Rapid factorization of structured matrices via randomized sampling

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Abstract: Randomized sampling has recently been demonstrated to be an efficient technique for computing approximate low-rank factorizations of matrices for which fast methods for computing matrix-vector products are available. This paper describes an extension of such techniques to a wider class of matrices that are not themselves rank-deficient, but have off-diagonal blocks that are. Such matrices arise frequently in numerical analysis and signal processing, and there exist several methods for rapidly performing algebraic operations (matrix-vector multiplications, matrix factorizations, matrix inversion, etc) on them once low-rank approximations to all off-diagonal blocks have been constructed. The paper demonstrates that if such a matrix can be applied to a vector in $O(N)$ time, where the matrix is of size $N \times N$, and if individual entries of the matrix can be computed rapidly, then in many cases, the task of constructing approximate low-rank factorizations for all off-diagonal blocks can be performed in $O(Nk^2)$ time, where $k$ is an upper bound for the numerical rank of the off-diagonal blocks.

1. INTRODUCTION

There has recently been much interest in the development of fast algorithms for structured matrices of different varieties. One class of such matrices is the class of “Hierarchically Semi-Separable” (HSS) matrices, [8, 25, 7]. These matrices are characterized by a specific type of rank deficiencies in their off-diagonal blocks (as described in Section 2.4) and arise upon the discretization of many of the integral operators of mathematical physics, in signal processing, in algorithms for inverting certain finite element matrices, and in many other applications, see e.g. [25, 6, 22, 20]. The common occurrence of such matrices in scientific computing motivates the development in [26, 7, 19, 10, 5] of fast algorithms for performing operations such as matrix-vector multiplies, matrix factorizations, matrix inversions, etc.

There currently is little consistency in terminology in discussing structured matrices. The property that we here refer to as the “HSS” property also arises under different names in a range of other publications, for instance [19, 24, 22, 20]. It is also closely related to the “$H^2$-matrices” discussed in [16, 4, 3]. The methods described in the present paper are directly applicable to the structures described in [19, 24, 22], and with minor modifications to the structures in [16, 4, 3].

The observation that many matrices that arise in scientific computing have off-diagonal blocks that can be approximated well by low-rank matrices underlies many “fast” methods such as the Fast Multipole Method [12, 13], panel clustering [15], Barnes-Hut [1], $H$-matrices [17], etc. It is important to note that the HSS property imposes stronger conditions on the off-diagonal blocks than any of the algorithms listed. We describe these conditions in detail in Section 2.4, but loosely speaking, the HSS property requires both that large blocks directly adjacent to the diagonal can be approximated by low rank matrices, and that the basis functions used be “nested”, i.e. that the basis functions on one level be expressed as linear combinations of the basis functions on the next finer level. The benefits obtained by imposing these stronger conditions in part derive from faster algorithms for matrix-vector multiplies [22], but more importantly from the fact that they allow other linear algebraic operations such as matrix factorizations and inversions to be performed in $O(N)$ time [7, 19, 2]. However, while there exist very fast algorithms for manipulating such matrices...
once the factors in the HSS representation are given, it is less well understood how to rapidly compute these factors in the first place. For matrices arising from the discretization of the boundary integral equations of mathematical physics, [21] describes a technique that is $O(N)$ in two dimensions and $O(N^{3/2})$ in three. In other environments, it is possible to use known regularity properties of the off-diagonal blocks in conjunction with standard interpolation techniques to obtain rough initial factorizations, and then recompress these to obtain factorizations with close to optimal ranks [3]. An approach of this kind with an $O(N \log N)$ or $O(N \log^2 N)$ complexity, depending on circumstances, is used in [22].

The purpose of the present paper is to describe a fast and simple randomized technique for computing all factors in the HSS representation of a large class of matrices. It works in any environment in which a fast matrix-vector multiplier is available (for instance, an implementation of the Fast Multipole Method, or some other legacy code) and it is possible and affordable to compute a small number of actual matrix elements. In order to describe the cost of the algorithm precisely, we must introduce some notation: We let $A$ be an $N \times N$ matrix whose off-diagonal blocks have maximal rank $k$ (in the “HSS”-sense, see Section 2.4), we let $T_{\text{mult}}$ denote the time required to perform a matrix-vector multiplication $x \mapsto Ax$, we let $T_{\text{rand}}$ denote the cost of constructing a pseudo random number from a normalized Gaussian distribution, we let $T_{\text{entry}}$ denote the computational cost of evaluating an individual entry of $A$, and $T_{\text{flop}}$ denote the cost of a floating point operation. The computational cost $T_{\text{total}}$ of the algorithm then satisfies

$$T_{\text{total}} \sim T_{\text{mult}} \times 2(k + 10) + T_{\text{rand}} \times N(k + 10) + T_{\text{entry}} \times 2Nk + T_{\text{flop}} \times cNk^2,$$

where $c$ is a small constant. In particular, if $T_{\text{mult}}$ is $O(N)$, then the method presented here is $O(N)$ as well.

The technique described in this paper utilizes recently published methods for computing approximate low-rank factorizations of matrices that are based on randomized sampling [23][18]. As a consequence, there is a finite probability that the method described here may fail in any given realization of the algorithm. This failure probability is a user specified parameter that in principle could be balanced against computational cost. In practice, the probability of failure can at a low cost be made entirely negligible. To be precise, in equation (1.1), the number “10” in the first and the second terms on the right hand side is chosen to yield a failure probability that is provably less than $10^{-5}$, and appears to actually be much smaller still. We note that when the method does not fail, the accuracy of the randomized scheme is very high; in the environment described in this paper, relative errors of less than $10^{-10}$ are easily obtained.

