Multiresolution Matrix Factorization

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Abstract

Large matrices appearing in machine learning problems often have complex hierarchical structures that go beyond what can be found by traditional linear algebra tools, such as eigendecomposition. Inspired by ideas from multiresolution analysis, this paper introduces a new notion of matrix factorization that can capture structure in matrices at multiple different scales. The resulting Multiresolution Matrix Factorizations (MMFs) not only provide a wavelet basis for sparse approximation, but can also be used for matrix compression (similar to Nyström approximations) and as a prior for matrix completion.

1. Introduction

Recent years have seen a surge of work on compressing and estimating large matrices in a variety of different ways, including (i) low rank approximations (Drineas et al., 2006; Halko et al., 2009), (ii) matrix completion (Achlioptas & McSherry, 2007; Candès & Recht, 2009); (iii) compression (Williams & Seeger, 2001; Kumar et al., 2012), and (iv) randomized linear algebra (see (Mahoney, 2011) for a review). Each of these requires some assumption about the matrix at hand, and invariably that assumption is that the matrix is of low rank. In this paper we offer an alternative to the low rank paradigm by introducing multiresolution matrices, which, we argue, in certain contexts better captures the true nature of matrices arising in learning problems.

To contrast the two approaches, recall that saying that a symmetric matrix $A \in \mathbb{R}^{n \times n}$ is of rank $r \ll n$ means that it can be expressed in terms of a dictionary of $r$ mutually orthogonal unit vectors $\{u_1, u_2, \ldots, u_r\}$ in the form

$$A = \sum_{i=1}^{r} d_i u_i u_i^\top, \quad (1)$$

where $d_1, \ldots, d_r$ are the normalized eigenvectors of $A$ and $u_1, \ldots, u_r$ are the corresponding eigenvalues. This is the decomposition that Principal Component Analysis (PCA) finds and it corresponds to the factorization

$$A = U^\top D U \quad (2)$$

with $D = \text{diag}(d_1, \ldots, d_r, 0, 0, \ldots, 0)$ and $U$ orthogonal.

The drawback of PCA is that eigenvectors are almost always dense, while matrices occurring in learning problems, especially those related to graphs, often have strong locality properties, whereby they more closely couple certain clusters of “nearby” coordinates than those farther apart with respect to some underlying topology. In such cases, modeling $A$ in terms of a basis of global eigenfunctions is both computationally wasteful and conceptually absurd: a localized dictionary would be more appropriate. This is part of the reason for the recent interest in sparse PCA (sPCA) algorithms (Jenatton et al., 2010), in which the $\{u_i\}$ dictionary vectors of (2) are constrained to be sparse, while the orthogonality constraint may be relaxed. However, sPCA is liable to suffer from the opposite problem of capturing structure locally, but failing to recover larger scale patterns in $A$.

In contrast to PCA and sPCA, the multiresolution factorizations introduced in this paper tease out structure at multiple different scales by applying not just one, but a sequence of sparse orthogonal transforms to $A$. After the first orthogonal transform, the subset of rows/columns of $U_1 A U_1^\top$ which interact the least with the rest of the matrix capture the finest scale structure in $A$, so the corresponding rows of $U_1$ are designated level one wavelets, and these dimensions are subsequently kept invariant. Then the process is repeated by applying a second orthogonal transform to yield $U_1 U_2 A U_2^\top U_2^\top$ and splitting off another subspace of $\mathbb{R}^n$ spanned by second level wavelets, and so on, ultimately resulting in an $L$ level factorization of the form

$$A = U_1^\top U_2^\top \cdots U_L^\top H U_L \cdots U_2 U_1. \quad (3)$$

For a given type of sparsity constraint on $U_1, \ldots, U_L$ and a given rate at which dimensions must be eliminated, matrices that are expressible in this form with $H$ diagonal ex-
cept, possibly, for a single small dense block on the diagonal) we call multiresolution factorizable.

Multiresolution matrix factorization (MMF) uncovers soft hierarchical organization in matrices, characteristic of naturally occurring large networks and the covariance structure of large collections of random variables, without enforcing a hard hierarchical clustering. In addition to using MMF as an exploratory tool, we suggest that

1. MMF structure may be used as a “prior” in matrix approximation and completion problems;
2. MMF can be used for matrix compression, since each intermediate \( U_1 U_2^\top \) is effectively a compressed version of \( A \);
3. The wavelet basis associated with MMF is a natural basis for sparse approximation of functions on a domain whose metric structure is given by \( A \).

In the following sections we discuss the relationship of MMF to classical multiresolution analysis (Section 3), propose algorithms for computing MMFs (Section 4), take the first steps to analyze their theoretical properties (Section 5) and provide some experiments (Section 6). The proofs of all propositions and theorems are in the Supplement.

## 1.1. Related work

Our work is related to several other recent lines of work on constructing wavelet bases on discrete spaces. The work of Coifman & Maggioni (2006) on Diffusion Wavelets was a major inspiration, especially in emphasizing the connection to classical harmonic analysis. The tree-like structure of MMFs relates them to the recent work of Greengard & Rokhlin (1987) on multiresolution on trees, and in particular to Treelets (Lee et al., 2008), which is a direct precursor to this paper. Hammond et al. (2011) propose a different approach to defining wavelets on graphs based on the analogy between spectral graph theory and Fourier analysis.

