cluster U into C clusters using k-means
2: sort descending list for each cluster per Equation 2
3: estimate costs of indexing and matrix multiply
4: if index cheaper, walk index for each user via Algorithm 1
5: if matrix multiply cheaper, call matrix multiply
return top-K lists for each user

3.4 Overview and Analysis

Overview. Algorithm 2 describes the three SIMDEX computation steps, which we analyze in the remainder of this section. As we discuss, the main impact on SIMDEX efficiency is the quality of clustering and the number of index lists per cluster. Fortunately, there are many existing high-quality clustering implementations that we can leverage, and, empirically, CF models are easily clustered; a small number of index lists suffices (Section 4).

Cluster Parameters. SIMDEX's index exposes one parameter: C, the number of clusters. The appropriate number of clusters is dataset-dependent. However, especially given the availability of highly optimized libraries for clustering, we find clustering (via k-means) typically represents a small $(1-10\%)$ fraction of SIMDEX's overall runtime, allowing substantial online experimentation. We vary this factor experimentally in Section 4.

Index Memory Requirement. The SIMDEX index requires $O(C|I|)$ storage, with one sorted list of length $|I|$ per cluster.

Index Serving Runtime. Given a k-means running time of $O(|C||U|)$ and $\bar{w}$, the average number of items visited per user in Algorithm 1, SIMDEX runs in time:

$$O(C|U| + C|I|\log|I| + |U|\bar{w}\log K), \tag{4}$$

where $C|I|\log|I|$ captures the index construction time (including sorting) and $|U|\bar{w}\log K$ captures the time to walk each list. Thus, SIMDEX is faster than brute force when Equation 4 is less than $O(|U||I| + |U||I|\log K)$. Therefore, minimizing $\bar{w}$ is instrumental in improving SIMDEX performance. In expectation, as θ_{uc} shrinks so will $\bar{w}$; thus, achieving a good clustering is highly important.

Optimization: sharing work across users for common items. In most MF prediction tasks, we found that, when using SIMDEX's index, many users would visit the same initial set of items (e.g., the first 100-1000) in computing their top-K. Therefore, to capitalize on this shared work, we introduce a small optimization to the SIMDEX index walk routine by sharing work for the first B items (in our evaluation, 4096). For the first B items in a cluster list, we perform a block matrix multiply between all user vectors in the cluster and the first B item vectors in the cluster item list. We refer to this optimization as *work sharing* during index serving.

Work sharing has two key consequences. First, work sharing allows SIMDEX's index traversal routine to make use of more hardware-efficient matrix-matrix multiply (instead of the less efficient matrix-vector or vector-vector multiply performed on a single, per-user basis) while still benefiting from SIMDEX's early termination routines. If a user only needs to visit fewer than B items, this will result in wasted work. However, on balance, for modest blocking sizes, we find that sharing the first B items is beneficial to end-to-end runtime.

Second, we need to explicitly account for this speedup in our cost model: the same hardware scaling constant h must be applied to the first B operations. By similar reasoning as in Equation 3, simple arithmetic shows that this semi-blocked SIMDEX traversal is in expectation more efficient than full matrix multiply when:

$$\frac{\hat{w} - B}{|I| - B} < h \tag{5}$$

That is, given that the work on the first B items in each cluster is shared via blocking, the hardware speedups of full blocked matrix multiply only apply to the $\hat{w} - B$ of $|I| - B$ remaining items. As we demonstrate in Section 4, this simple modification preserves the accuracy of the SIMDEX cost model and, in turn, the optimizer's decision accuracy.

Parallelization. To provide an apples-to-apples comparison to existing work, we focus on single-threaded execution in this paper. However, SIMDEX's index admits parallelization. Blocked matrix multiply routines are the subject of considerable study in parallel algorithms. In addition, SIMDEX's index structure permits embarrassingly parallel construction and querying. For index construction, there are many existing algorithms and implementations for parallel k-means, and computing each index list can be performed independently on a per-cluster basis. At serving time, we can partition clusters across cores (or machines) and route users to cores based on their cluster assignments, providing a natural basis for parallelization. All data structures are read-only, allowing replication in the event of hot-spots.

Cold Start and Incremental Maintenance. If we wish to add a new user to SIMDEX's index, we can add them to the nearest cluster and serve their queries by computing θ_{uc}. Provided $\theta_{uc} \leq \theta_b$, we can serve the new user with the existing index. Over time, if we add many users that are significantly different from the users that were present for the initial clustering, performance for these new users may degrade, but correctness will be maintained. To improve performance in the presence of severe drift, we can rebuild the indices. If we wish to add a new item to SIMDEX, we can compute Equation 2 for each cluster and insert the item in the correct position within each cluster's sorted item list.