2. Preliminaries

In this section, we introduce some notation, and list a number of known results regarding low rank factorizations, and hierarchical factorizations of matrices.

2.1. Notation. Throughout the paper, we measure vectors in $\mathbb{R}^n$ using their Euclidean norm, and matrices using the corresponding operator norm.

For an $m \times n$ matrix $A$, and an integer $k = 1, 2, \ldots, \min(m, n)$, we let $\sigma_k(A)$ (or simply $\sigma_k$ when it is obvious which matrix is being referred to) denote the $k$’th singular value of $A$. We assume that these are ordered so that $\sigma_1(A) \geq \sigma_2(A) \geq \cdots \geq \sigma_{\min(m,n)}(A) \geq 0$. We say that a matrix $A$ has “$\varepsilon$-rank” $k$ if $\sigma_{k+1}(A) < \varepsilon$.

We use the notation of Golub and Van Loan [11] to specify submatrices. In other words, if $A$ is an $m \times n$ matrix with entries $a_{ij}$, and $I = [i_1, i_2, \ldots, i_k]$ and $J = [j_1, j_2, \ldots, j_l]$ are
two index vectors, then we let \( A(I, J) \) denote the \( k \times l \) matrix
\[
A(I, J) = \begin{bmatrix}
a_{i1j1} & a_{i1j2} & \cdots & a_{i1jl} \\
a_{i2j1} & a_{i2j2} & \cdots & a_{i2jl} \\
\vdots & \vdots & & \vdots \\
a_{ikj1} & a_{ikj2} & \cdots & a_{ikjl}
\end{bmatrix}.
\]

We let the shorthand \( A(I,:) \) denote the matrix \( A(I,[1, 2, \ldots, n]) \), and define \( A(:,J) \) analogously.

Given a set of matrices \( \{X_j\}_{j=1}^l \) we let \( \text{diag}(X_1, X_2, \ldots, X_l) \) denote the block diagonal matrix
\[
\text{diag}(X_1, X_2, \ldots, X_l) = \begin{bmatrix}
X_1 & 0 & 0 & \cdots & 0 \\
0 & X_2 & 0 & \cdots & 0 \\
0 & 0 & X_3 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & X_l
\end{bmatrix}.
\]

2.2. Low rank factorizations. We say that an \( m \times n \) matrix \( A \) has exact rank \( k \) if there exist an \( m \times k \) matrix \( E \) and a \( k \times n \) matrix \( F \) such that
\[
A = EF.
\]

In this paper, we will utilize three standard matrix factorizations. In describing them, we let \( A \) denote an \( m \times n \) matrix of rank \( k \). The first is the so called “QR” factorization:
\[
A = QR
\]
where \( Q \) is an \( m \times k \) matrix whose columns are orthonormal, and \( R \) is a \( k \times n \) matrix with the property that a permutation of its columns is upper triangular. The second is the “singular value decomposition” (SVD):
\[
A = UDV^t,
\]

where the \( m \times k \) matrix \( U \) and the \( n \times k \) matrix \( V \) have orthonormal columns, and the \( k \times k \) matrix \( D \) is diagonal. The third factorization is the so called “interpolatory decomposition”:
\[
A = A(:, J) X,
\]

where \( J \) is a vector of indices marking \( k \) of the columns of \( A \), and the \( k \times n \) matrix \( X \) has the \( k \times k \) identity matrix has a submatrix and has the property that all its entries are bounded by 1 in magnitude. In other words, the interpolatory decomposition picks \( k \) columns of \( A \) as a basis for the column space of \( A \) and expresses the remaining columns in terms of the chosen ones.

The existence for all matrices of the QR factorization and the SVD are well-known, as are techniques for computing them accurately and stably, see e.g. [11]. The interpolatory decomposition is slightly less well known but it too always exists, and there are stable and accurate techniques for computing it, see e.g. [11] 9. (Practical algorithms for computing the interpolatory decomposition may produce a matrix \( X \) whose elements slightly exceed 1 in magnitude.) In the pseudo code we use to describe the methods of this paper, we refer to such algorithms as follows:
\[
[Q, R] = \text{qr}(A), \quad [U, D, V] = \text{svd}(A), \quad [X, J] = \text{interpolate}(A).
\]

In the applications under consideration in this paper, matrices that arise are typically only approximately of low rank. Moreover, their approximate ranks are generally not known
à priori. As a consequence, the algorithms will typically invoke versions of the factorization algorithms that take the computational accuracy $\varepsilon$ as an input parameter. For instance,

$$[U, D, V] = \text{svd}(A, \varepsilon)$$

results in matrices $U$, $D$, and $V$ of sizes $m \times k$, $n \times k$, and $k \times k$, such that

$$\|UDV^t - A\| \leq \varepsilon.$$ 

In this case, the number $k$ is the $\varepsilon$-rank of $A$, and is of course an output of the algorithm. The corresponding functions for computing an approximate QR factorization or an interpolatory decomposition are denoted

$$[Q, R] = \text{qr}(A, \varepsilon), \quad [X, J] = \text{interpolate}(A, \varepsilon).$$

**Remark 2.1.** Standard techniques for computing partial QR and interpolatory factorizations (Gram-Schmidt, Householder, etc) produce results that are guaranteed in the Frobenius norm (or some related matrix norm that can be computed via $O(mn)$ methods). It is possible to modify such techniques to measure remainders in the $l^2$-operator norm, but we have found no need to utilize such techniques since in all the applications that we have studied so far, the relevant matrix norms are excellent predictors for each other.