More generally, the idea of multilevel operator compression is related to both algebraic multigrid methods (e.g., Livne & Brandt, 2011) and fast multipole expansions (Greengard & Rokhlin, 1987). In the machine learning community, ideas of multiscale factorization and clustering have appeared in (Dhillon et al., 2007), (Savas & Dhillon, 2011) and (Zhong et al., 2012), amongst other works.

## 2. Notation

We define \([n] = \{1, 2, \ldots, n\}\). The \( n \) dimensional identity matrix we denote \( I_n \) unless \( n \) is obvious from the context, in which case we will just use \( I \). The \( i \)’th row of a matrix \( M \) is \( M_{\cdot i} \); and the \( j \)’th column is \( M_{j \cdot} \). We use \( \cup \) to denote the disjoint union of two sets, so \( S_1 \cup \ldots \cup S_m = T \) is a partition of \( T \). The group of \( n \) dimensional orthogonal matrices is \( SO(n) \).

Given a matrix \( M \in \mathbb{R}^{n \times m} \) and two sequences of indices \( I = (i_1, \ldots, i_k) \subseteq [n] \) and \( J = (j_1, \ldots, j_l) \subseteq [m] \), \( M_{I,J} \) will denote the \( k \times l \) submatrix of \( M \) cut out by rows \( i_1, \ldots, i_k \) and columns \( j_1, \ldots, j_l \), i.e., the matrix whose entries are \([M_{I,J}]_{i,j} = M_{i,a,j,b} \). Similarly, if \( S = \{i_1, \ldots, i_k\} \subseteq [n] \) and \( T = \{j_1, \ldots, j_l\} \subseteq [m] \) (assuming \( i_1 < i_2 < \ldots < i_k \) and \( j_1 < j_2 < \ldots < j_k \)), \( M_{S,T} \) will be the \( k \times l \) matrix with entries \([M_{S,T}]_{i,j} = M_{i,a,j,b} \).

Given \( M_1 \in \mathbb{R}^{n_1 \times m_1} \) and \( M_2 \in \mathbb{R}^{n_2 \times m_2} \), \( M_1 \oplus M_2 \) is the \((n_1 + n_2) \times (m_1 + m_2)\) dimensional matrix with entries

\[
[M_1 \oplus M_2]_{i,j} = \begin{cases} 
[M_1]_{i,j} & \text{if } i \leq n_1 \text{ and } j \leq m_1 \\
[M_2]_{i - n_1, j - m_1} & \text{if } i > n_1 \text{ and } j > m_1 \\
0 & \text{otherwise}.
\end{cases}
\]

A matrix \( M \) is said to be block diagonal if it is of the form

\[
M = M_1 \oplus M_2 \oplus \ldots \oplus M_p
\]

for some sequence of smaller matrices \( M_1, \ldots, M_p \). We will only deal with block diagonal matrices in which each of the blocks is square. To remove the restriction that each block in (4) must involve a contiguous set of indices we introduce the notation

\[
M = \oplus_{(i_1, \ldots, i_k)} M_1 \oplus \oplus_{(q_1, \ldots, q_k)} M_2 \ldots \oplus_{(u_p, \ldots, u_p)} M_p
\]

for the generalized block diagonal matrix whose entries are

\[
M_{a,b} = \begin{cases} 
[M_{a,q,r}] & \text{if } i^a_w = a \text{ and } i^q_v = b \text{ for some } u, q, r, \\
0 & \text{otherwise}.
\end{cases}
\]

We will sometimes abbreviate expressions like (5) by dropping the first \( \oplus \) operator and its indices.

## 3. Multiresolution Analysis

Given a measurable space \( X \), Fourier analysis filters functions on \( X \) according to smoothness by expressing them in the eigenbasis of an appropriate self-adjoint smoothing operator \( T \). On \( X = \mathbb{R}^d \), for example, \( T \) might be the inverse of the Laplacian \( \nabla^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \ldots + \frac{\partial^2}{\partial x_d^2} \), leading to the Fourier transform \( \hat{f}(k) = \int f(x) e^{-2\pi i k \cdot x} \, dx \). When \( X \) is a graph and \( T \) is the graph Laplacian or a diffusion operator, the same ideas lead to spectral graph theory. Thus, Fourier analysis corresponds to the eigendecomposition \( T = U^\top DU \) or its operator counterpart.

In contrast, Multiresolution Analysis (MRA) constructs a sequence of spaces of functions of increasing smoothness

\[
L_2(X) \supseteq \ldots \supseteq V_0 \supseteq V_1 \supseteq V_2 \supseteq \ldots
\]

![Figure 1. Multiresolution analysis repeatedly splits \( V_0, V_1, \ldots \) into a smoother part \( V_{j+1} \) and a rougher part \( W_{j+1} \).](image-url)
by repeatedly splitting each \( V_j \) into a smoother part \( V_{j+1} \), and a rougher part \( W_{j+1} \) (Figure 1). The further we go down this sequence, the longer the length scale over which typical functions in \( V_j \) vary, thus, projecting a function to \( V_j, V_{j+1}, \ldots \) amounts to analyzing it at different levels of resolution. This inspired Mallat to define multiresolution analysis on \( X = \mathbb{R} \) directly in terms of dilations and translations by the following axioms (Mallat, 1989):

1. \( \bigcap_j V_j = \{0\} \),
2. \( \bigcup_j V_j = L^2(\mathbb{R}) \),
3. If \( f \in V_k \) then \( f(x) = f(x - 2^j m) \) is also in \( V_k \) for any \( m \in \mathbb{Z} \),
4. If \( f \in V_k \), then \( f(x) = f(2x) \) is in \( V_{k-1} \).

