Abstract. A randomized algorithm for computing a compressed representation of a given rank structured matrix $A \in \mathbb{R}^{N \times N}$ is presented. The algorithm interacts with $A$ only through its action on vectors. Specifically, it draws two tall thin matrices $\Omega, \Psi \in \mathbb{R}^{N \times s}$ from a suitable distribution, and then reconstructs $A$ by analyzing the matrices $A\Omega$ and $A^*\Psi$. For the specific case of a “Hierarchically Block Separable (HBS)” matrix (a.k.a. Hierarchically Semi-Separable matrix) of block rank $k$, the number of samples $s$ required satisfies $s = O(k)$, with $s \approx 3k$ being a typical scaling. While a number of randomized algorithms for compressing rank structured matrices have previously been published, the current algorithm appears to be the first that is both of truly linear complexity (no $N \log(N)$ factors) and fully black-box in nature (in the sense that no matrix entry evaluation is required).

Key words. randomized approximation of matrices; rank-structured matrices; HODLR matrix; hierarchically block separable matrix; hierarchically semiseparable matrix; randomized SVD; fast direct solver.

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1. Introduction. This work describes a set of efficient algorithms for handling large dense matrices that have rank structure. To simplify slightly, this means that an $N \times N$ matrix can be tessellated into $O(N)$ blocks in such a way that each block is either small or of low numerical rank, cf. Figure 2. This structure allows the matrix to be stored and applied to vectors efficiently, often with cost that scales linearly or close to linearly with $N$. Sometimes, it is also possible to compute an approximate inverse or LU factorization in linear or close to linear time. Matrices of this type have turned out to be ubiquitous in both engineering and data sciences, and have been the subject of much research in recent decades, going under names such as $H$-matrices [2, 3, 12]; HODLR matrices [1, 18], Hierarchically Block Separable (HBS) or Hierarchically Semi-Separable (HSS) matrices [4, 5, 24], Recursive Skeletonization [8, 14, 17, 23], and many more.

The specific problem we address is the following: Suppose that $A$ is an $N \times N$ matrix that we know has HBS structure, but we do not have direct access to the low-rank factors that define the compressible off-diagonal blocks. Instead, we have access to fast “black-box” algorithms that given tall thin matrices $\Omega, \Psi \in \mathbb{R}^{N \times s}$, evaluate the matrix-matrix products

$$Y = A\Omega, \quad \text{and} \quad Z = A^*\Psi.$$  

The problem is then to recover $A$ from the information in the set $\{Y, \Omega, Z, \Psi\}$. The algorithms described here solve the reconstruction problem using $s = O(k)$ sample vectors, where $k$ is an upper bound on the ranks of the off-diagonal blocks. (The pre-factor hidden in the formula $s = O(k)$ is often modest, with $s \approx 3k$ being representative.)

The scheme presented has several important applications. First, it can be used to derive a rank-structured representation of any integral operator for which a fast
matrix-vector multiplication algorithm, such as the Fast Multipole Method [10, 11], is available. Such a representation opens the door to a wider range of matrix operations such as LU factorization, matrix inversion, and sometimes even full spectral decompositions. Second, it can greatly simplify algebraic operations involving products of rank-structured matrices. For instance, the perhaps key application of rank-structured matrix algebra is the acceleration of sparse direct solvers, as the dense matrices that arise during LU factorization are often rank-structured. In the course of such a solver, a typical operation would be to form a Schur complement such as $S_{22} = A_{22} - A_{21}A_{11}^{-1}A_{12}$ that would arise when the top left block $A_{11}$ is eliminated from a $2 \times 2$ blocked matrix. If $A_{11}$ is rank-structured, then $A_{11}^{-1}$ can easily be applied to vectors via an LU factorization. If, additionally, $A_{12}$ and $A_{21}$ are either sparse or rank-structured, then $S_{22}$ can easily be applied to a vector. The technique described will then enable one to construct a data-sparse representation of $S_{22}$. In contrast, to directly evaluate the product $A_{21}A_{11}^{-1}A_{12}$ is both onerous to code and slow to execute.