### 2.3. Construction of low-rank approximations via randomized sampling.

Let $A$ be a given $m \times n$ matrix that we know can accurately be approximated by a matrix of rank $k$ (which we do not know), and suppose that we seek to determine a matrix $Q$ with orthonormal columns (as few as possible) such that

$$\|A - QQ^t A\|$$

is small. (In other words, we seek a matrix $Q$ whose columns form an approximate ON-basis for the column space of $A$.) When we have access to a fast technique for computing matrix vector products $x \mapsto Ax$, this task can efficiently be solved using randomized sampling via the following steps:

1. Pick an integer $l$ that is slightly larger than $k$ (the choice $l = k + 10$ will turn out to be a good one).
2. Form an $n \times l$ matrix $R$ whose entries are drawn independently from a normalized Gaussian distribution.
3. Form the product $S = AR$.
4. Construct a matrix $Q$ whose columns form an ON-basis for the columns of $S$.

Note that each column of the “sample” matrix $S$ is a random linear combination of the columns of $A$. We would therefore expect the algorithm described to have a high probability of producing an accurate result provided that $l$ is sufficiently much larger than $k$. It is perhaps less obvious that this probability depends only on the difference between $l$ and $k$ (not on $m$ or $n$, or any other properties of $A$), and that it approaches $1$ extremely rapidly as $l - k$ increases. The details are given in the following theorem from [23]:

**Theorem 2.1.** Let $A$ be an $m \times n$ matrix, and let $l$ and $k$ be integers such that $l \geq k$. Let $R$ be an $n \times l$ matrix whose entries are drawn independently from a normalized Gaussian distribution. Let $Q$ be an $m \times l$ matrix whose columns form an ON-basis for the columns of $AR$. Let $\sigma_{k+1}$ denote the minimal error in approximating $A$ by a matrix of rank $k$:

$$\sigma_{k+1} = \min_{\text{rank}(B) = k} \|A - B\|.$$ 

Then

$$\|A - QQ^t A\|_2 \leq 10 \sqrt{\frac{k}{n}} \sigma_{k+1}.$$
with probability at least
\[ 1 - \varphi(l - k), \]
where \( \varphi \) is a decreasing function satisfying, for instance, \( \varphi(8) < 10^{-5} \) and \( \varphi(20) < 10^{-17} \).

In this paper, we always set \( l = k + 10 \); note however that \( l - k \) is a user defined parameter that can be set to balance the risk of failure against computational cost.

**Remark 2.2.** In practical applications, it is in Step (4) of the algorithm described above sufficient to construct an ON-basis for the columns of the sample matrix \( S \) that is accurate to precision \( \varepsilon \). Under very moderate conditions on decay of the singular values of \( A \), the number of basis vectors actually constructed will be extremely close to the optimal number, regardless of the number \( l \).

**Remark 2.3.** The approximate rank \( k \) is rarely known in advance. In a situation where a single matrix \( A \) is to be analyzed, it is a straight-forward matter to modify the algorithm described here to an algorithm that adaptively determines the numerical rank by generating a sequence of samples from the column space of \( A \) and simply stopping when no more information is added. In the application we have in mind in this paper, however, the randomized scheme will be used in such a way that a single random matrix will be used to create samples of a large set of different matrices. In this case, we choose a number \( l \) of random samples that we are confident exceeds the numerical rank of all the matrices by at least 10. Note that the bases constructed for the various matrices will have the correct number of elements due to the observation described in Remark 2.2.

**Remark 2.4.** The randomized sampling technique is particularly effective when used in conjunction with the interpolatory decomposition. To illustrate, let us suppose that \( A \) is an \( n \times n \) matrix of rank \( k \) for which we can rapidly evaluate the maps \( x \mapsto A x \) and \( x \mapsto A^t x \). Using the randomized sampling technique, we then construct matrices \( S^{\text{col}} = A R \) and \( S^{\text{row}} = A^t R \) whose columns span the column and the row spaces of \( A \), respectively. If we seek to construct a factorization of \( A \) without using the interpolatory decomposition, we would then orthonormalize the columns of \( S^{\text{col}} \) and \( S^{\text{row}} \),

\[
[Q^{\text{col}}, Y^{\text{col}}] = \text{qr}(S^{\text{col}}), \quad \text{and} \quad [Q^{\text{row}}, Y^{\text{row}}] = \text{qr}(S^{\text{row}}),
\]

whence

\[ (2.1) \quad A = Q^{\text{col}} ( (Q^{\text{col}})^t A Q^{\text{row}} ) Q^{\text{row}}. \]

Note that the evaluation of (2.1) requires \( k \) matrix-vector multiplies involving the large matrix \( A \) in order to compute the \( k \times k \) matrix \( (Q^{\text{col}})^t A Q^{\text{row}} \). Using the interpolatory decomposition instead, we simply determine the \( k \) rows of \( S^{\text{col}} \) and \( S^{\text{row}} \) that span their respective row spaces,

\[
[X^{\text{col}}, J^{\text{col}}] = \text{interpolate}((S^{\text{col}})^t), \quad \text{and} \quad [X^{\text{row}}, J^{\text{row}}] = \text{interpolate}((S^{\text{row}})^t).
\]

Then we immediately obtain the factorization

\[ (2.2) \quad A = X^{\text{col}} A(J^{\text{col}}, J^{\text{row}}) (X^{\text{row}})^t. \]

Note that the factorization (2.2) is obtained by simply extracting the \( k \times k \) submatrix \( A(J^{\text{col}}, J^{\text{row}}) \) from \( A \).