These imply the existence of a so-called “mother wavelet” \( \psi \) such that each \( V_k \) is spanned by an orthonormal basis

\[
\Psi_k = \{ \psi_{\ell,m}(x) = 2^{-\ell/2} \psi(2^{-\ell} x - m) \}_{m \in \mathbb{Z}}
\]

and a “father wavelet” \( \phi \) such that each \( V_k \) is spanned by an orthonormal basis

\[
\Phi_k = \{ \phi_{\ell,m}(x) = 2^{-\ell/2} \phi(2^{-\ell} x - m) \}_{m \in \mathbb{Z}}.
\]

The wavelet transform (up to level \( L \)) of a function \( f : X \to \mathbb{R} \) residing at a particular level of the hierarchy (6), without loss of generality \( f \in V_0 \), expresses it as

\[
f(x) = \sum_{\ell=1}^L \sum_m \alpha_{\ell,m} \psi_{\ell,m}(x) + \sum_m \beta_m \phi_{\ell,m}(x),
\]

with \( \alpha_{\ell,m} = \langle f, \psi_{\ell,m} \rangle \) and \( \beta_m = \langle \phi_{\ell,m}, f \rangle \). Multiresolution owes much of its practical usefulness to the fact that \( \psi \) can be chosen in such a way that (a) it is localized in both space and frequency, (b) the individual \( U_\ell : V_{\ell-1} \to V_\ell \oplus W_\ell \) basis transforms are sparse. Thus, (7) affords a computationally efficient way of decomposing functions into components at different levels of detail, and provides an excellent basis for sparse approximations.

3.1. Multiresolution on discrete spaces

The problem with extending multiresolution to less structured and discrete spaces, such as graphs, is that in these settings there are no obvious analogs of translation and dilation, required by Mallat’s third and fourth axioms. Rather, similarly to (Coifman & Maggioni, 2006), assuming that \( |X| = n \) is finite, we adopt the view that multiresolution analysis with respect to a symmetric smoothing matrix \( A \in \mathbb{R}^{n \times n} \) now consists of finding a sequence of spaces

\[
V_L \subset \ldots \subset V_2 \subset V_1 \subset V_0 = L(X) \cong \mathbb{R}^n
\]

where each \( V_\ell \) has an orthonormal basis \( \Phi_\ell := \{ \phi^\ell_m \}_m \) and each complementary space \( W_\ell \) has an orthonormal basis \( \Psi_\ell := \{ \psi^\ell_m \}_m \) satisfying the following conditions:

MRA1. The sequence (8) is a filtration of \( \mathbb{R}^n \) in terms of smoothness with respect to \( A \) in the sense that

\[
\eta_\ell = \sup_{v \in V_\ell} \langle v, Au \rangle / \langle v, v \rangle
\]

decays at a given rate.

MRA2. The wavelets are localized in the sense that

\[
\mu_\ell = \max_{m \in \{1, \ldots, d_\ell \}} \| \psi^\ell_m \|_0
\]

increases no faster than a certain rate.

MRA3. Letting \( U_\ell \) be the matrix expressing \( \Phi_\ell \cup \Psi_\ell \) in the previous basis \( \Phi_{\ell-1} \), i.e.,

\[
\phi^\ell_m = \sum_{i=1}^{\dim(V_{\ell-1})} [U_\ell]_{m,i} \phi^{\ell-1}_i
\]

and

\[
\psi^\ell_m = \sum_{i=1}^{\dim(V_{\ell-1})} [U_\ell]_{m+i} \phi^{\ell-1}_i,
\]

each \( U_\ell \) is sparse, guaranteeing the existence of a fast wavelet transform (\( \Phi_0 \) is taken to be the standard basis, \( \phi^0_m = e_m \)).

3.2. Multiresolution Matrix Factorization

The central idea of this paper is to convert multiresolution analysis into a matrix factorization problem by focusing on how it compresses the matrix \( A \). In particular, extending each \( U_\ell \) matrix to size \( n \times n \) by setting \( U_\ell \leftarrow U_\ell \oplus I_{n-\dim(V_{\ell-1})} \), we find that in the \( \Phi_1 \cup \Psi_1 \) basis \( A \) becomes \( U_1 A U_1^\top \). In the \( \Phi_2 \cup \Psi_2 \cup \Psi_3 \) basis it becomes \( U_2 U_1 A U_1^\top U_2^\top \), and so on, finally in the \( \Phi_L \cup \Psi_L \cup \ldots \cup \Psi_1 \) basis it takes on the form

\[
H = U_L \ldots U_2 U_1 A U_1^\top U_2^\top \ldots U_L.
\]

Therefore, similar to the way that Fourier analysis corresponds to eigendecomposition, multiresolution analysis effectively factorizes \( A \) in the form

\[
A = U_1^\top U_2^\top \ldots U_L^\top H \ldots A U_2 U_1
\]

with the constraints that (a) each \( U_\ell \) orthogonal matrix must be sufficiently sparse, (b) outside its top left \( \dim(V_{\ell-1}) \times \dim(V_{\ell-1}) \) block, each \( U_\ell \) is the identity. Furthermore, by (9–10), the first \( \dim(V_L) \) rows of \( U_L \ldots U_2 U_1 \) are the \( \{ \phi^L_m \}_m \) scaling functions, whereas the rest of its rows return the \( \{ \psi^L_m \}, \{ \psi^{L-1}_m \}, \ldots, \{ \psi_1^L \} \) wavelets.

