Parallel MMF: a Multiresolution Approach to Matrix Computation

Risi Kondor† Nedelina Teneva* and Pramod K. Mudrakarta*
*Department of Computer Science, †Department of Statistics
{risi,nteneva,pramodkm}@cs.uchicago.edu
The University of Chicago

Abstract

Multiresolution Matrix Factorization (MMF) was recently introduced as a method for finding multiscale structure and defining wavelets on graphs/matrices. In this paper we derive pMMF, a parallel algorithm for computing the MMF factorization. Empirically, the running time of pMMF scales linearly in the dimension for sparse matrices. We argue that this makes pMMF a valuable new computational primitive in its own right, and present experiments on using pMMF for two distinct purposes: compressing matrices and preconditioning large sparse linear systems.

1 Introduction

While the size of machine learning datasets continues to increase at the rate an order of magnitude or more every few years, the clock speed of commodity hardware has all but plateaued. Thus, increasingly, real world learning problems can only be tackled by algorithms that implicitly or explicitly exploit parallelism.

Broadly speaking, there are two main approaches to parallelizing the optimization problems at the heart of machine learning algorithms. In the data parallel model, the dataset is divided into batches (shards) that are processed independently by separate processing units, but all processing units have (synchronous or asynchronous) access to a central resource that stores the current values of all the optimization variables, i.e., the model’s parameters [1]. In the parameter parallel approach, all processing units operate on the same data, but each one of them optimizes only a subset of the parameters [2, 3]. Data parallel algorithms often exploit the assumption that data subsets are i.i.d. given the model parameters. However, such trivial parallelization is not suitable for model parallel algorithms, since it fails to capture the often non-trivial interactions between parameters and so taking independent parameter subsets could lead to flawed estimates. On the other hand, model parallelization is often achieved by course graining the parameter space (e.g., topological order or imposing some constraints on the graph induces by the parameter interaction), which might not be sufficient to discover the finer and more complex interactions between the parameters.

In contrast, in this paper we advocate a multiresolution approach to parallelism, in which both the data and the parameters are parallelized, and communication between processing units is minimized. At the finest level of resolution, the data is divided into many shards, which are processed independently, determining the “high frequency” parameters of the model. These parameters are local to each shard, obviating the need for a central parameter server. Additionally, the data in each shard is compressed, so when it is redistributed across the cores for the second level, each shard becomes a compressed sketch of a larger subset of the original dataset, making it possible for the second level processing units to “learn” parameters that capture lower frequency, less localized features. Iterating this process leads to a multi-level algorithm that simultaneously uncovers the structure of the original data, and fits a model.

The specific algorithm that we focus on in this paper is a parallelized version of the Multiresolution Matrix Factorization (MMF) process first described in [4]. By itself, MMF is not a learning algorithm. However, parallel MMF is a gateway to efficiently performing a range of fundamental
computational tasks, such as matrix compression, inversion, and solving linear systems. These tasks are critical building blocks of most learning algorithms. Due to space restrictions, the bulk of our numerical experiments, as well as the implementation details of our algorithm, which are critical to making pMMF scale to large problems, are relegated to the Supplement.

**Notations.** In the following, \([n]\) will denote the set \(\{1, 2, \ldots, n\}\). Given a matrix \(A \in \mathbb{R}^{n \times n}\) and two (ordered) sets \(S_1, S_2 \subseteq [n]\), \(A_{S_1,S_2}\) will denote the \(|S_1|\times|S_2|\)-dimensional submatrix of \(A\) cut out by the rows indexed by \(S_1\) and the columns indexed by \(S_2\). \(\overline{S}_1\) will denote \([n]\setminus S_1\). \(B_1 \otimes B_2 \otimes \ldots \otimes B_m = [n]\) denotes that the sets \(B_1, \ldots, B_m\) form a partition of \([n]\). \(A_{:,i}\) or \([A]_{:,i}\) denotes the \(i^{\text{th}}\) column of \(A\).