**Remark 2.5.** In practical application, the entries of the random matrix \( R \) are not “true” random numbers, but numbers from a “pseudo random number generator”. Empirical experiments indicate that the algorithm is not at all sensitive to the quality of the random number generator.
2.4. Hierarchically Semi-Separable matrices. In this section, we define the class of “Hierarchically Semi-Separable” (HSS) matrices, and introduce notation for keeping track of various blocks of structured matrices. A more detailed discussion of this topic can be found in e.g. [7, 25].

In order to define the HSS property for an $N \times N$ matrix $A$, we first partition the index vector $I = [1, 2, \ldots, N]$ in a hierarchy of index sets. For simplicity, we limit attention to binary tree structures in which every level is fully populated. We use the integers $p = 0, 1, \ldots, P$ to label the different levels, with $P$ denoting the finest level. Thus at level $P$, we partition $I$ into $2^P$ disjoint vectors $\{I(P,j)\}_{j=1}^{2^P}$ so that $I = [I(P,1), I(P,2), \ldots, I(P,2^P)]$.

We then merge the index vectors by twos, so that for each $p = 0, 1, \ldots, P-1$, and each $j = 1, 2, \ldots, 2^p$, we have $I(P,j) = [I(p+1,2j-1), I(p+1,2j)]$.

For a given node $\tau = (p, j)$, we call the two nodes $\sigma_1 = (p+1, 2j-1)$ and $\sigma_2 = (p+1, 2j)$ the “children” of $\tau$, and we say that $\sigma_1$ and $\sigma_2$ are “siblings”. The tree structure is illustrated in Figure 2.1.

For any node $\tau = (p, j)$ in the tree, we define the corresponding diagonal block of $A$ via $D_\tau = A(I_\tau, I_\tau)$, and let $D^{(p)}$ denote the $N \times N$ matrix with the matrices $\{D(p,j)\}_{j=1}^{2^p}$ as its diagonal blocks,

$$D^{(p)} = \text{diag}(D(p,1), D(p,2), \ldots, D(p,2^p)).$$

For a node $\tau = (p, j)$, we now define the corresponding “HSS row block” $A^{\text{row}}_\tau$ and “HSS column block” $A^{\text{col}}_\tau$ by

$$A^{\text{row}}_\tau = A(I_\tau, :) - D^{(p)}(I_\tau, :) \quad \text{and} \quad A^{\text{col}}_\tau = A(:, I_\tau) - D^{(p)}(:, I_\tau).$$

These definitions are illustrated in Figure 2.2.

**Definition 2.1.** A matrix $A$ is an “HSS matrix” if for some given positive integer $k$, every HSS block has rank at most $k$.

It is convenient to construct factorizations for the HSS blocks that are “nested” in the sense that the bases on one level are expressed in terms of the bases on the next finer level. To express this concept in formulas, we suppose that for each node $\tau$, $U_\tau$ denotes a matrix whose columns form a basis for the column space of the HSS row block $A^{\text{row}}_\tau$. It is possible...
to construct the set of bases \{U_\tau\} in such a way that for every non-leaf node \tau, there exists a \(2k \times k\) matrix \(\hat{U}_\tau\) such that

\[
U_\tau = \begin{bmatrix} U_{\sigma_1} & 0 \\ 0 & U_{\sigma_2} \end{bmatrix} \hat{U}_\tau,
\]

where \(\sigma_1\) and \(\sigma_2\) denote the two children of \(\tau\). We analogously construct a set \{V_\tau\} of bases for the row spaces of the HSS column blocks \(A^\text{col}_{\sigma_2}\) for which there exist \(2k \times k\) matrices \(\hat{V}_\tau\) such that

\[
V_\tau = \begin{bmatrix} V_{\sigma_1} & 0 \\ 0 & V_{\sigma_2} \end{bmatrix} \hat{V}_\tau.
\]

Next, let \(\{\sigma_1, \sigma_2\}\) denote a sibling pair in the tree, and consider the offdiagonal block

\[
A_{\sigma_1, \sigma_2} = A(I_{\sigma_1}, I_{\sigma_2}).
\]

Since \(A_{\sigma_1, \sigma_2}\) is a submatrix of the HSS row block \(A^\text{row}_{\sigma_1}\) and the HSS column block \(A^\text{col}_{\sigma_2}\), there must exist a \(k \times k\) matrix \(B_{\sigma_1, \sigma_2}\) such that

\[
A_{\sigma_1, \sigma_2} = U_{\sigma_1} B_{\sigma_1, \sigma_2} (V_{\sigma_2})^t.
\]

An HSS matrix \(A\) is completely described if for every leaf node \(\tau\), we are given the matrices \(D_\tau\) and the basis matrices \(U_\tau\) and \(V_\tau\), and for all sibling pairs \(\{\sigma_1, \sigma_2\}\) we are given the matrices \(B_{\sigma_1, \sigma_2}\) and if for each non-leaf node \(\tau\) we are given the matrices \(\hat{U}_\tau\) and \(\hat{V}_\tau\). In particular, given a vector \(x\), the vector \(b = Ax\) can be evaluated via the following steps:

1. For every leaf node \(\tau\), calculate \(\tilde{x}_\tau = V^t_\tau x(I_\tau)\).

2. Looping over all non-leaf nodes \(\tau\), from finer to coarser, calculate

\[
\tilde{x}_\tau = \hat{V}_\tau \begin{bmatrix} \tilde{x}_{\sigma_1} \\ \tilde{x}_{\sigma_2} \end{bmatrix},
\]

where \(\sigma_1\) and \(\sigma_2\) are the children of \(\tau\).