Correctness of Index. SIMDEX's index returns exact top-K results. The intuition behind this is that each SIMDEX index traversal visits a sequence of items with a *monotonically decreasing* upper bound on the true rating for each user-item pair. We state this more formally in the following two Lemmas below, which highlight in reasoning about the behavior of SIMDEX's querying:

LEMMA 1 (MONOTONICITY OF SORTED INDEX LISTS). *Let L_c be a sorted index list constructed by* SIMDEX. *For each pair of items* $\mathbf{i}$,$\mathbf{j}$ *in L_c, if* $\mathbf{i}$ *appears before* $\mathbf{j}$ *in L_c, then $r^*_{ci} \geq r^*_{cj}$.*

PROOF. This is by construction: Algorithm 1 sorts each list in descending order by the corresponding r^*_{ci}. □

This fact, coupled with the fact that each $\hat{r}^b_i$ is a true upper bound on the rating for item i for each user u assigned to $\mathbf{c}$, establishes our correctness criteria. First, we prove the upper bound:

LEMMA 2 (UPPER BOUND IN INDEX LISTS). *Given r^*_{ci} corresponding to item* $\mathbf{i}$, $\forall$ *users* $\mathbf{u}$ *assigned to* $\mathbf{c}$, $r^*_{ci} \geq \frac{\mathbf{u} \cdot \mathbf{i}}{\|\mathbf{u}\|}$.

PROOF. This is also by construction. Recall that $\mathbf{u} \cdot \mathbf{i} = \|\mathbf{u}\|\,\|\mathbf{i}\| \cos(\theta_{ui})$, where θ_{ui} is the angular distance between $\mathbf{u}$ and $\mathbf{i}$. Therefore, we have $\frac{\mathbf{u} \cdot \mathbf{i}}{\|\mathbf{u}\|} = \|\mathbf{i}\| \cos(\theta_{ui})$. By the triangle inequality, given θ_{ic}, the angular distance between item $\mathbf{i}$ and cluster $\mathbf{c}$, we have

$$\|\mathbf{i}\| \cos(\theta_{ui}) \leq \|\mathbf{i}\| \max_{\theta \in [\theta_{ic} \pm \theta_{uc}]} \cos\theta$$

For all $c_i, c_j \in [0, \pi]$, if $c_i > c_j$, then $\cos(c_i) < \cos(c_j)$. In our case, $\theta_{uc}, \theta_b \in [0, \pi]$ by construction, and θ_b is chosen to be larger than all $\theta_{u'c}$ for all $\mathbf{u}'$ assigned to the cluster.

$$\|\mathbf{i}\| \max_{\theta \in [\theta_{ic} \pm \theta_{uc}]} \cos\theta \leq \|\mathbf{i}\| \max_{\theta \in [\theta_{ic} \pm \theta_b]} \cos\theta = r^*_{ci}.$$

Therefore, $r^*_{ci} \geq \frac{\mathbf{u} \cdot \mathbf{i}}{\|\mathbf{u}\|}$, as desired. □

Finally, we can prove that SIMDEX's index is exact:

THEOREM 1. SIMDEX*'s index returns exact top-K results for Maximum Inner Product Search.*

PROOF. Suppose there exists user $\mathbf{u}$ such that Algorithm 2 returns a set of items I' that is not the true top-K result I^* for MIPS for $\mathbf{u}$. Then there exists at least one item $\mathbf{i}_w \in I'$ such that $\mathbf{i}_w \notin I^*$. $|I'| = |I^*| = k$ because Algorithm 1 always returns k items. Therefore, there must also exist at least one item $\mathbf{i}_r \in I^*$ such that $\mathbf{i}_r \notin I'$. Because $\mathbf{i}_r$ is part of the true top-K for $\mathbf{u}$ and $\mathbf{i}_w$ is not, it must be the case that $\mathbf{u} \cdot \mathbf{i}_r > \mathbf{u} \cdot \mathbf{i}_w$. Algorithm 1 computes $\mathbf{u} \cdot \mathbf{i}$ for each $\mathbf{i}$ it visits, and, had it visited $\mathbf{i}_r$, then $\mathbf{i}_r$ would have been added to the min-heap and eventually returned as I'. Therefore, Algorithm 1 must not have visited $\mathbf{i}_r$ in the corresponding L_{cm} sorted index list. This implies that there exists some item $\mathbf{i}_s$ in L_{cm} appearing before $\mathbf{i}_r$ such that $r^*_{ci_s} < \frac{\mathbf{u} \cdot \mathbf{i}_w}{\|u\|}$, thus causing Algorithm 1 to return I' without visiting $\mathbf{i}_r$. Per Lemma 1, this implies $r_{ci_s} \geq r^*_{ci_r}$, so $\frac{\mathbf{u} \cdot \mathbf{i}_w}{\|u\|} > r^*_{ci_r}$. However, per Lemma 2, $r^*_{ci_r} \geq \frac{\mathbf{u} \cdot \mathbf{i}_r}{\|\mathbf{u}\|}$. This implies $\mathbf{u} \cdot \mathbf{i}_w > \mathbf{u} \cdot \mathbf{i}_r$, a contradiction, and so I' must contain the true top-K result. □

Recall that blocked matrix multiply is also exact, so, given Theorem 1, SIMDEX returns exact top-K MIPS solutions independent of the SIMDEX optimizer's selection of SIMDEX's index or matrix multiply.