## 2 Parallel Multiresolution Matrix Factorization

The Multiresolution Matrix Factorization (MMF) of a symmetric matrix \(A \in \mathbb{R}^{n \times n}\) is a multi-level factorization of the form

\[
A \approx Q_1^T \ldots Q_L^T A L \ldots Q_L^T H Q_L Q_{L-1} \ldots Q_1,
\]

where \(Q_1, \ldots, Q_L\) is a sequence of carefully chosen orthogonal matrices (rotations) obeying a number of constraints:

1. Each \(Q_\ell\) is chosen from some subclass \(Q\) of highly sparse orthogonal matrices. In the simplest case, \(Q\) is the class of **Givens rotations**, i.e., orthogonal matrices that only differ from the identity matrix in four matrix elements

\[
\begin{align*}
Q_\ell (i, i) &= \cos \theta, \\
Q_\ell (i, j) &= \sin \theta,
\end{align*}
\]

for some pair of indices \((i, j)\) and rotation angle \(\theta\). Slightly more generally, \(Q\) can be the class of so-called **\(k\)-point rotations**, which rotate not just two, but \(k\) coordinates, \((i_1, \ldots, i_k)\).

2. The effective size of the rotations decreases according to a set schedule \(\delta_0 \geq \delta_1 \geq \ldots \geq \delta_L\), i.e., there is a nested sequence of sets \([n] = S_0 \supseteq S_1 \supseteq \ldots \supseteq S_L\) with \(|S_\ell| = \delta_\ell\) such that \([Q_\ell]_{S_{\ell-1}, S_{\ell-1}}\) is the \(n - \delta_{\ell-1}\) dimensional identity. \(S_\ell\) is called the **active set** at level \(\ell\). In the simplest case, exactly one row/column is removed from the active set after each rotation.

3. \(H\) is **\(S_L\)-core-diagonal**, which means that it is all zero, except for (a) the submatrix \([H]_{S_L,S_L}\) called the core and (b) the rest of the diagonal.

Moving the rotations in (1) over onto the left hand side, the structure implied by the above conditions can be represented graphically as

\[
\begin{array}{cccccccc}
Q_L^T & \ldots & Q_2^T & Q_1^T & P & A & P^T & Q_2 & \ldots & Q_L^T \\
Q_L & \ldots & Q_2 & Q_1 & A & H & A & \ldots & Q_L
\end{array}
\]

(2)

Here, for ease of visualization, \(A\) is conjugated by a permutation matrix \(P\), which ensures that \(S_\ell = \{1, \ldots, \delta_\ell\}\) for each \(\ell\). However, an actual MMF would not contain such an explicit permutation. In general, MMF is only an approximate factorization, because there is no guarantee that using a given number of rotations \(A\) can be brought into core-diagonal form with zero error. Most MMF factorization algorithms try to find \(Q_1, \ldots, Q_L\) and \(H\) so as to minimize the squared Frobenius norm of the difference between the l.h.s and r.h.s of (2), called the **residual**.

The original motivation for MMF in (4) was to mimic the structure of fast orthogonal wavelet transforms. For example, when \(A\) is the Laplacian matrix of a graph \(G\) and \(U = Q_L \ldots Q_2 Q_1\), the rows of \(U\) are interpreted as wavelets on the vertices of \(G\). Those rows whose indices lie in \(S_0\), \(S_1\) are set by the first rotation matrix \(Q_1\), and are not modified by the rest of the rotations. (If \(Q_1\) is a Givens rotation, there is only one such row, but for the more complicated rotations there might be several.) These rows are very sparse, and provide the lowest level, most local, highest frequency wavelets. The rows indexed by \(S_1 \setminus S_2\) are determined by \(Q_2 Q_1\), and correspond to level 2 wavelets, and so on. Writing the MMF as \(A \approx U^T H U\) suggests that the rows of \(U\) can also be interpreted as a hierarchically sparse PCA basis for \(A\). Finally, since the size of the active set decreases after each rotation, defining \(A_\ell = Q_\ell \ldots Q_1 A Q_1^T \ldots Q_\ell^T\), the sequence of transformations

\[
A = A_0 \mapsto A_1 \mapsto A_2 \mapsto \ldots \mapsto A_L \mapsto H
\]

(3)
is effectively a matrix compression scheme, which, according to [4], often significantly outperforms, for example, Nyström methods. MMF is closely related to Diffusion Wavelets [5] and Treelets [6].