In the Fourier case, \( H \) would be diagonal. In the multiresolution case the situation is slightly more complicated since \( H \) consists of four distinct blocks:

\[
H = \begin{pmatrix}
H_{\phi,\phi} & H_{\phi,\psi} \\
H_{\psi,\phi} & H_{\psi,\psi}
\end{pmatrix}
= \begin{pmatrix}
H_{1:d_L,1:d_L} & H_{1:d_L,1:d_L+1:n} \\
H_{d_L+1:n,1:d_L} & H_{d_L+1:n,1:d_L+1:n}
\end{pmatrix},
\]

with \( d_L = \dim(V_L) \). Here \( H_{\phi,\phi} \) is effectively \( A \) compressed to \( V_L \), and is therefore dense. The structure of the
other three matrices, however, reflects to what extent the MRA criterion is satisfied. In particular, the closer the wavelet lengths are to being eigenfunctions, the better they can filter the space by smoothness, as defined by $A$. Below, we define multiresolution factorizable matrices as those for which this is perfectly satisfied, i.e., which have a factorization with $H_{\Phi, \Psi} = H_{\Phi, \Psi}^*$ diagonal.

In the following, we relax the form of (12) somewhat by allowing each $U_{\ell}$ to fix some set $[n] \setminus \mathcal{S}_{\ell}$ of $n - \dim(V_{\ell-1})$ coordinates rather than necessarily the last $n - \dim(V_{\ell-1})$ (as long as $S_0 \supseteq S_1 \supseteq \ldots$). This also affects the order in which rows are eliminated as wavelets, and the criterion $S_n$ coordinates rather than necessarily the last $d_n$.

We define multiresolution factorizable matrices as those for which each $U_{\ell}$ is an orthogonal matrix of the form $U_{\ell} = I_{n - d_{\ell}}$ for some nested sequence of sets $[n] = S_0 \supseteq S_1 \supseteq \ldots \supseteq S_L$.

**Definition 1** Given an appropriate subset $\mathcal{O}$ of the group $\text{SO}(n)$ of $n$-dimensional rotation matrices, a depth parameter $L \in \mathbb{N}$, and a sequence of integers $n = d_0 \geq d_1 \geq d_2 \geq \ldots \geq d_L \geq 1$, a **Multiresolution Matrix Factorization (MMF)** of a symmetric matrix $A \in \mathbb{R}^{n \times n}$ over $\mathcal{O}$ is a factorization of the form

$$A = U_1^T U_2^T \ldots U_{L-2}^T H U_{L-1}^T U_L U_1,$$

where each $U_{\ell} \in \mathcal{O}$ satisfies $[U_{\ell}]_{[n]\setminus \mathcal{S}_{\ell-1}, [n]\setminus \mathcal{S}_{\ell-1}} = I_{n - d_{\ell}}$ for some nested sequence of sets $[n] = S_0 \supseteq S_1 \supseteq \ldots \supseteq S_L$ with $|\mathcal{S}_{\ell}| = d_{\ell}$ and $H \in H_{\mathcal{S}_L}^n$.

**Definition 2** We say that a symmetric matrix $A \in \mathbb{R}^{n \times n}$ is fully multiresolution factorizable over $\mathcal{O} \subseteq \text{SO}(n)$ with $(d_1, \ldots, d_L)$ if it has a decomposition of the form described in Definition 1.

The sequence $(d_1, \ldots, d_L)$ may follow some predefined law, such as geometric decay, $d_{\ell} = \lfloor mn^{\ell} \rfloor$ or arithmetic decay, $d_\ell = n - \ell m$. The major difference between different types of MMFs, however, is in the definition of the set $\mathcal{O}$ of sparse rotations. In this regard we consider two alternatives: elementary and compound $k$'th order rotations.

**Definition 3** We say that $U \in \mathbb{R}^{n \times n}$ is an elementary rotation of order $k$ (sometimes also called a $k$-point rotation) if it is an orthogonal matrix of the form

$$U = I_{n-k} \oplus_{i_1=1}^{i_k} O$$

for some $\{i_1, \ldots, i_k\} \subseteq [n]$ and $O \in \text{SO}(k)$. The set of all such matrices we denote $\text{SO}_k(n)$.

A $k$'th order elementary rotation is very local, since it only touches coordinates $\{i_1, \ldots, i_k\}$, and leaves the rest invariant. The simplest case are second order rotations, which are of the form

$$U = U_{i,j}^\theta = \begin{pmatrix} c & -s \\ s & c \end{pmatrix}, \quad c = \cos \theta, \quad s = \sin \theta,$$

where the dots denote that apart from rows/columns $i$ and $j$, $U_{i,j}^\theta$ is the identity, and $\theta$ is some angle in $[0, 2\pi]$. Such matrices are called Givens rotations, and they play an important role in numerical linear algebra. Indeed, Jacobi’s algorithm for diagonalizing symmetric matrices (Jacobi, 1846), possibly the first matrix algorithm to have been invented, works precisely by constructing an MMF factorization over Givens rotations. Inspired by this connection, we will call any MMF with $\mathcal{O} = \text{SO}_k(n)$ a $k$'th order Jacobi MMF.