4. EXPERIMENTAL EVALUATION

In this section, we evaluate SIMDEX's efficiency at answering top-K queries across varying datasets, regularizations, and serving methods. We answer the following questions:

1. Does SIMDEX improve the runtime of computing exact top-K recommendations on standard datasets?
2. Between blocked matrix multiply and SIMDEX's index, can SIMDEX identify the optimal serving strategy?
3. How fast is SIMDEX's entire index construction pipeline—user clustering, executing the cost-based optimizer, computing and sorting the upper bounds, then computing the exact top-K?
4. How sensitive is SIMDEX's index to clustering parameters?

We answer these questions via experimental analysis on reference benchmark datasets from the literature and via comparison to several state-of-the-art methods. Our results show that SIMDEX delivers an average of 2× and up to 6× speedups over existing, highly-optimized baselines. Furthermore SIMDEX identifies the optimal serving strategy with an average of only 1.86% overhead.

4.1 Experimental Setup

Datasets. We use three reference benchmark datasets for our experimental evaluation (Table 1). These are widely used throughout

Dataset	# users	# items	# ratings
Netflix Prize [7] (Netflix)	480,189	17,770	100,480,507
Yahoo Music KDD [16] (KDD)	1,000,990	624,961	252,810,175
Yahoo Music R2 [42] (R2)	1,823,179	136,736	699,640,226

Table 1: Reference standard collaborative filtering datasets for evaluation.

the literature to evaluate collaborative filtering models; related work has also benchmarked their systems against these datasets, and we consider them the reference standard.

The authors of [37] provided the models used in their evaluation of LEMP, which were trained using Distributed Stochastic Gradient Descent [38]; we denote these models as $\star$-DSGD throughout this section. For the remaining datasets, we train models using the NOMAD toolkit [44] (denoted $\star$-NOMAD), using the regularization parameter and hyperparameters settings reported in [44] as the starting point for a grid search for the optimal test RMSE. For the Yahoo Music R2 dataset[1], the literature did not contain any previously reported hyperparameter settings; therefore, we performed an expanded grid search. For all datasets, we report results from the best trained models for each value of f.

Implementation. We implemented SIMDEX in C++. For a fair comparison to the baselines below, we use double floating point precision with single-threaded execution. We use the open source Armadillo library [33] for k-means and Intel MKL [19] for blocked matrix multiply (both configured for single-threaded execution). Our source code is available online[2] and we have also validated the correctness of SIMDEX's exact top-K results by comparing with the top-K results of the brute-force approach.

Benchmarking. To benchmark SIMDEX, we compared our implementation against LEMP and FEXIPRO, the current state of the art in top-K serving.

For LEMP, we use the publicly available source code provided by the LEMP authors to reproduce their benchmarks using our target models; the LEMP authors' recent work [37] shows that it outperforms all prior solutions to the MF MIPS setting, providing a gold standard for evaluation. We compile LEMP with SIMD optimizations enabled for maximum performance.

For FEXIPRO, we were unable to obtain the source code and/or target models from the authors. Therefore, we re-implemented FEXIPRO in C++, following the description in [25]. We included all three pruning transformations (i.e., SVD, integer, monotonic) and used the same the linear algebra libraries (i.e., Armadillo[3]) to compute the thin SVD operation, a necessary step in FEXIPRO's algorithm. In our experiments, we were unable to reproduce FEXIPRO's speedups over LEMP reported in [25]. As a result, we provided the FEXIPRO authors both our source code and experimental results, but have not yet received a response. Therefore, in this section, we report runtimes from our own implementation of FEXIPRO, which is available as open source online[4].

Environment. We report results on a single Intel Xeon E7-4850 v3 2.20 GHz processor with 1 TB of RAM. We allow Intel MKL to use the entire 1TB memory in blocking, however SIMDEX's index only uses a small fraction and, on the largest dataset, MKL uses no more than 80GB for blocked matrix multiply. Although the processor has multiple cores, we report only the single-threaded performance for SIMDEX's index, blocked matrix multiply, and LEMP. By default, SIMDEX uses a work-sharing block size of 4096 items and uses an index size of 8 clusters for each model.

[1]https://webscope.sandbox.yahoo.com/catalog.php?datatype=r&did=2
[2]https://github.com/stanford-futuredata/simdex
[3]http://arma.sourceforge.net
[4]https://github.com/stanford-futuredata/fexipro-benchmarking

4.2 Results

End-to-End Performance. To begin, we examine end-to-end performance of SIMDEX compared to alternative, exact methods. Figure 4 depicts the results across all three datasets and all target models, varying the target K in top-K and the number of latent factors. By using its optimizer to select between clustering users and blocked matrix multiply, SIMDEX computes top-K an average of $2\times$ (and up to $6\times$) faster than LEMP and substantially (> $10\times$) faster than FEXIPRO. These runtime improvements are especially significant because each model depicted in Figure 4 is the *optimal* choice of model hyperparameters for the given training method; SIMDEX is able to efficiently and accurately identify the appropriate serving strategy independent of the regime (i.e., high similarity or low similarity) of the optimal model, a phenomenon we study in detail in the remainder of this section.