3. Looping over all non-leaf nodes \(\tau\), from coarser to finer, calculate

\[
\begin{bmatrix} \tilde{b}_{\sigma_1} \\ \tilde{b}_{\sigma_2} \end{bmatrix} = \begin{bmatrix} 0 & B_{\sigma_1, \sigma_2} \\ B_{\sigma_2, \sigma_1} & 0 \end{bmatrix} \begin{bmatrix} \tilde{x}_{\sigma_1} \\ \tilde{x}_{\sigma_2} \end{bmatrix} + \hat{U}_\tau \tilde{b}_\tau \text{ (where } \tilde{b}_\tau = 0 \text{ for the root node).}
\]

4. For every leaf node \(\tau\), calculate \(b(I_\tau) = U_\tau \tilde{b}_\tau + D_\tau x(I_\tau)\).

The computational cost of performing these steps is \(O(Nk)\).

**Remark 2.6.** The matrix \(A\) can be expressed in terms of the matrices \(D_\tau, U_\tau, V_\tau,\) and \(B_{\sigma_1, \sigma_2}\) as a telescoping factorization. To demonstrate this, we introduce for each level
$p = 1, 2, \ldots, P$ the block-diagonal matrices
\[
U^{(p)} = \text{diag}(U_{(p,1)}, U_{(p,2)}, \ldots, U_{(p,2^p)}), \quad \text{and} \quad V^{(p)} = \text{diag}(V_{(p,1)}, V_{(p,2)}, \ldots, V_{(p,2^p)}).
\]
Moreover, we define for each non-leaf node $\tau$ the $2k \times 2k$ matrices
\[
B_{\tau} = \begin{bmatrix}
0 & B_{\sigma_1 \sigma_2} \\
B_{\sigma_2 \sigma_1} & 0
\end{bmatrix}
\]
where $\sigma_1$ and $\sigma_2$ are the children of $\tau$, and set for $p = 0, 1, \ldots, P - 1$
\[
B^{(p)} = \text{diag}(B_{(p,1)}, B_{(p,2)}, \ldots, B_{(p,2^p)}).
\]
Finally, recall from (2.3) that
\[
D^{(P)} = \text{diag}(D_{(P,1)}, D_{(P,2)}, \ldots, D_{(P,2^P)}).
\]
For simplicity, we give the factorization for the specific value $P = 3$:
\[
A = U^{(3)}(U^{(2)}(U^{(1)}B^{(0)}(V^{(1)})^t + B^{(1)}(V^{(2)})^t + B^{(2)}(V^{(3)})^t + D^{(3)}).
\]

\textbf{Remark 2.7.} For notational simplicity, we consider only the case where all HSS blocks are approximated by factorizations of the same rank $k$. In practice, it is a simple matter to implement algorithms that use variable ranks.

\textbf{Remark 2.8.} It is common to require the matrices $U_{\tau}$ and $V_{\tau}$ that arise in an HSS factorization of a given matrix to have orthonormal columns. We have found it convenient to relax this assumption and allow the use of other well-conditioned bases. In particular, the use of interpolative decompositions (as described in Section 2.2) is essential to the performance of the fast factorization technique described in Section 2.1. A simple algorithm for switching between the two formulations (using orthonormal bases, or interpolatory ones) is described in Section 3.2.

\textbf{3. Fast computation of HSS approximations}

The straight-forward way of computing the HSS factorization of matrix would be to form all HSS blocks, and then perform dense linear algebra operations on them to construct the required basis functions. This approach would require at least $O(N^2 k)$ algebraic operations to factorize an $N \times N$ matrix of HSS rank $k$. In this section, we describe how the randomized sampling techniques described in Section 2.3 can be used to reduce this cost to $O(N k^2)$.

The technique described relies crucially on the use of the interpolatory decompositions described in Section 2.2 in the HSS factorization. The advantage is that the matrices $B_{\sigma_1 \sigma_2}$ are then submatrices of the original matrix $A$ and can therefore be constructed directly without a need for projecting the larger blocks onto the bases chosen, cf. Remark 2.4.

Section 3.1 describes a scheme for rapidly computing the HSS factorization of a symmetric matrix. The scheme described in Section 3.1 results in a factorization based on interpolatory bases and the blocks $B_{\sigma_1 \sigma_2}$ are submatrices of the original matrix; Section 3.2 describes how such a factorization can be converted to one in which the bases for the HSS blocks are
orthonormal, and the blocks $B_{\sigma_1 \sigma_2}$ are diagonal. Section 3.3 describes how to extend the methods to non-symmetric matrices.

3.1. A scheme for computing an HSS factorization of a symmetric matrix. Let $A$ be an $N \times N$ symmetric matrix that has an HSS factorization of rank $k$. Suppose further that:

(a) Matrix vector products $x \mapsto A x$ can be evaluated at a cost $T_{\text{mult}}$.

(b) Individual entries of $A$ can be evaluated at a cost $T_{\text{entry}}$.

In this section, we will describe a scheme for computing an HSS factorization of $A$ in time

$$T_{\text{total}} \sim T_{\text{mult}} \times (k + 10) + T_{\text{rand}} \times N (k + 10) + T_{\text{entry}} \times 2 N k + T_{\text{flop}} \times c N k^2,$$

where $T_{\text{rand}}$ is the time required to generate a pseudo random number, $T_{\text{flop}}$ is the CPU time requirement for a floating point operation and $c$ is a small number that does not depend on $N$ or $k$.