**Definition 4** We say that $U \in \mathbb{R}^{n \times n}$ is a compound rotation of order $k$ if it is an orthogonal matrix of the form

$$U = \oplus_{i_1=1}^{i_k} O_{1} \oplus_{i_2=1}^{i_k} O_{2} \ldots \oplus_{i_m=1}^{i_m} O_{m}$$

for some partition $\{i_1, \ldots, i_k\} \cup \ldots \cup \{i_m, \ldots, i_m\}$ of $[n]$ with $k_1 + \ldots + k_m \leq k$, and some sequence of orthogonal matrices $O_1, \ldots, O_m$ of the appropriate sizes. The set of all such matrices we denote $\text{SO}_k(n)$.

Intuitively, compound rotations consist of many elementary rotations executed in parallel, and can consequently lead to much more compact factorizations.

**4. Computing MMFs**

Much like how low rank methods express matrices in terms of a small dictionary of vectors as in (1), MMF approximates $A$ in the form

$$A^* = \sum_{i,j=1}^{d_L} \beta_{i,j} \phi_i^L \phi_j^L \top + \sum_{\ell=1}^{L} \sum_{i=1}^{d_{\ell}} \eta^\ell_i \psi_i^\ell \psi_i^\ell \top,$$

where the $\phi_i^\ell$ and $\psi_i^\ell$ are wavelet frequencies that are the diagonal elements of the $H_{\Phi, \Psi}$ block of $H$, whereas the $\beta_{i,j}$ are the entries of the $H_{\Phi, \Psi}$ block. Thus, given $\mathcal{O}$ and $(d_1, \ldots, d_L)$, finding the best MMF factorization to a symmetric matrix $A$ requires solving

$$\min_{H \in H_{\mathcal{S}_L}^n; U_1, \ldots, U_L \in \mathcal{O}} \| A - U_1^T \ldots U_{L-1}^T H U_L U_1 \|_F.$$

Assuming that we measure error in the Frobenius norm, which is rotationally invariant, this is equivalent to

$$\min_{H \in H_{\mathcal{S}_L}^n; U_1, \ldots, U_L \in \mathcal{O}} \| U_L \ldots U_1 A U_1^T \ldots U_L^T \|_F^2,$$

where $\| \cdot \|_F^2$ is the squared “residual norm”

$$\| H \|_F^2 = \sum_{i \neq j \in \mathcal{S}_L} | H_{i,j} |^2.$$

Defining $A_\ell = U \ldots U_1 A U_1^T \ldots U_L$, intuitively, our objective is to find a series of sparse rotations

$$A \equiv A_0 \xrightarrow{U_1} A_1 \xrightarrow{U_2} \ldots \xrightarrow{U_L} A_L$$
that bring $A$ to a form as close to diagonal as possible. The following Proposition tells us that as soon as we designate a certain set $J_ℓ := S_{ℓ-1} \setminus S_ℓ$ of rows/columns in $A_ℓ$ wavelets, the $ℓ_2$-norm of these rows/columns (discounting the diagonal and those parts that fall outside the $S_{ℓ-1} \times S_{ℓ-1}$ active submatrix) is already committed to the final error.

**Proposition 1** Given an MMF as defined in Definition 1, the objective function of (17) is expressible as $\sum_{ℓ=1}^L \mathcal{E}_ℓ$, where $\mathcal{E}_ℓ = \| [A_ℓ]_{i,j}, [i,j] \|_{\text{off-diag}}^2 + 2 \| [A_ℓ]_{i,j}, [i,j] \|_{\text{Frob}}^2$, and $\| M \|_{\text{off-diag}} := \sum_{i\neq j} |M_{i,j}|^2$.

The following algorithms for finding MMFs all follow the greedy approach suggested by this proposition of finding at each level a rotation $U_ℓ$ that produces $d_ℓ - d_{ℓ-1}$ rows/columns that are as close to diagonal as possible, and then designating these as the level $ℓ$ wavelets.

### 4.1. Jacobi MMFs

In Jacobi MMFs, where each $U_ℓ$ is an $I_{n-k} \oplus (i_1, \ldots, i_k)O$ elementary rotation, we set $(d_1, \ldots, d_L)$ so as to split off some constant number $m < k$ of wavelets at each level. For simplicity, for now we take $m = 1$. Furthermore, we make the natural assumption that this wavelet is one of the rows involved in the rotation, w.l.o.g. $J_ℓ = \{i_1\}$.

**Proposition 2** If $U_ℓ = I_{n-k} \oplus O$ with $I = (i_1, \ldots, i_k)$ and $J_ℓ = \{i_k\}$, then the contribution of level $ℓ$ to the MMF approximation error is

$$\mathcal{E}_ℓ = \mathcal{E}_ℓ^O = 2 \sum_{p=1}^{k-1} [O[A_{ℓ-1}],i,O]_k^2 \| k,p + 2 [OBO^T],k,k \|
$$

where $B = [A_{ℓ-1}]_{i,S_ℓ} ([A_{ℓ-1}]_{i,S_ℓ})^T$. (19)

**Corollary 1** In the special case of $k = 2$ and $I_ℓ = (i, j)$, $\mathcal{E}_ℓ = \mathcal{E}_ℓ^{O,(i,j)} = 2 [O[A_{ℓ-1}],(i,j),O]_k,1^2 \| 1,2 + 2 [OBO^T],k,k \|

$$ (20)$$

with $B = [A_{ℓ-1}]_{(i,j),S_ℓ} ([A_{ℓ-1}]_{(i,j),S_ℓ})^T$.

According to the greedy strategy, at each level $ℓ$, the $I$ index tuple and $O$ rotation must be chosen so as to minimize (19). The resulting algorithm is given in Algorithm 1, where $A_L \downarrow H_{nL}$ stands for zeroing out all the entries of $A_ℓ$ except those on the diagonal and in the $S_ℓ \times S_ℓ$ block.