The method we describe is inspired by the randomized compression algorithms of [19]. The algorithms described in that work require only $O(k)$ samples to compress an HBS matrix, and they have linear complexity when the cost of applying $A$ to a vector is $O(N)$. However, they are not true black-box algorithms since, in addition to randomized samples, they also require direct evaluation of a small number of entries of the matrix. In contrast, the method presented here is truly black-box.

**Remark 1.1 (Peeling algorithms).** A related class of algorithms for randomized compression of rank-structured matrices is described in [16, 20]. These techniques are “true” black-box algorithms in that they only access the matrix through the black-box matrix-vector multiplication routines, but they require $O(k \log(N))$ samples and $O(k^2 N \log(N))$ floating point operations, so they do not have linear complexity.

The manuscript is structured as follows: Section 2 surveys some basic linear algebraic techniques that we rely on. Section 3 introduces our formalism for HBS matrices. Section 4 describes the new algorithm, and analyzes its asymptotic complexity. Section 5 describes numerical results.

2. Preliminaries. In introducing well-known material, we follow the presentation of [20].

2.1. Notation. Throughout the paper, we measure a vector $x \in \mathbb{R}^n$ by its Euclidean norm $\|x\| = \left(\sum_i |x_i|^2\right)^{1/2}$. We measure a matrix $A \in \mathbb{R}^{m \times n}$ with the corresponding operator norm $\|A\| = \sup_{\|x\|=1} \|Ax\|$, and in some cases with the Frobenius norm $\|A\|_{\text{Fro}} = \left(\sum_{i,j} |A(i,j)|^2\right)^{1/2}$. To denote submatrices, we use the notation of Golub and van Loan [9]: If $A$ is an $m \times n$ matrix, and $I = [i_1, i_2, \ldots, i_k]$ and $J = [j_1, j_2, \ldots, j_k]$, then $A(I, J)$ denotes the $k \times l$ matrix

$$A(I, J) = \begin{bmatrix}
A(i_1, j_1) & A(i_1, j_2) & \cdots & A(i_1, j_l) \\
A(i_2, j_1) & A(i_2, j_2) & \cdots & A(i_2, j_l) \\
\vdots & \vdots & \ddots & \vdots \\
A(i_k, j_1) & A(i_k, j_2) & \cdots & A(i_k, j_l)
\end{bmatrix}$$

We let $A(I, :)$ denote the column submatrix $A(I, [1, 2, \ldots, n])$ and let $A(:, J)$ denote the analogous row submatrix of $A$. We let $A^T$ denote the transpose of $A$, and we say that matrix $U$ is orthonormal if its columns are orthonormal, $U^TU = I$. 

2.2. The QR factorization. The full QR factorization of a matrix \( A \) of size \( m \times n \) takes the form
\[
A = Q R, \quad m \times n \quad m \times m \quad m \times n
\]
where \( Q \) is orthonormal and \( R \) is upper-triangular. For a matrix of rank \( k \), the rank-\( k \) partial QR factorization of \( A \) is given by
\[
A = Q(:, 1 : k) R(1 : k, 1 : k), \quad m \times n \quad m \times k \quad k \times n
\]
and the last \( m - k \) columns of \( Q \) contain an orthonormal basis of the nullspace of \( A \),
\[
\text{span}(Q(:, (k + 1) : m)) = \mathcal{N}(A).
\]

2.3. Randomized compression. Let \( A \) be an \( m \times n \) matrix that can be accurately approximated by a matrix of rank \( k \), and suppose we seek to determine a matrix \( Q \) with orthonormal columns (as few as possible) such that \( \| A - QQ^* A \| \) is small. In other words, we seek a matrix \( Q \) whose columns form an approximate orthonormal basis (ON-basis) for the column space of \( A \). This task can efficiently be solved via the following randomized procedure:

1. Pick a small integer \( p \) representing how much “oversampling” is done. (\( p = 10 \) is often good.)
2. Form an \( n \times (k + p) \) matrix \( G \) whose entries are independent and identically distributed (i.i.d.) normalized Gaussian random numbers.
3. Form the “sample matrix” \( Y = AG \) of size \( m \times (k + p) \).
4. Construct an \( m \times (k + p) \) matrix \( Q \) whose columns form an ON basis for the columns of \( Y \).