Due to the above properties, MMF is an attractive tool for uncovering the structure of large datasets. However, it has one fundamental limitation, which is its computational cost. The greedy factorization algorithm described in [4] essentially follows the sequence of transformations in (3), at each level choosing \( Q_\ell \) and a set of rows/columns to be eliminated from the active set, so as to minimize their contribution to the final approximation error. Assuming the simplest case of each \( Q_\ell \) being a Givens rotation, this involves (a) finding the pair of vertices \((i, j)\) involved in \( Q_\ell \), and (b) finding the rotation angle \( \theta \). In general, the latter is easy. However, finding the optimal choice of \((i, j)\) (or, in the case of \( k \)-point rotations, \((i_1, \ldots, i_k)\)) is a combinatorial problem that scales poorly with \( n \).

The first obstacle is that the optimization is based on inner products between columns, so it requires computing the Gram matrix \( G_\ell = A_{\ell -1}^T A_{\ell -1} \) at a complexity of \( O(n^3) \). Note that this need only be done once: since rotations act on \( G_\ell \) the same way that they act on \( A \), once we have \( G_1 = A^T A \), each subsequent \( G_\ell \) can be efficiently derived via the recursion \( G_{\ell+1} = Q_{\ell} G_\ell Q_{\ell}^T \). The second obstacle is that searching for the optimal \((i_1, \ldots, i_k)\) has complexity \( O(n^k) \).

The objective of the present paper is to construct a parallel MMF algorithm, pMMF, which, on typical matrices, assuming access to a sufficient number of processors, runs in time close to linear in \( n \). The ideas behind the new algorithm exploit the very structure in \( A \) that MMF factorizations pursue in the first place, namely locality at multiple levels of resolution.

### 2.1 Clustering

The first and crucial step towards pMMF is to cluster the rows/columns of \( A \) into \( m \) clusters and only consider rotations between \( k \)-sets of rows/columns that belong to the same cluster. Letting \( B_u \) be the indices of the rows/columns belonging to cluster \( u \), clustering has three immediate benefits:

1. Instead of having to compute the full Gram matrix \( G = A^T A \), it is sufficient to compute the local Gram matrices \( \{G^u = A^T B_u A_{B_u}\} \). Assuming that the clustering is even, i.e., \( |B_u| = \Theta(c) \) for some typical cluster size \( c \) (and therefore, \( m = \Theta(n/c) \)), this reduces the overall complexity of computing the Gram matrices from \( O(n^3) \) to \( O(mcn^2n) = O(cn^3) \).

2. The complexity of the index search problem involved in finding each \( Q_\ell \) is reduced from \( O(n^k) \) to \( O(c^k) \). In typical MMFs \( \delta_L = O(n) \), and the total number of rotations, \( L \), scales linearly with \( n \). Therefore, the total complexity of searching for rotations in the unclustered case is \( O(n^{k+1}) \), whereas with clustering it is \( O(c^k n) \).

3. The Gram matrices and the rotations of the different clusters are completely decoupled, therefore, on a machine with at least \( m \) cores, they can be computed in parallel, reducing the computation time of the above to \( O(cn^2/m) = O(cn^2) \) and \( O(c^k n/m) = O(c^k + 1) \), respectively.

Using the clustering \( B_1 \cup B_2 \cup \ldots \cup B_m = [n] \) results in an MMF in which each of the \( Q_\ell \) matrices (and hence, also their product) are \((B_1, \ldots, B_m)\)-block-diagonal, as defined below.

**Definition 1** Given a partition \( B_1 \cup B_2 \cup \ldots \cup B_m \) of \([n]\), we say that \( M \in \mathbb{R}^{n \times n} \) is \((B_1, \ldots, B_m)\)-block-diagonal if \( M_{i,j} = 0 \) unless \( i \) and \( j \) fall in the same cluster \( B_u \) for some \( u \).