The optimal choice of technique (SIMDEX's index, matrix multiply, or LEMP) varies by dataset. We show in the next subsection that SIMDEX's optimizer automatically identifies the optimal choice between SIMDEX's index and matrix multiply. Moreover, for 49 of 64 model configurations, SIMDEX is either within 5% of LEMP or is faster. Most notably, LEMP outperforms SIMDEX by an average of 7% on Netflix-DSGD, $f = 10$ and by an average of 67% on R2-NOMAD, $f = 100$. Unsurprisingly, these models are trained with higher regularization, so matrix multiply is not chosen and LEMP is able to prune more computation than SIMDEX's index. As shown in Section 1, the best choice of technique varies heavily based on dataset, training method (i.e., DSGD or NOMAD), and regularization; no one choice dominates. To better understand these factors, we performed a series of additional microbenchmarks below.

Impact of regularization. We return to the question of regularization raised in Section 1, Figure 1, this time comparing to SIMDEX's index. Figure 5 illustrates the trade-off between regularization and running time for SIMDEX's index, matrix multiply, and LEMP: the fastest serving method for the most accurate model varies substantially. However, because SIMDEX is able to accurately identify the fastest method, it can optimally decide between SIMDEX's index and matrix multiply on a per-model basis. Given the high degree of heterogeneity in model training routines and appropriate hyperparameters for each dataset, this is an important property if one wishes to serve the *best* (most accurate) models fast.

Optimizer Quality. Table 2 illustrates the accuracy of SIMDEX's optimizer in selecting between SIMDEX's index and matrix multiply. We apply a base hardware factor h of 0.05, indicating a $20\times$ benefit for blocking on our current hardware, due to both increased memory bandwidth (due to sequential access) and floating point operations (due to matrix multiply's lack of control flow) resulting in increased effective FLOPS. Because matrix multiply performs priority queue-based selection sort to find the true top-K items after multiplication, we add a corrective $\log_2(K)$ factor as we increase K. As a result, SIMDEX's cost model is able to recover the optimal decision for all but one dataset, Netflix-NOMAD, $f = 25$. For this dataset, SIMDEX selects matrix multiply, which is an average of 9.3% slower than SIMDEX's index. We believe this margin of error is reasonable (e.g., compared to conventional query processing cost estimates) and, for Netflix-NOMAD, $f = 25$, the resulting (sub-optimal) choice is still substantially faster than LEMP and FEXIPRO. This demonstrates that SIMDEX can make accurate, *model-specific* decisions, enabling substantial end-to-end performance improvements.

Clustering sensitivity. To understand the effect of SIMDEX's clustering on end-to-end runtime, we varied the number of clusters