When $k = 2$, the rotations $U_1, \ldots, U_L$ form a binary tree, in which each $U_ℓ$ takes two scaling functions from level $ℓ-1$ and passes on a single linear combination of them to the next level (Figure 2). In general, the more similar two rows $A_{1,j}$ and $A_{2,j}$ are to each other, the smaller we can make $d_ℓ - d_{ℓ-1}$ in some metric the entries in row $i$ measure the similarity of vertex $i$ to all the other vertices, this means that Algorithm 1 will tend to pick pairs of adjacent or nearby vertices and then produce scaling functions that represent linear combinations of those vertices. Thus, second order MMFs effectively perform a hierarchical clustering on the rows/columns of $A$. Uncovering this sort of hierarchical structure is one of the goals of MMF analysis.

The idea of constructing wavelets by forming a tree of Givens rotations was first introduced under the name “Treelets” by Lee et al. (2008). Their work, however, does not make a connection to matrix factorization. In particular, instead of minimizing the contribution of each rotation to the matrix approximation error, the Treelets algorithm chooses $I$ and $O$ so as to zero out the largest off-diagonal entry of $A_ℓ-1$. This pivoting rule is the same as in Jacobi’s classical algorithm, so if one of the two indices $\{i, j\}$ was not always eliminated from the active set, we would eventually diagonalize $A$ to arbitrary precision.

**Algorithm 1** **GREEDYJACOBI** computing the Jacobi MMF of $A$ with $d_ℓ = n - ℓ$.

**Input:** $k, L$, and a symmetric matrix $A_0 = A \in \mathbb{R}^{n \times n}$

set $S_0 := \{n\}$

for $(ℓ = 1$ to $L$) {

foreach $I_ℓ = (i_1, \ldots, i_k) \in (S_{ℓ-1})^k$ with $i_1 < \ldots < i_k$

compute $\mathcal{E}_ℓ = \min_{O \in SO(k)} \mathcal{E}_ℓ^O$ (as defined in (19))

set $I_ℓ := \arg \min I_ℓ \mathcal{E}_ℓ$

set $O_ℓ := \arg \min_{O \in SO(k)} \mathcal{E}_ℓ^O$

set $U_ℓ := I_{n-k} \oplus I_ℓ O_ℓ$

set $S_ℓ := S_{ℓ-1} \setminus I_ℓ$

set $A_ℓ := U_ℓ A_{ℓ-1} U_ℓ^\top$

}

**Output:** $U_1, \ldots, U_L$ and $H = A_L \downarrow H_{nL}$

Jacobi MMFs with $k \geq 3$ are even more interesting because they correspond to a lattice in which each $U_ℓ$ now has $k$ children and $k - 1$ parents (Figure 2). In the $k = 2$ case the supports of any two wavelets $ψ^{i}_1$ and $ψ^{i}_2$ are either disjoint or one is contained in the other. In contrast, for $k \geq 3$, a single original coordinate, such as $δ_6$ in Figure 2 can contribute to multiple wavelets ($ψ^{i}_5$ and $ψ^{i}_6$, for example) with different weights, determined by all the orthogonal matrices along the corresponding paths in the lattice. Thus, higher order MMFs are more subtle than just a single hierarchical clustering: by building a lattice of subspaces they capture a softer notion of hierarchy, and can uncover multiple overlapping hierarchical structures in $A$. 

![Figure 2: Left: Example of the tree induced by a second order Jacobi MMF of a six dimensional matrix. Right: Example of a Jacobi MMF with $k = 3$ of a 10 dimensional matrix.](image)
The reason that (21) involves the matrix elements \( \{A_j\}_{k_j,k_j'} \) \( j \neq j' \) at the intersection of pairs of wavelet rows/columns. Accounting for these elements explicitly would introduce interactions between the \( O_j \) rotations, leading to a difficult optimization problem. Therefore, both for finding the optimal partition \( 1 \cup \ldots \cup I_m \) and for finding the optimal \( O_1, \ldots, O_m \) rotations, we use the right hand side of (21) as a proxy for \( E_\ell \).

Once again, the binary \( (k = 2) \) case is the simplest, since optimizing \( 1 \cup \ldots \cup I_m \) then reduces to finding a minimal cost matching amongst the indices in the active set \( S_{\ell-1} \) with cost matrix

\[
W_{i,j} = 2 \min_{O \in SO(2)} \left[ \sum_{r=1}^k |O[A_{\ell-1}\{i,j\}]_{1,1} O^\top_{1,1}| + |OBO^\top_{k,k}| \right],
\]

where \( B = [A_{\ell-1}\{i,j\}]^{S_{\ell-1}\{i,j\}} \) \( (A_{\ell-1})^{T} \).

An exact solution to this optimization problem can be found in time \( O(|S_{\ell-1}|^3) \) using a modified weighted version of the famous “Blossom algorithm” by Edmonds (1965). However, it is also known that the simple greedy strategy of setting \( \{i_1,j_1\} = \arg \min_{i,j} W_{i,j} \), then \( \{i_2,j_2\} = \arg \min_{i,j} W_{i,j} \), etc., yields a 2-approximation in linear time. In general, the most expensive component of MMF factorizations is forming the \( B \) matrices (which naïvely takes \( O(n^k) \) time), however, in practice techniques like locality sensitive hashing allow this (as well as the entire algorithm) to run in time close to linear in \( n \).