Clustering, in the form described above, decouples MMF into \( m \) completely independent subproblems. Besides the inherent instability of such an algorithm due to the vagaries of clustering algorithms, this approach is antithetical to the philosophy of multiresolution, since it cannot discover global features in the data: by definition, every wavelet will be local to only one cluster. The natural solution is to soften the clustering by repeatedly re-clustering the data after a certain number of rotations. Writing out the full MMF again and grouping together rotations with the same clustering structure

\[
A \approx Q_1^T H Q_1 \cdots Q_{i_1 +1}^T H Q_{i_1} \cdots Q_{i_p +1}^T H Q_{i_p} \cdots Q_1^T H Q_1
\]

results in a factorization

\[
A \approx \overline{Q}_1^T \overline{Q}_2^T \cdots \overline{Q}_p^T H \overline{Q}_p \cdots \overline{Q}_1, \tag{4}
\]

where each \( \overline{Q}_p \), which we call a *stage*, is now a product of many \( Q_\ell \) elementary rotations, all conforming to the same block diagonal structure \((B_{i_1}^p, \ldots, B_{i_p}^p)\). Note that the number of clusters,
In a given cluster

2.3 Blocked matrices

the criterion for elimination is minimal off-diagonal norm, $\| A_{i,i} \|$, finding each rotation to $O$ rotations, the $k$th order rotations need to be further computed.

Algorithm 1 pMMF (top level of the algorithm)

Input: a symmetric matrix $A \in \mathbb{R}^{n \times n}$

Set $A_0 \leftarrow A$

for ($p = 1$ to $P$) {
    cluster the active columns of $A_{p-1}$ to get $(B_{p1}^1, \ldots, B_{pm}^1)$
    reblock $A_{p-1}$ according to $(B_{p1}^1, \ldots, B_{pm}^1)$
    for ($u = 1$ to $m$) $Q_{p,u} \leftarrow \text{FindRotationsInCluster}(p, u)$
    for ($u = 1$ to $m$) for ($v = 1$ to $m$) set $[A_p]_{u,v} \leftarrow Q_{p,u} [A_{p-1}]_{u,v} Q_{p,v}^T$
    merge $(Q_{p,1}, \ldots, Q_{p,m})$ into $Q_p$
}

$H \leftarrow$ the core of $A_L$ plus its diagonal

Output: $(H, Q_1, \ldots, Q_p)$

$m_p$, might not be the same across stages. In particular, since the active part of $A_t$ progressively gets smaller and smaller, $m_p$ will usually decrease with $p$. The top level pseudocode of pMMF, driven by this repeated clustering process, is given in Algorithm 1.

2.2 Randomized greedy search for rotations

The second computational bottleneck in MMF is finding the $k$ rows/columns involved in each rotation. To address this, we use a randomized strategy, whereby first a single row/column $i_1$ is chosen from the active set (within a given cluster) uniformly at random, and then $k-1$ further rows/columns $i_2, \ldots, i_k$ are selected from the same cluster according to some separable objective function $\phi(i_2, \ldots, i_k)$ related to minimizing the contribution to the final error. For simplicity, in pMMF we use

$$\phi(i_2, \ldots, i_k) = \sum_{r=2}^{k} \frac{\| A_{i_1} : i_r \|}{\| A_{i_1} : i_r \|}$$

i.e., $[A_{i_1}]_{i_1}$ is rotated with the $k-1$ other columns that it has the highest normalized inner product with in absolute value. Similarly to 4, the actual rotation angle (or, in the case of $k$th order rotations, the $k \times k$ non-trivial submatrix of $Q_i$) is determined by diagonalizing $[G_i]_{(i_1, \ldots, i_k),(i_1, \ldots, i_k)}$ at a cost of only $O(k^2)$. This aggressive randomized-greedy strategy reduces the complexity of finding each rotation to $O(c)$, and in our experience does almost as well as exhaustive search. The criterion for elimination is minimal off-diagonal norm, $\| A_{i,i} \|_{\text{off-diag}} = (\| A_{i,i} \|^2 - A_{i,i}^2)^{1/2}$, because $\| A_{i,i} \|_{\text{off-diag}}$ is the contribution of eliminating row/column $i$ to the final error.