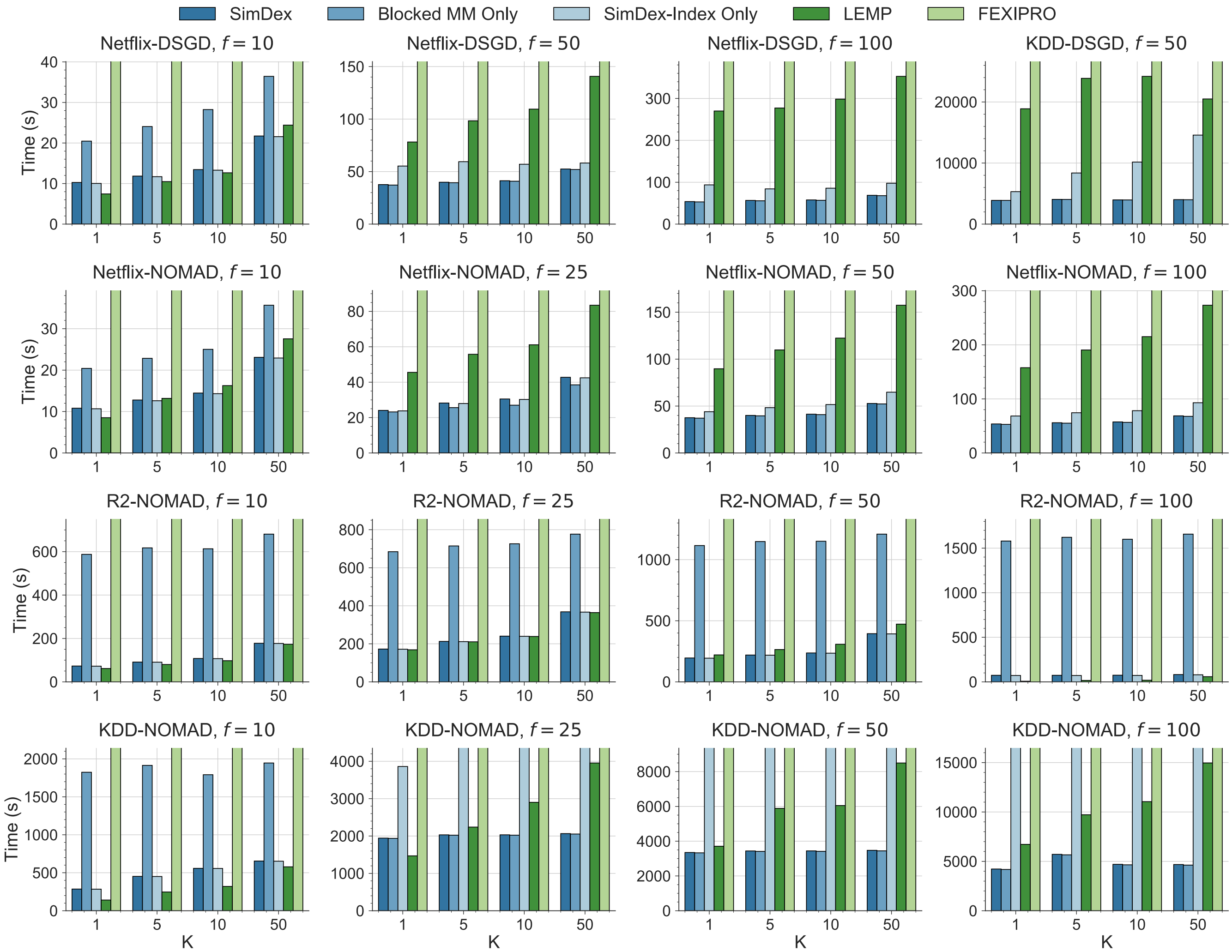


Figure 4: Wall-clock time of SIMDEX compared to LEMP and FEXIPRO for computing top-K (lower is better). For each model, we tuned the hyperparameters during training to yield the optimal test RMSE. On average, SIMDEX is $2\times$ faster than LEMP and substantially faster than FEXIPRO, which fails to complete in the time intervals depicted.

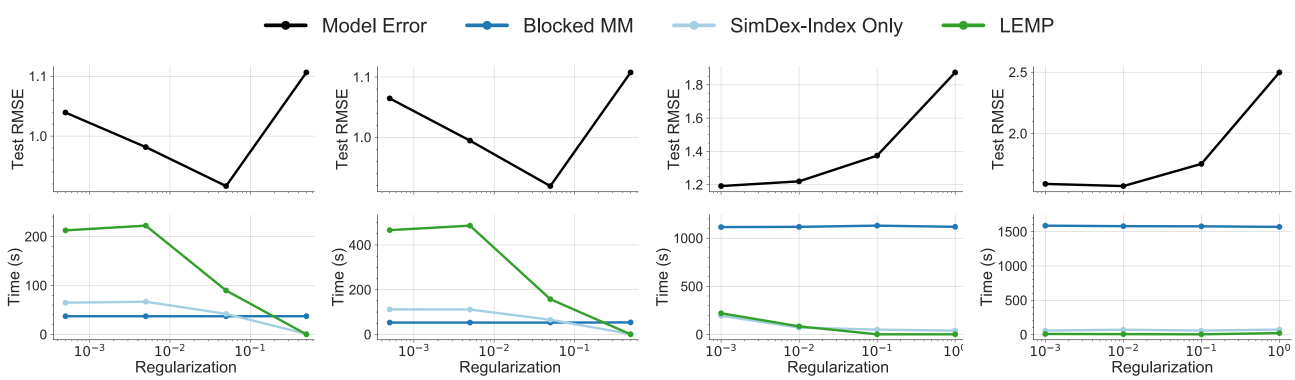


Figure 5: Impact of regularization (λ) on runtime performance of SIMDEX's index, blocked matrix multiply, and LEMP. As λ increases, SIMDEX's index obtains a better clustering of the user vectors, which leads to tighter bounds and improved performance.

SIMDEX uses. Figure 7 illustrates the trade-off between clustering time and computation time for each dataset: more clusters require more time to compute but subsequently reduce the computational overhead of later steps, while fewer clusters require less time to compute but increase the computational overhead of later steps. Clustering time increases roughly proportionally to the number of