The core idea of the method is to construct an $N \times (k + 10)$ random matrix $R$, and then construct for each level $p$, the "sample" matrices

$$S^{(p)} = (A - D^{(p)}) R,$$

via a procedure to be described. Then for any cell $\tau$ on level $p$,

$$S^{(p)}(I_\tau, :) = A^{\text{row}}_\tau R,$$

and since $A^{\text{row}}_\tau$ has rank $k$, the columns of $S^{(p)}(I_\tau, :)$ span the column space of $A^{\text{row}}_\tau$ according to Theorem 2.1. We can then construct a basis for the column space of the large matrix $A^{\text{row}}_\tau$ by analyzing the small matrix $S^{(p)}(I_\tau, :)$.

What makes the procedure fast is that the sample matrices $S^{(p)}$ can be constructed by means of an $O(N)$ process from the result of applying the entire matrix $A$ to $R$,

$$S = A R.$$

At the finest level, $p = P$, we directly obtain $S^{(P)}$ from $S$ by simply subtracting the contribution from the diagonal blocks of $A$,

$$S^{(P)} = S - D^{(P)} R. \quad (3.1)$$

Since $D^{(P)}$ is block diagonal with small blocks, equation (3.1) can be evaluated cheaply. To proceed to the next coarser level, $p = P - 1$, we observe that

$$S^{(P-1)} = (A - D^{(P-1)}) R = (A - D^{(P)}) R - (D^{(P-1)} - D^{(P)}) R = S^{(P)} - (D^{(P-1)} - D^{(P)}) R. \quad (3.2)$$

Now $(D^{(P-1)} - D^{(P)})$ has only $2^P$ non-zero blocks. The pattern of these blocks is illustrated for $P = 3$ below:

![Pattern of non-zero blocks](image)

Each of these blocks were compressed in the computation at level $P$ so (3.2) can also be evaluated rapidly. The algorithm then proceeds up towards coarser levels via the formula

$$S^{(p-1)} = S^{(p)} - (D^{(p-1)} - D^{(p)}) R,$$
**Input:** A fast means of computing matrix-vector products \(x \mapsto Ax\).
A method for computing individual entries of \(A\).
The HSS-rank \(k\) of \(A\).
A partitioning \(\{I_{(P,j)}\}_{j=1}^{2P}\) of the interval \([1, 2, \ldots, N]\).

**Output:** Matrices \(\hat{U}_\tau, B_{\sigma_1, \sigma_2}, D_\tau\) that form an HSS factorization of \(A\).
(Note that \(\hat{V}_\tau = \hat{U}_\tau\) for a symmetric matrix.)

Generate an \(N \times (k + 10)\) Gaussian random matrix \(R\).
Evaluate \(S = AR\) using the fast matrix-vector multiplier.

```
loop over levels, finer to coarser, \(p = P : (-1) : 1\)
  loop over all nodes \(\tau\) on level \(p\)
    if \(\tau\) is a leaf node then
      \(I_{\text{loc}} = I_\tau\)
      \(R_{\text{loc}} = R(I_\tau,:)
      \(S_{\text{loc}} = S(I_\tau,: - A(I_\tau, I_\tau) R_{\text{loc}}
    else
      Let \(\sigma_1\) and \(\sigma_2\) be the two children of \(\tau\).
      \(I_{\text{loc}} = [\tilde{I}_{\sigma_1}, \tilde{I}_{\sigma_2}]
      R_{\text{loc}} = \begin{bmatrix} R_{\sigma_1} \\
      R_{\sigma_2} \end{bmatrix}
      S_{\text{loc}} = \begin{bmatrix} S_{\sigma_1} - A(\tilde{I}_{\sigma_1}, \tilde{I}_{\sigma_2}) R_{\sigma_2} \\
      S_{\sigma_2} - A(\tilde{I}_{\sigma_2}, \tilde{I}_{\sigma_1}) R_{\sigma_1} \end{bmatrix}
    end if

  \[\hat{U}_\tau, J_\tau\] = interpolate\((S_{\text{loc}}^t)\)
  \(R_\tau = \hat{U}_\tau^t R_{\text{loc}}\)
  \(S_\tau = S_{\text{loc}}(J_\tau,:)
  \(\tilde{I}_\tau = I_{\text{loc}}(J_\tau)
  end loop
end loop
```

For all leaf nodes \(\tau\), set \(D_\tau = A(I_\tau, I_\tau)\).
For all sibling pairs \(\{\sigma_1, \sigma_2\}\) set \(B_{\sigma_1, \sigma_2} = A(\tilde{I}_{\sigma_1}, \tilde{I}_{\sigma_2})\).

**Algorithm 1:** Computing the HSS factorization of a symmetric matrix.

which can be evaluated rapidly since the blocks of \((D^{(p-1)} - D^{(p)})\) have at this point been compressed.

The condition that the bases be “nested” in the sense of formula (2.4) can conveniently be enforced by using the interpolative decompositions described in Section 2.2. At the finest level, we pick \(k\) rows of each HSS row block that span its row space. At the next coarser level, we pick in each HSS row block \(k\) rows that span its row space *out of the 2k rows that span its two children*. By proceeding analogously throughout the upwards pass, (2.4) will be satisfied.

The use of interpolatory decompositions has the additional benefit that we do not need to form the entire matrices \(S^{(p)}\) when \(p < P\). Instead, we work with the submatrices formed by keeping only the rows of \(S^{(p)}\) corresponding to the spanning rows at that step.

A complete description of the methods is given with the caption “Algorithm 1”.