2.3 Blocked matrices

In a given cluster $u$ of a given stage $p$, the local Gram matrix $G_u$, and the rotations can be determined from the columns belonging to just that cluster. However, subsequently, these rotations need to be

Algorithm 2 FindRotationsInCluster$(p, u)$ — here $k = 2$ and $\eta$ is the compression ratio

Input: a matrix $A = [A_p]_{i,u} \in \mathbb{R}^{n \times c}$ made up of the $c$ columns of $A_{p-1}$ forming cluster $u$ in $A_p$

compute the Gram matrix $G = A^T A$

set $I = [c]$ (the active set)

for ($s = 1$ to $[\eta c]$) {
    select $i \in I$ uniformly at random
    find $j = \arg \max_{j \in I \setminus \{i\}} \| A_{i,i} A_{i,j} \| / \| A_{i,j} \|$
    find the Givens rotation $q_{ij}$ of columns $(i,j)$ as described in the text
    set $A \leftarrow q_{ij} A q_{ij}^T$
    set $G \leftarrow q_{ij} G q_{ij}^T$
    if $\| A_{i,i} \|_{\text{off-diag}} < \| A_{j,j} \|_{\text{off-diag}}$ eliminate $i$; otherwise eliminate $j$
}

Output: $Q_{p,u} = q_{[\eta c]} \ldots q_2 q_1$

4
applied to the entire matrix, from both the right and the left, which cuts across clusters. To be able to perform this part of the algorithm in parallel as well, we partition the original matrix, and the second operation is done in parallel for each row of blocks.

To perform this efficiently, the first operation is done in parallel for each column of blocks of the resulting data structure is called a symmetrically blocked matrix (c.f., [7]).

Definition 2 Given a matrix $A \in \mathbb{R}^{n \times n}$ and a partition $B_1 \cup B_2 \cup \ldots \cup B_m$ of $n$, the $(u, v)$ block of $A$ is the submatrix $[A]_{u,v} := A_{B_u,B_v}$. The symmetric blocked matrix form of $A$ consists of the $m^2$ separate matrices $\{([A]_{u,v})_i\}_{u,v=1}^m$.

In pMMF, the matrix $A_p$ is always maintained in blocked matrix form, where the block structure is dictated by the clustering of the current stage. For large matrices, the individual blocks can be stored on separate cores or separate machines, and all operations, including computing the Gram matrices, are performed in a block-parallel fashion. This further reduces the time complexity of the Gram matrix computation from $O(n^2)$ to $O(c^3)$. Assuming $m^2_p$-fold parallelism, and a total of $\eta_c$ rotations in stage $p$, the overall time needed to apply all of these rotations to the entire matrix scales with $O(\eta n c^2)$.

The blocked matrix data structure is ideally suited to carrying out each stage of MMF on a parallel system, because (except for summary statistics) no data needs to be communicated between the different blocks. However, changing the block structure of the matrix from one clustering to another can incur a large communication overhead. To retain $m$-fold parallelism, the reblocking is carried out in two phases: first, each column of blocks is reblocked row-wise, then each row of blocks in the resulting new blocked matrix is reblocked column-wise (Figure 1).

2.4 Sparsity and matrix-free MMF arithmetic

Ultimately, pMMF is intended for factoring matrices that are sparse, but whose dimensionality is in the hundreds of thousands or millions. As the factorization progresses, the fill-in (fraction of non-zeros) in $A_p$ will increase, but at the same time, the active part of $A_p$ will progressively shrink. This means that in practice, given a sufficiently highly parallel system, the overall complexity can still scale roughly linearly with the number of non-zeros in $A$.