We remark that the fast Haar transform is nothing but a binary MMF, and the Cooley–Tukey FFT is a degenerate MMF (where \( d_0 = \ldots = d_L \)) of a complex valued matrix.

### 4.3. Computational details

Problems of the form \( \min_{O \in SO(k)} \|OBO^\top C\| \), called Procrustes problems, generally have easy, \( O(k^3) \) time closed form solutions. Unfortunately, both (19) and (21) involve mixed linear/quadratic versions of this problem, which are much more challenging. However, the following result shows that in the \( k = 2 \) case this may be reduced to solving a simple trigonometric equation.

**Proposition 4** Let \( A \in \mathbb{R}^{2 \times 2} \) be diagonal, \( B \in \mathbb{R}^{2 \times 2} \) symmetric and \( O = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \). Set \( a = (A_{1,1} - A_{2,2})^2 / 4 \\ b = B_{1,2} \\
\left. e = \sqrt{b^2 + c^2}, \quad \theta = 2\alpha \right) \) and \( \omega = \arctan(c/b) \). Then if \( \alpha \) minimizes \( \|OAO^\top\|_{2,2} \), then \( \theta \) satisfies

\[
(\alpha/e) \sin(2\theta) + \sin(\theta + \omega + \pi/2) = 0.
\]

Putting \( A \) and \( B \) in the diagonal form required by this proposition is easy. While (23) is still not an explicit expression for \( \alpha \), it is trivial to solve with iterative methods.

### 4.4. Comparison to Treelets

Since Treelets (Lee et al., 2008) are a special case of MMF, it is natural to compare the two approaches:

1. In Treelets, the choice of \( (i,j) \) coordinates to rotate and the rotation angle \( \theta \) are chosen based on an analogy with Jacobi’s algorithm. In contrast, in MMF they are optimized to reduce the algorithm’s objective function, which is approximation error.

2. The Treelets algorithm has a tendency to lead to cascades, where the same coordinate is involved in a long series of rotations, and this can ruin multiresolution. Parallel MMFs avoid this problem.

3. MMFs extend to \( k \geq 3 \), which is what enables imputing more subtle structure than just a single hierarchy.
5. Theoretical analysis

MMFs satisfy properties MRA2 and MRA3 of Section 3.1 by construction. Showing that they also satisfy MRA1 requires, roughly, to prove that the smoother a function is, the smaller its high frequency wavelet coefficients are. For this purpose the usual notion of smoothness with respect to a metric $d$ is Hölder continuity, defined

$$|f(x) - f(y)| \leq c_H \, d(x, y)^\alpha \quad \forall x, y \in X,$$

with $c_H$ and $\alpha > 0$ constant. In classical wavelet analysis one proves that the wavelet coefficients of ($c_H$, $\alpha$)-Hölder functions decay at a certain rate, for example, $|\langle f, \psi^m \rangle| \leq c' \ell^{\alpha+\beta}$ for some $\beta$ and $c'$ (Daubechies, 1992).

As we have seen, MMFs are driven by the similarity between the rows/columns of the matrix $A$. Therefore, relaxing the requirement that $d$ must be a metric, we now take

$$d(i, j) = |\langle A_{i,:}, A_{j,:} \rangle|^{-1}. \quad (24)$$

One must also make some assumptions about the structure of the underlying space, classically that $X$ is a so-called space of homogeneous type (Deng & Han, 2009), which means that for some constant $c_{\text{hom}}$

$$\text{Vol}(B(x, 2r)) \leq c_{\text{hom}} \text{Vol}(B(x, r)) \quad \forall x \in X, \forall r > 0.$$ 

To capture the analogous structural property for matrices, we introduce a concept with connections to the R.I.P condition in compressed sensing (Candès & Tao, 2005).

**Definition 5** We say that a symmetric matrix $A \in \mathbb{R}^{n \times n}$ is $\Lambda$–rank homogeneous up to order $K$, if for any $S \subseteq [n]$ of size at most $K$, letting $Q = A_S \cdot A_{S,:}$, setting $D$ to be the diagonal matrix with $D_{ii} = \|Q_{i,:}\|_1$, and $\bar{Q} = D^{-1/2}QD^{-1/2}$, the $\lambda_1, \ldots, \lambda_{|S|}$ eigenvalues of $\bar{Q}$ satisfy $\Lambda < |\lambda_i| < 1 - \Lambda$, and furthermore $c^{-1}_{\text{T}} \leq D_{ii} \leq c_T$ for some constant $c_T$.

Recall that the spectrum of the normalized adjacency matrix of a graph is bounded in $[-1, 1]$ (Chung, 1997). Definition 5 asserts that if we form a graph with vertex set $S$ and edge weights $(A_{i,:}, A_{j,:})$, its eigenvalues in absolute value are bounded away from both 0 and 1. Definition 5 then roughly corresponds to asserting that $A$ does not have clusters of rows that are either almost identical (an incoherence condition) or completely unrelated. This allows us to now state the matrix analog of the Hölder condition.

**Theorem 1** Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix that is $\Lambda$–rank homogeneous up to order $K$ and has an MMF factorization $A = U_1^T \cdots U_L^T H U_L \cdots U_1$. Assume $\psi^m_i$ is a wavelet in this factorization arising from row $i$ of $A_{k-1}$ supported on a set $S$ of size $K \leq \overline{K}$ and that $\|H_{i,:}\|^2 \leq \epsilon$.