**Remark 3.1.** For simplicity, Algorithm 1 is described for the case where the off-diagonal blocks of \(A\) has exact rank at most \(k\), and the number \(k\) is known in advance. In actual
applications, one typically is given a matrix $A$ whose off-diagonal blocks are not necessarily rank-deficient in an exact sense, but can to high accuracy be approximated by low-rank matrices. In this case, Algorithm 1 needs to be modified slightly to take as an input the computational accuracy $\varepsilon$ instead of the rank $k$, and the line
\[ [\hat{U}_\tau, J_\tau] = \text{interpolate}(S_{\text{loc}}^t) \]
needs to be replaced by the line
\[ [\hat{U}_\tau, J_\tau] = \text{interpolate}(S_{\text{loc}}^t, \varepsilon). \]
This directly leads to a variable rank algorithm that is typically far more efficient than the fixed rank algorithm described.

3.2. Recompression into orthonormal basis functions. In this section, we describe a simple post-processing step that converts the HSS factorization resulting from Algorithm 1 (which is based on interpolatory factorizations) into a factorization with orthonormal basis functions. This process also diagonalizes all matrices $B_{\sigma_1 \sigma_2}$.

Suppose that the matrices $U_\tau$, $D_\tau$, and $B_{\sigma_1 \sigma_2}$ in an HSS factorization of a symmetric matrices have already been generated (for instance by the algorithm of Section 3.1). The method described here produces new matrices $U_{\tau}^{\text{new}}$ and $B_{\sigma_1 \sigma_2}^{\text{new}}$ with the property that each $U_{\tau}^{\text{new}}$ has orthonormal columns, and each $B_{\sigma_1 \sigma_2}^{\text{new}}$ is diagonal.

**Remark 3.2.** The method described here does not in any way rely on particular properties of the interpolative decomposition. In fact, it works for any input matrices $U_\tau$, $D_\tau$, $B_{\sigma_1 \sigma_2}$ for which the factorization (2.5) holds.

The orthonormalization procedure works hierarchically, starting at the finest level and working upwards. At the finest level, it loops over all sibling pairs $\{\sigma_1, \sigma_2\}$. It orthonormalizes the basis matrices $U_{\sigma_1}$ and $U_{\sigma_2}$ by computing their QR factorizations,
\[ [W_1, R_1] = \text{qr}(U_{\sigma_1}) \quad \text{and} \quad [W_2, R_2] = \text{qr}(U_{\sigma_2}), \]
so that
\[ U_{\sigma_1} = W_1 R_1 \quad \text{and} \quad U_{\sigma_2} = W_2 R_2, \]
and $W_1$ and $W_2$ have orthonormal columns. The matrices $R_1$ and $R_2$ are then used to update the diagonal block $B_{\sigma_1 \sigma_2}$ to reflect the change in basis vectors, \[ \tilde{B}_{12} = R_1 B_{\sigma_1 \sigma_2} R_2^t. \]
Then $\tilde{B}_{12}$ is diagonalized via a singular value decomposition, \[ \tilde{B}_{12} = \tilde{W}_1 B_{\sigma_1 \sigma_2}^{\text{new}} \tilde{W}_2. \]
The new bases for $\sigma_1$ and $\sigma_2$ are constructed by updating $W_1$ and $W_2$ to reflect the diagonalization of $\tilde{B}_{12}$,
\[ U_{\sigma_1}^{\text{new}} = W_1 \tilde{W}_1, \quad \text{and} \quad U_{\sigma_2}^{\text{new}} = W_2 \tilde{W}_2. \]
Finally, the basis vectors for the parent $\tau$ of $\sigma_1$ and $\sigma_2$ must be updated to reflect the change in bases at the finer level,
\[ \hat{U}_\tau \leftarrow \begin{bmatrix} \tilde{W}_1^t & 0 \\ 0 & \tilde{W}_2^t \end{bmatrix} \hat{U}_\tau. \]

Once the finest level has been processed, simply move up to the next coarser one and proceed analogously. A complete description of the recompression scheme is given with the caption “Algorithm 2”.
Input: The matrices $\hat{U}_\tau$, $B_{\sigma_1\sigma_2}$, $D_\tau$ in an HSS factorization of a symmetric matrix $A$.

Output: Matrices $\hat{U}^\tau_{\text{new}}$, $B^\tau_{\sigma_1\sigma_2}$, and $D_\tau$ that form an HSS factorization of $A$ such that all $\hat{U}^\tau_{\text{new}}$ have orthonormal columns and all $B^\tau_{\sigma_1\sigma_2}$ are diagonal.

(The matrices $D_\tau$ remain unchanged.)

Set $U^\tau_{\text{tmp}} = U_\tau$ for all leaf nodes $\tau$.

loop over levels, finer to coarser, $p = P - 1, P - 2, \ldots, 0$

loop over all nodes $\tau$ on level $p$

Let $\sigma_1$ and $\sigma_2$ denote the two sons of $\tau$.

$[W_1, R_1] = \text{qr}(U^\tau_{\text{tmp}})$

$[W_2, R_2] = \text{qr}(U^\tau_{\text{tmp}})$

$[\tilde{W}_1, B^\tau_{\sigma_1\sigma_2}, \tilde{W}_2] = \text{svd}(R_1 B_{\sigma_1\sigma_2} R_2^*)$

$\hat{U}^\tau_{\sigma_1} = W_1 \tilde{W}_1$

$\hat{U}^\tau_{\sigma_2} = W_2 \tilde{W}_2$

$\hat{U}^\tau_{\text{tmp}} = \begin{bmatrix} \tilde{W}_1^t R_1 & 0 \\ 0 & \tilde{W}_2^t R_2 \end{bmatrix} \hat{U}_\tau$

end loop

end loop

Remark: In practice, we let the matrices $U^\tau_{\text{tmp}}$ and $U^\tau_{\text{new}}$ simply overwrite $U_\tau$.