The complete factorization appearing on the r.h.s. of (1) we denote $\tilde{A}$. Storing $\tilde{A}$ by storing $H$ and the $\{Q_r\}$ matrices separately, the space complexity scales roughly linearly in the dimension. On the other hand, computing $\tilde{A}$ explicitly as a dense $\mathbb{R}^{n \times n}$ matrix is usually unfeasible. Therefore, when applying the computed factorization, for example, as a preconditioner (Section 4), which requires repeatedly multiplying a vector $v$ by $\tilde{A}$, we use the so-called matrix-free approach: $v$ is stored in the same blocked form as $\tilde{A}$, the rotations are applied individually, and as the different stages are applied to $v$, the vector goes through an analogous reblocking process to that described for $\tilde{A}$. The complexity of matrix-free MMF/vector multiplication is $O(kpn)$. Inverting $\tilde{A}$, which is also critical for downstream applications, involves inverting the entries on the diagonal of $H$ and inverting the core matrix, thus the overall complexity of MMF inversion is $O(n + \delta_L^2)$.

The theoretical complexity of the main components of pMMF are summarized in Table 1. Of course, requiring $m^2$-fold parallelism as $m \to \infty$ is an abstraction. Note, however, that even the total operation count scales with $\gamma m^2$, which is just the number of non-zeros in the original matrix. The plots in Figure 2 and similar plots in the Supplement confirm that on many real world datasets,
pMMF often scales linearly in the number of nonzeros, hence, for bounded degree graphs, also in $n$. Particularly, matrices coming from sparse network graphs, the wall clock time of pMMF tends to scale linearly with the dimension. Also note that in these experiments $n$ is on the order of $10^4 \sim 10^5$, yet the factorization time is on the order of just one minute.

3 pMMF Compression

Most, if not all, machine learning algorithms reduce to linear algebra operations or optimization over large instance/feature matrices or instance-instance similarity matrices. The classical example is, of course, kernel methods, which reduce to convex optimization involving the so-called Gram matrix, a symmetric positive semi-definite (p.s.d.) matrix of size $n \times n$, where $n$ is the number of training examples. Despite their many attractive properties and their large literature, the applicability of kernel methods to today’s large datasets is limited by the fact that “out of the box” their computation times scale with about $n^3$. This issue (not just for kernel methods, but more broadly) has catalyzed an entire area focused on compressing or “sketching” matrices with minimal loss.

In the symmetric (and p.s.d) case, most sketching algorithms approximate $A \in \mathbb{R}^{n \times n}$ in the form $\tilde{A} = CW^\dagger C^\top$, where $C$ is a judiciously chosen $\mathbb{R}^{n \times m}$ matrix with $m \ll n$, and $W^\dagger$ is computed by taking the pseudo-inverse of a certain matrix that is of size only $m \times m$. The algorithms mainly differ in how they define $C$:

(i) Projection based methods set each column of $C$ to be a random linear combination of the columns of the original matrix $A$, and use Johnson–Lindenstrauss type arguments to show that the resulting low dimensional random sketch preserves most of the information at least about the part of $A$ spanned by its high eigenvalue eigenvectors [8]. These methods come with strong guarantees, but suffer from the cost of having to compute $m$ dense linear combinations of the columns of $A$. Even if $A$ was sparse, this process destroys the sparsity.

(ii) Structured projections are a twist on the above idea, replacing the random projection with a fixed, dense, but efficiently computable, basis transformation (and subsampling in that basis), such as the fast Hadamard transform or the fast Fourier transform [9, 10].

(iii) In contrast to (i) and (ii), Nyström algorithms construct $C$ by choosing a certain number of actual columns of $A$, usually by random sampling. Here, the focus has shifted from uniform sampling [11][12], via $l_2$–norm sampling [13], to sampling based on so-called leverage scores [14][15][16], which, for low rank matrices, can be shown to be optimal. Further recent developments include the ensemble Nyström method [17] and the clustered Nyström algorithm [18]. Finally, a number of adaptive algorithms have also been proposed [19][20][21].

pMMF can also be regarded as a sketching method, in the sense that it compresses $A$ into an $m := \delta_L \ll n$ dimensional core via a very fast series of orthogonal transforms $Q_L \ldots Q_2 Q_1$, which play a role analogous to $C^\top$. In contrast to the other methods, however, MMF also retains the entries on the diagonal of $H$. From the point of view of downstream computation, this incurs very little extra cost. For example, if the purpose of sketching $A$ is to compute its inverse, maybe for use in a Gaussian process or ridge regression, then $\tilde{A}^{-1}$ can be easily computed by inverting the core of $H$ (as in the Nyström methods), and just taking the inverse of all other matrix elements on the diagonal.