	$K=1(h=0.05)$			$K=5(h=0.11)$			$K=10(h=0.16)$			$K=50(h=0.28)$		
Model	$\frac{\hat{w}-B}{\lvert I\rvert-B}$	MM	SDI	$\frac{\hat{w}-B}{\lvert I\rvert-B}$	MM	SDI	$\frac{\hat{w}-B}{\lvert I\rvert-B}$	MM	SDI	$\frac{\hat{w}-B}{\lvert I\rvert-B}$	MM	SDI
Netflix-DSGD, $f=10$	0.032	20.47	**6.27**	0.058	24.06	**7.42**	0.092	28.24	**8.82**	0.176	36.44	**17.21**
Netflix-DSGD, $f=50$	0.375	**37.20**	48.36	0.477	**39.45**	41.37	0.542	**40.85**	45.33	0.700	**51.99**	57.20
Netflix-DSGD, $f=100$	0.699	**52.99**	77.7	0.786	**55.72**	80.41	0.842	**56.89**	85.53	0.898	**67.94**	97.68
KDD-DSGD, $f=50$	0.135	**3879.4**	5311.8	0.210	**4040.02**	8373.12	0.241	**3959.36**	10160.29	0.339	**3994.79**	14577.1
Netflix-NOMAD, $f=10$	0.039	20.42	**6.46**	0.109	22.85	**8.11**	0.112	25.02	**9.19**	0.231	35.66	**18.83**
Netflix-NOMAD, $f=25$	0.358	**23.19**	20.77	0.440	**25.63**	22.56	0.515	**27.01**	24.68	0.676	**38.50**	37.49
Netflix-NOMAD, $f=50$	0.570	**37.14**	41.90	0.668	**39.59**	43.10	0.712	**40.87**	44.56	0.817	**52.31**	58.64
Netflix-NOMAD, $f=100$	0.576	**52.89**	65.46	0.651	**55.16**	73.47	0.697	**56.67**	76.86	0.827	**67.78**	85.75
R2-NOMAD, $f=10$	0.022	587.649	**72.46**	0.036	617.48	**90.64**	0.044	613.28	**107.09**	0.069	680.90	**177.11**
R2-NOMAD, $f=25$	0.050	684.40	**171.56**	0.063	714.75	**211.62**	0.074	726.2	**239.46**	0.104	776.98	**366.93**
R2-NOMAD, $f=50$	0.0317	1115.71	**193.96**	0.038	1148.41	**218.14**	0.043	1150.89	**234.96**	0.067	1209.32	**392.78**
R2-NOMAD, $f=100$	0.0	1587.27	**58.79**	0.0	1611.96	**68.87**	0.0	1623.97	**59.49**	0.0	1659.32	**66.472**
KDD-NOMAD, $f=10$	0.0482	1823.83	**289.428**	0.092	1914.22	**450.93**	0.117	1790.98	**557.36**	0.168	1945.63	**652.28**
KDD-NOMAD, $f=25$	0.271	**1937.96**	3860.57	0.358	**2023.2**	5967.71	0.403	**2023.16**	6910.16	0.500	**2053.55**	9220.97
KDD-NOMAD, $f=50$	0.503	**3329.06**	19612.4	0.597	**3412.78**	23245.40	0.618	**3416.58**	24487.09	0.691	**3445.22**	30286.40
KDD-NOMAD, $f=100$	0.552	**4178.61**	-	0.623	**5660.329**	-	0.649	**4646.53**	-	0.716	**4623.21**	-

Table 2: SIMDEX optimizer quality: SIMDEX's relative cost estimate for matrix multiply versus index serving (via Equation 5) as well as actual runtimes for matrix-multiply (MM) and SIMDEX index-only serving (SDI). For R2-NOMAD, $f = 100$, $\hat{w} = B = 4096$. In addition, we omit timing for SDI KDD-NOMAD, $f = 100$, which did not complete within $10\times$ of MM. With a hardware factor of $h = 0.05 \log_2(K)$, SIMDEX's optimizer selects a serving strategy (choice depicted in bold) that is optimal for all but one dataset, Netflix-NOMAD, $f = 25$, in which SIMDEX's choice of matrix multiply is an average of 9.3% slower than SIMDEX's index. These results demonstrate the utility and accuracy of SIMDEX's cost model.

clusters, while computational time decreases in a dataset-dependent manner. Overall, we find that a small number of clusters ($C = 8$) performs well across datasets (including those not depicted in this plot), and, given the relative robustness of this parameter to mild perturbations, we believe that a small amount of tuning (if any) beyond this reasonable default will perform well in practice.

Point Queries. One aspect of SIMDEX's index that is unique compared to LEMP and matrix multiply is its amenability to point queries (i.e., online queries, without pre-computing all users and all items). That is, following index construction, SIMDEX can stop processing and instead only compute user predictions on demand. To investigate the performance implications of this option, we measured the latency of SIMDEX's index for point queries with work-sharing disabled. Figure 8 depicts the results for single-user queries across several models; we plot a CDF of the query latencies to show the distribution of runtime performance for the users in the dataset. For two Netflix models, SIMDEX's index performs well, averaging 1.7 ms per user (which, again does not include the pre-processing time to construct the index, which ranges from a few hundred milliseconds to a few seconds). In contrast, the KDD and R2 models have more items, resulting in query times in the tens of milliseconds. These latencies are lower than waiting to compute a full, batched matrix multiply (or LEMP) for all users (tens to thousands of seconds) but in turn incur a throughput penalty as depicted in Figure 4.

Runtime analysis. Finally, to better understand the impact of each stage of SIMDEX's execution and to analyze its overhead, we measured the running time of each component. On average, SIMDEX incurs an overhead of 1.82% for clustering, constructing its index, and performing cost estimation. We illustrate a breakdown for Netflix-NOMAD, $f = 50$ and R2-NOMAD, $f = 50$ in Figure 6, both of which use SIMDEX's index; for Netflix, SIMDEX spends 0.79 seconds in the first three stages, and over 43 seconds in the final stage when computing predictions using the index. We also illustrate the effect of work sharing, which delivers $2.43\times$ and $1.38\times$ speedups for these datasets; the effect for Netflix is more pronounced because the average number of items visited in the index for each user (i.e., $\bar{w}$) is larger than in R2. Sharing a single, small blocked matrix multiply at the start of index traversal allows SIMDEX's index to benefit from hardware-efficient BLAS. Overall, SIMDEX's overheads are small, especially relative to the speedups that SIMDEX's optimizer enables by choosing between SIMDEX's index and matrix multiply.