![Figure 3. Comparison with the Treelets algorithm. Zachary’s Karate Club graph (left) and a matrix of genetic relationship between 50 individuals from (Crossett et al., 2013) (right).](image)

Then if $f : [n] \to \mathbb{R}$ is $(c_H, 1/2)$–Hölder with respect to (24), then

$$|\langle f, \psi^m \rangle| \leq cT \sqrt{cHCA} \epsilon^{1/2} K \quad (25)$$

with $c_A = 4/(1 - (2\Lambda)^2)$.

Here $\epsilon$ is closely related to the MMF approximation error and is therefore expected to be small. Eq. (25) then says that, as we expect, if $f$ is smooth, then its “high frequency” local wavelet coefficients (low $K$ and $\ell$) will be small.

6. Experiments

In a toy example we consider the diffusion kernel of the Laplacian of a cycle graph ($C_n$) on $n = 16$ vertices. Applying Algorithm 2, we compute the binary parallel MMF up to depth $L = 5$, and find that MMF recovers the Haar wavelets (see Figure 6 in the supplement). Similar results can be obtained for any cycle graph, except that for large $n$ the longest wavelength wavelets cannot be fully reconstructed due to issues of numerical precision.

We also evaluate the performance of GREEDYJACOBI by comparing it with Treelets on two small matrices. Note that in the greedy setting, similar to the Treelets, MMF removes one dimension at a time, and thus in both algorithms, the off-diagonal part of the rows/columns designated as wavelets contributes to the error. The first dataset is the well-known Zachary’s Karate Club (Zachary, 1977) social network ($N = 34$, $E = 78$) for which we set $A$ to be the heat kernel. The second one is constructed using simulated data from the family pedigrees in (Crossett et al., 2013): 5 families were randomly selected, and 10 individuals from the 15 related individuals were randomly selected independently in each family. The resulting relationship matrix represents the estimated kinship coefficient and is calculated via the GCTA software of Yang et al. (2011).

Figure 4 shows that GREEDYJACOBI outperforms Treelets for a wide range of compression ratios.

**6.1. Comparison to Other Factorization Methods**

To verify that MMF produces meaningful factorizations, we measure the approximation error of factoring two
1024 × 1024 matrices: a matrix consisting of i.i.d. normal random variables and a Kronecker graph, $K^k$, of order $k = 5$, where $K_1$ is a 2 × 2 seed matrix (Leskovec et al., 2010). Figure 4 shows that MMF performs suboptimally when the matrix lacks an underlying multiresolution structure. However, on matrices with multilevel structure MMF systematically outperforms other algorithms.

In order to evaluate MMF for matrix compression, we use several large datasets: GR (arXiv General Relativity collaboration graph, $N = 5242$) (Leskovec et al., 2007), Dexter (bag of words, $N = 2000$) (Asuncion & Newman, 2012), and HEP (arXiv High Energy Physics collaboration graph, $N = 9877$, see Supplement). The first two are normalized graph Laplacians of real-world networks and the third one is a linear kernel matrix constructed from a 20000-feature dataset. By virtue of its design, MMF operates only on symmetric matrices, so we compare its performance to different variants of the so-called Nyström method, which in machine learning is considered standard for compressing symmetric matrices (Figure 5).

The Nyström method involves randomly sampling rows/columns of the matrix to be compressed, and its variants differ mainly in the sampling technique (uniform at random without replacement, non-uniform leverage score probabilities, Gaussian or SRFT mixtures of the columns). The MMF approximation error is measured by summing the $\ell_2$ norm (except for the diagonal element) of the rows/columns that are designated wavelets at each iteration of the algorithm (Proposition 1). For the Nyström method, the compression error $\|A - CW'C\|^\text{Frob}$ is a function of the number of columns sampled, as well as, potentially, the desired rank $r$ of the approximation (which leads to a distinction between rank-restricted and non-rank-restricted variants) (Gittens & Mahoney, 2013). Similarly, at every level of the MMF compression, the approximation error is a function of $|S_t|$, the number of dimensions that have not yet been eliminated. The results in Figure 5 suggest that, despite similar wall clock times,

2 Note that compressing a matrix to size $d \times d$ means something slightly different for Nyström methods and MMF: in the latter case, in addition to the $d \times d$ core, we also preserve a sequence of $n - d$ wavelet frequencies.

Figure 5. Comparison of the Frobenius norm error of the binary parallel MMF (Algorithm 2 with $k = 2$) and different flavors of the Nyström method on two real datasets. In the rank-restricted cases $r = 20$ for GR and $r = 8$ for Dexter.

by leveraging more nuanced structure in matrices arising from data than just low rank, MMF factorization can potentially outperform standard compression techniques by a large margin.

7. Conclusions

The interplay between the geometry of a space $X$ and the structure of function spaces on $X$ is a classical theme in harmonic analysis (Coifman & Maggioni, 2006). As an instance of this connection, this paper developed the matrix factorization analog of multiresolution analysis on finite sets. The resulting factorizations, on the one hand, provide a natural way to define multiresolution on graphs, correlated sets of random variables, and so on. On the other hand, they lead to new classes of structured matrices and new matrix compression algorithms.

What classes of naturally occurring matrices exhibit MMF structure is an important question. From the algorithmic point of view, devising fast randomized version of MMFs will be critical. Finally, from the theoretical point of view, one of the biggest challenges is to relate the new concepts of multiresolution factorizable and $\Lambda$–rank homogenous matrices to the existing body of work in harmonic analysis, algebra and compressed sensing.

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