The main distinction between pMMF and other matrix sketching methods is that while the latter, implicitly or explicitly, make the assumption that $A$ is low rank, or close to low rank, MMF makes a different structural assumption about $A$, namely that it has hidden hierarchical or multiresolution structure. Figure 3 shows the results of experiments comparing the performance of MMF to other
matrix sketching algorithms on some standard datasets. As in panes 1–3, on most datasets that we tried, pMMF significantly outperforms the other sketching methods in both Frobenius norm error and spectral norm error (plots of the latter can be found in the Supplement). The advantage of pMMF seems to be particularly great on network graphs, perhaps not surprisingly, since it has long been conjectured that networks have multiresolution structure [23, 24]. However, we find that pMMF often outperforms other methods on kernel matrices in general. On the other hand, on a small fraction of datasets, typically those which explicitly have low rank or are very close to being low rank (e.g., the fourth pane of Figure 3), pMMF performs much worse than expected. In such cases, a combination of the low rank and multiresolution approaches might be most advantageous, which is the subject of ongoing work.

It is important to emphasize that pMMF is very scalable. Many other Nyström methods are implemented in MATLAB, which limits the size of datasets on which they can be feasibly ran on. Moreover, leverage score methods require estimating the singular vectors of $A$, which, unless $A$ is very low rank, can be a computational bottleneck. Several of the Nyström experiments took 30 minutes or more to run on 8 cores, whereas our custom C++ pMMF implementation compressed the matrix in at most one or two minutes (see more timing results in the Supplement). Hence, pMMF addresses a different regime than many other Nyström papers: whereas the latter often focus on compressing $\sim 10^3$ dimensional matrices to just 10–100 dimensions, we are more interested in compressing $\sim 10^4–10^5$ dimensional matrices to $\sim 10^1$ dimensions.

## 4 pMMF Preconditioning

Given a large matrix $A \in \mathbb{R}^{n \times n}$, and a vector $b \in \mathbb{R}^n$, solving the linear system $Ax = b$ is one of the most fundamental problems in computational mathematics. In the learning context, solving linear systems is the computational bottleneck in a range of algorithms. When $A$ is sparse, $Ax = b$ is typically solved with iterative methods, such as conjugate gradients. However, it is well known that the number of iterations needed for such methods to converge scales badly with $\kappa$, where $\kappa$ is the ratio of the largest and smallest eigenvalues of $A$, called the **condition number**.

The idea of **preconditioning** is to solve instead of $Ax = b$ the related system $(M^{-1}A)x = M^{-1}b$, where $M^{-1}$ is an easy to compute rough approximation to $A^{-1}$. A good preconditioner will ensure that $M^{-1}A$ is fast to multiply with the current vector iterate, while the condition number of $M^{-1}A$ is much better than that of the original matrix $A$. At the same time, it is important that $M^{-1}$ be easily computable for massive matrices. For symmetric matrices, a variation on the above is to solve $(M^{-1/2}AM^{-1/2})y = M^{-1/2}b$, and then set $x = M^{-1/2}y$, which retains symmetry. pMMF is a natural candidate preconditioner for symmetric matrices since (a) the pMMF factorization can be computed very fast (b) as evidenced by the previous section, $\tilde{A}$ is a good approximation to $A$, (c) $\tilde{A}^{-\xi}$ (with $\xi \in \{1, 1/2\}$) can be computed from $\tilde{A}$ in just $O(n + \delta n^3)$ time. However, unlike some other preconditioners, $\tilde{A}^{-\xi}$ is generally not sparse. Therefore, in MMP preconditioning one never expands $\tilde{A}^{-\xi}$ into a full matrix, but rather $\tilde{A}^{-\xi}$ is applied to the vectors involved in the iterative method of choice as a sequence of rotations, as described in Section 2.4.