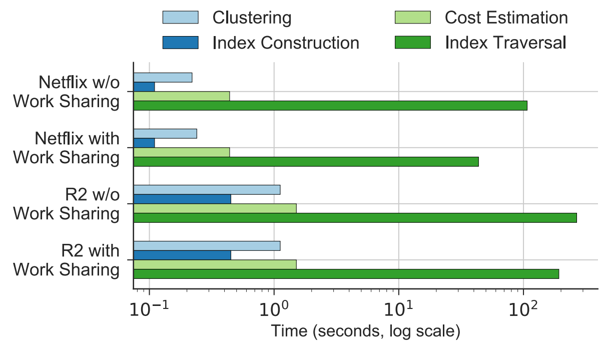


Figure 6: Runtime breakdown of SIMDEX top-1 execution for Netflix-NOMAD, $f = 50$ and R2-NOMAD, $f = 50$ datasets, both of which execute using SIMDEX's index. Enabling blocking improves execution time by $2.43\times$ and $1.38\times$, respectively. In deciding to make predictions using SIMDEX's index, SIMDEX's optimizer incurs overheads of 1.78% and 1.58%.

5. RELATED WORK

We survey the prior literature on Maximum Inner Product Search (MIPS) to provide a more thorough overview of the various strategies used to improve the runtime performance of top-K. For a given strategy (e.g., tree-based indexes), we focus our attention on the best representative solutions found in the literature and describe the relative advantages and disadvantages between them and SIMDEX.

Many of the standard high-dimensional clustering and search techniques found in the literature, such as nearest-neighbor search (NNS) [12, 43], cosine similarity search [5, 11, 24, 36, 41], and Locality Sensitive Hashing (LSH) [3, 10], have been applied to MIPS. As discussed in Section 2, classic techniques target distance functions that obey the triangle inequality. However, inner product does not obey the triangle inequality, so traditional approaches to NNS, cosine similarity search, and LSH can only compute the approximate—not exact—top K. In this direction, recent work has extended LSH to support asymmetric hash functions [35], which reduce the approximate MIPS problem to a sublinear nearest-neighbor search. Similarly, Bachrach et al. [4] also reduce MIPS to NNS using a novel Euclidean transformation, while Zhang et al. [45] use hashing to approximate MIPS. However, these techniques compute an approximate top K. We provide an exact top-K method.

Several authors have proposed using tree-based indexes to im-

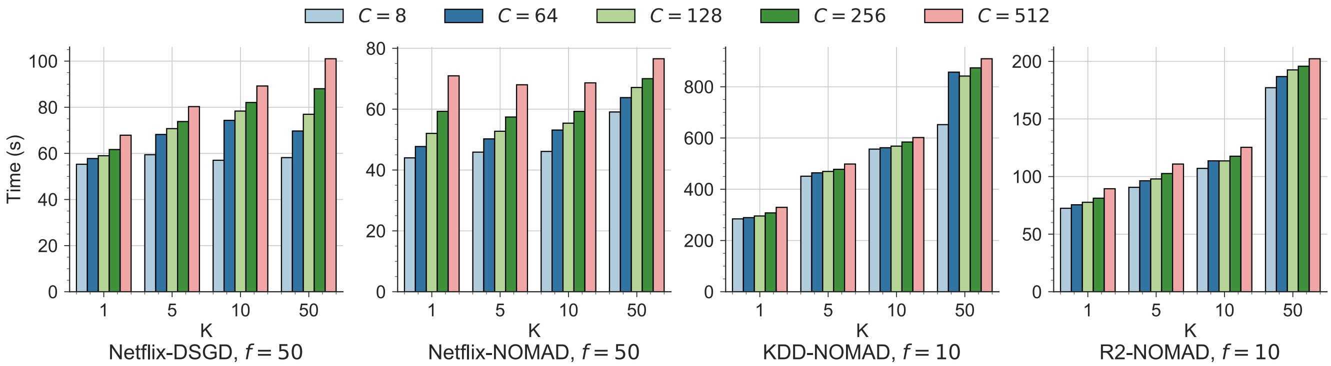


Figure 7: Runtime vs number of clusters for SIMDEX's index. A choice of $C = 8$ delivers robust performance across datasets.

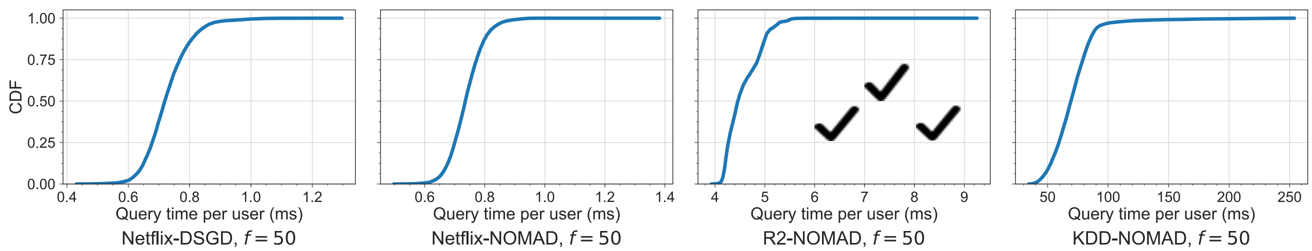


Figure 8: Distribution of point query times for $K = 1$ using SIMDEX's index. While SIMDEX's optimizer chooses between SIMDEX's index and batch matrix multiply, SIMDEX's index can also be used to serve point (i.e., online) queries for users with low latency if desired.