Algorithm 2: Orthonormalizing an HSS factorization

3.3. Non-symmetric matrices. The extension of Algorithms 1 and 2 to the case of non-symmetric matrices is straight-forward. In Algorithm 1, we construct a set of sample matrices $\{S_\tau\}$ with the property that the columns of each $S_\tau$ span the column space of the corresponding HSS row block $A^{\text{row}}_\tau$. Since $A$ is in that case symmetric, the columns of $S_\tau$ automatically span the row space of $A^{\text{col}}_\tau$ as well. For non-symmetric matrices, we need to construct different sample matrices $S^{\text{row}}_\tau$ and $S^{\text{col}}_\tau$ whose columns span the column space of $A^{\text{row}}_\tau$ and the row space of $A^{\text{col}}_\tau$, respectively. Note that in practice, we work only with the subsets of all these matrices formed by the respective spanning rows and columns; in the non-symmetric case, these may be different. The algorithm is described in full with the caption “Algorithm 3”.

The generalization of the orthonormalization technique is entirely analogous.

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Input: A fast means of computing matrix-vector products $x \mapsto Ax$ and $x \mapsto A^t x$.
A method for computing individual entries of $A$.
The HSS-rank $k$ of $A$.
A partitioning $\{I_{(p,j)}\}_{j=1}^P$ of the interval $[1, 2, \ldots, N]$.
Output: Matrices $\hat{U}_\tau, B_{\sigma_1,\sigma_2}, D_\tau$ that form an HSS factorization of $A$.

Generate two $N \times (k + 10)$ Gaussian random matrices $R_{\text{row}}$ and $R_{\text{col}}$.
Evaluate $S_{\text{row}} = A^t R_{\text{row}}$ and $S_{\text{col}} = A R_{\text{col}}$ using the fast matrix-vector multiplier.

**loop** over levels, finer to coarser, $p = P : (-1) : 1$

**loop** over all nodes $\tau$ on level $p$

if $\tau$ is a leaf node then

$R_{\text{row}}^\text{loc} = I_{\tau}$

$R_{\text{col}}^\text{loc} = R(I_{\tau}, :)$

$S_{\text{row}}^\text{loc} = S_{\text{row}}(I_{\tau}, :) - A(I_{\tau}, I_{\tau}) R_{\text{row}}^\text{loc}$

$S_{\text{col}}^\text{loc} = S_{\text{col}}(I_{\tau}, :) - A(I_{\tau}, I_{\tau})^t R_{\text{col}}^\text{loc}$

else

Let $\sigma_1$ and $\sigma_2$ be the two sons of $\tau$.

$R_{\text{row}}^\text{loc} = [\hat{I}_{\text{row}}^\text{loc}, \hat{J}_{\text{row}}^\text{loc}]$

$R_{\text{col}}^\text{loc} = [\hat{R}_{\text{col}}^\text{loc}, \hat{R}_{\text{col}}^\text{loc}]$

$S_{\text{row}}^\text{loc} = \begin{bmatrix}
S_{\sigma_1}^\text{row} - A(\hat{I}_{\text{row}}^\text{loc}, \hat{R}_{\text{row}}^\text{loc}) R_{\text{row}}^\text{loc}
S_{\sigma_2}^\text{row} - A(\hat{I}_{\text{row}}^\text{loc}, \hat{R}_{\text{row}}^\text{loc}) R_{\text{row}}^\text{loc}
\end{bmatrix}$

$S_{\text{col}}^\text{loc} = \begin{bmatrix}
S_{\sigma_1}^\text{col} - A(\hat{I}_{\text{col}}^\text{loc}, \hat{R}_{\text{col}}^\text{loc}) R_{\text{col}}^\text{loc}
S_{\sigma_2}^\text{col} - A(\hat{I}_{\text{col}}^\text{loc}, \hat{R}_{\text{col}}^\text{loc}) R_{\text{col}}^\text{loc}
\end{bmatrix}$

end if

$[\hat{X}_{\tau}^\text{row}, \hat{J}_{\tau}^\text{row}] = \text{interpolate}(S_{\text{row}}^\text{loc})$

$[\hat{X}_{\tau}^\text{col}, \hat{J}_{\tau}^\text{col}] = \text{interpolate}(S_{\text{col}}^\text{loc})$

$P_{\tau}^\text{row} = (\hat{X}_{\tau}^\text{row})^t R_{\text{row}}^\text{loc}$

$S_{\tau}^\text{row} = S_{\text{row}}^\text{loc}(\hat{J}_{\tau}^\text{row}, :)$

$\hat{I}_{\tau}^\text{row} = R_{\text{row}}^\text{loc}(\hat{J}_{\tau}^\text{row})$

$P_{\tau}^\text{col} = (\hat{X}_{\tau}^\text{col})^t R_{\text{col}}^\text{loc}$

$S_{\tau}^\text{col} = S_{\text{col}}^\text{loc}(\hat{J}_{\tau}^\text{col}, :)$

$\hat{I}_{\tau}^\text{col} = R_{\text{col}}^\text{loc}(\hat{J}_{\tau}^\text{col})$

end loop

For all leaf nodes $\tau$, set $D_{\tau} = A(I_{\tau}, I_{\tau})$.
For all sibling pairs $\{\sigma_1, \sigma_2\}$ set $B_{\sigma_1,\sigma_2} = A(\hat{I}_{\sigma_1}^\text{row}, \hat{I}_{\sigma_2}^\text{row})$.

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