A large number of different preconditioners have been proposed in the literature, and even for a given type of problem there is often no single best choice, rather the choice reduces to experimentation.
In our experiments our goal was to show that pMMF preconditioning can improve the convergence of linear solvers in learning problems, and that it is competitive with other preconditioners. Figure 4 compares the performance of pMMF as a preconditioner to other standard preconditioners, such as incomplete Cholesky and SSOR. Several more preconditioning results are presented in the Supplement. In summary, pMMF appears competitive with other preconditioners on network and kernel matrices, and sometimes outperforms other methods. In each of our experiments, the time required to compute the pMMF preconditioner was less than a minute, which is amortized over the number of linear solves. We are still experimenting with how much pMMF as a preconditioner can be improved by fine tuning its parameters, and how well it will perform coupled with other solvers.

5 Conclusions

The most common structural assumption about large matrices arising in learning problems is that they are low rank. This paper explores the alternative approach of assuming that they have multiresolution structure. Our results suggest that not only is the multiresolution model often more faithful to the actual structure of data (e.g., as evidenced by much lower approximation error in compression experiments), but it also lends itself to devising efficient parallel algorithms, which is critical to dealing with large scale problems. Our approach bears some similarities to multigrid methods [26] and structured matrix decompositions [27][28][29], which are extremely popular in applied mathematics, primarily in the context of solving systems of partial differential equations. A crucial difference, however, is that whereas in these algorithms the multiresolution structure is suggested by the geometry of the domain, in learning problems the structure itself has to be learnt “on the fly”. Empirically, the pMMF algorithm described in this paper scales linearly in the size of the data. Further work will explore folding entire learning and optimization algorithms into the multiresolution framework, while retaining the same scaling behavior.

|                         | serial MMF | pMMF operations | pMMF time | N_{\text{proc}} |
|-------------------------|------------|-----------------|-----------|-----------------|
|                         | dense      | sparse          | dense     | sparse          |                 |
| Computing Grams         | $O(n^4)$   | $O(\gamma n^3)$ | $O(\text{pen}^2)$ | $O(\text{pen}^2)$ | $m^2$           |
| Finding Rotations       | $O(n^3)$   | $O(\gamma n^3)$ | $O(\text{cn})$   | $O(\text{cn})$   | $m$             |
| Updating Grams          | $O(n^3)$   | $O(\gamma n^3)$ | $O(\text{en})$   | $O(\text{en})$   | $m$             |
| Applying rotations      | $O(\gamma kn^2)$ | $O(\gamma kn^2)$ | $O(\text{kn}^2)$ | $O(\text{kn}^2)$ | $m^2$           |
| Clustering              | $O(pn^2)$  | $O(\gamma pn^2)$ | $O(\text{pen})$  | $O(\text{pen})$  | $m^2$           |
| Reblocking              | $O(pn^2)$  | $O(\gamma pm^2)$ | $O(\text{pen})$  | $O(\text{pen})$  | $m$             |
| Factorization total     | $O(n^4)$   | $O(\gamma n^3)$ | $O(\text{pen}^2)$ | $O(\text{pen}^2)$ | $m^2$           |

Table 1: The rough complexity of different subtasks in pMMF vs. in the original serial MMF algorithm of [4]. Here $n$ is the dimensionality of the original matrix, $A$, $k$ is the order of the rotations, and $\gamma$ is the fraction of non-zero entries in $A$, when $A$ is sparse. We neglect that during the course of the computation $\gamma$ tends to increase, because concomitantly $A_k$ shrinks, and computation time is usually dominated by the first few stages. We also assume that entries of sparse matrices can be accessed in constant time. In pMMF, $p$ is the number of stages, $m$ is the number of clusters in each stage, and $\epsilon$ is the typical cluster size (thus, $\epsilon = \theta(n/m)$). The “pMMF time” columns give the time complexity of the algorithm assuming an architecture that affords $N_{\text{proc}}$-fold parallelism. $g = \delta_k$ is the size of the dense core in $H$. It is assumed that $k \leq p \leq c \leq n$, but $n = o(c^2)$. 

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