prove the runtime of top-K computation. Ram and Gray [29] present three different techniques for indexing the items of the dataset: single-ball trees, dual-ball trees, and cone trees. All three data structures share a similar strategy: they recursively subdivide the metric space of items into hyperspheres. Every node in the tree represents a set of points, and each node is indexed with a center and a ball enclosing all the points in the node. Of the three, the cone tree offers the fastest speedups. All of these data structures compute the exact top-K; however, the speedups they attain are limited for high-dimensional and large datasets. For K=1 and F=51, they achieve a 1.98× speedup on Netflix and a 2.16× speedup on Yahoo KDD. Follow-on work by Curtin et al. [15] extend this method using cover trees [8] but the result (and follow-on results from Curtin and Ram [14] using dual-trees [18]) are still empirically slower than alternatives due to high index construction and traversal time [37]. Unlike SIMDEX, none of the these approaches utilize the commonalities among users to prune the search space of items.

Teflioudi et al. [37] present LEMP, an index on item vectors to speed up top-K computation. LEMP sorts the item vectors by length and partitions them into buckets: each bucket is sized to fit in the processor's cache and contains a set of item vectors of roughly equal magnitude. After this discretization step, LEMP computes an exact top-K by using the angles of the item vectors to solve a smaller cosine similarity search problem within each bucket, thus taking advantage of both the direction and length of each item vector. If the variance of the item vector norms is sufficiently high within a single bucket, LEMP eschews cosine similarity search in favor of a more suitable search technique, such as an incremental pruning of the candidate items based on partial inner products and the Cauchy-Schwarz inequality. Thus, LEMP exploits similarities among *item vectors* but does not exploit the similarities between *user vectors* that are found in collaborative filtering models. In contrast, SIMDEX clusters users and analyzes the direction and length *between* centroids and the item vectors in the dataset. This strategy enables SIMDEX to leverage these user similarities effectively.

Most recently, FEXIPRO [25] combines several pruning techniques to reduce computation during predictions. First, FEXIPRO computes the thin SVD on the item matrix and uses the output to apply lossless transformation to the user and item matrices. This transformation places larger weights in the first few dimensions of each vector, thus improving on the incremental pruning techniques first suggested by LEMP. Second, FEXIPRO applies integer-based quantization to enable more efficient integer-based CPU instructions for inner product computations. Third, FEXIPRO applies a final transformation that ensures the inner product will always increase monotonically by removing negative weights. Combined, [25] reports substantial speedups over LEMP. However, as we have discussed in Section 4, we were unable to reproduce these results. Nevertheless, we believe that similar types of transformations—especially SVD transformations and integer pruning—are noteworthy contributions to the MIPS problem, and are likely complementary optimizations one could apply to SIMDEX during index-based serving.

Finally, Koenigstein et al. [22] introduce two methods for indexing Matrix Factorization models: i) indexing the items with metric trees, and ii) clustering users using spherical clustering. The first approach builds a metric tree on the items in the dataset similar to Ram et al.; once constructed, they employ a branch-and-bound algorithm to compute the top-K for each user as they traverse through the tree. While the exact top-K is always found, their approach also yields limited speedups on large datasets: for K=50 and F=50, they achieve a 1.31× speedup for Netflix and a 3.01× speedup for Yahoo KDD. The second method they present is an approximate approach that is closely related to SIMDEX: in this method, users are placed into cones of similar "taste" and then recommendations for each of these cones are pre-computed. Given these cones, the top-K for a given user is the top-K of the cone the user belongs to. While this strategy provides a significantly means way of retrieving the top-K, the results are not accurate: for example, on Yahoo KDD, they achieve a 4.45× speedup with 75% accuracy. SIMDEX also clusters users; however, we use the resulting clusters to produce a conservative upper bound the predicted ratings for user-item pairs, enabling us to filter out items that cannot be in a user's top-K, thus preserving exact top-K while achieving faster query speed.

6. CONCLUSION

Collaborative filtering and matrix factorization models are a critical component of recommender systems at scale. In this work, we draw a connection between the degree of similarity in a model—induced by model training parameters such as regularization—and the ability to efficiently utilize it in predicting new recommendations using existing techniques. Specifically, for several of the most accurate models, brute-force matrix multiply outperforms prior state of the art. To capitalize on this observation, we introduced SIMDEX, a new method for serving top-K queries over matrix factorization models that measures and optimizes for the similarity in a given model. SIMDEX combines clustering with a new bound on predicted ratings to quickly determine whether to attempt to prune computation or to perform blocked matrix multiply, subsequently performing well in both high-similarity and low-similarity regimes. Our implementation demonstrates accurate decision-making and achieves substantial speedups over alternatives across a range of models produced by different datasets, training hyperparameters, and training algorithms. These results indicate a fundamental connection between model training and model serving at scale. SIMDEX is open source at https://github.com/stanford-futuredata/simdex.

Acknowledgments. We thank the many members of the Stanford InfoLab for providing feedback on this work. This research was supported in part by Toyota Research Institute, Intel, the Army High Performance Computing Research Center, RWE AG, Visa, Keysight Technologies, Northrop Grumman, Facebook, and VMWare.

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