Note that each column of the sample matrix \( Y \) 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 when \( p \) is a large number. It is perhaps less obvious that this probability depends only on \( p \) (not on \( m \) or \( n \), or any other properties of \( A \)) and that it approaches 1 extremely rapidly as \( p \) increases. In fact, one can show that the basis \( Q \) determined by the scheme above satisfies
\[
\| A - QQ^* A \| \leq [1 + 11 \sqrt{k + p} \cdot \sqrt{\min\{m,n\}}] \sigma_{k+1}
\]
with probability at least \( 1 - 6 \cdot p^{-p} \) (see [13, sec. 1.5]), where \( \sigma_{k+1} \) is the \((k+1)\)-largest singular value of \( A \). The error bound (2.2) indicates that the error produced by the randomized sampling procedure can be larger than the theoretically minimal error \( \sigma_{k+1} \) by a factor of \( 1 + 11 \sqrt{k + p} \cdot \sqrt{\min\{m,n\}} \). This crude bound is typically very pessimistic, in particular for matrices whose singular values decay rapidly; cf. [13].

2.4. Functions for computing orthonormal bases. We write
\[
Q = \text{qr}(B, k),
\]
for a function call that returns the first \( k \) columns of \( Q \) in a QR factorization, and we write
\[
Q = \text{null}(B, k),
\]
for a function call that returns the last \( k \) columns of \( \mathbf{Q} \) in a QR factorization. We only call \texttt{null} with inputs \( \mathbf{B}, k \) for a matrix \( \mathbf{B} \) that is known to have a nullspace of dimension at least \( k \).

3. Hierarchically block separable matrices. In this section, we review important concepts relating to HBS matrices, based on the presentation of [21]. We introduce a binary tree structure that specifies the tessellation of an HBS matrix, give the precise definition of an HBS matrix, and describe telescoping factorizations of HBS matrices.

3.1. A tree structure. Let \( I = [1, 2, \ldots, N] \) be a vector of indices corresponding to the rows and columns of an \( N \times N \) matrix. We define a tree \( T \), in which each node \( \tau \) is associated with a contiguous subset of the indices \( I_\tau \). To the root node of the tree, we assign the full set of indices \( I \). The two children of the root node are given index vectors \([1, \ldots, \lceil N/2 \rceil] \) and \([ \lceil N/2 \rceil + 1, \ldots, N] \). We continue evenly splitting the indices of each node to form two child nodes until we reach a level of the tree in which the size of each node is below some given threshold \( m \). We refer to a node with children as a parent node, and a node with no children as a leaf node. The depth of a node is defined as its distance from the root node, and level \( \ell \) of the tree is defined as the set of nodes with depth \( \ell \), so that level 0 consists of only the root node, level 1 consists of the two children of the root node, and so on. The levels of the tree represent successively finer partitions of \( I \). The depth of the tree is defined as the maximum node depth, denoted by \( L \approx \log_2 N/m \). For simplicity, we only consider fully populated binary trees. An example tree structure is depicted in Figure 1.

3.2. The HBS matrix format. Let \( T \) be a tree defined on index vector \( I = [1, 2, \ldots, N] \). Matrix \( \mathbf{A} \) of size \( N \times N \) is said to be hierarchically block separable with block rank \( k \) with respect to \( T \) if the following conditions are satisfied.

(1) Assumptions on the ranks of off-diagonal blocks of the finest level: For every pair of distinct leaf nodes \( \tau \) and \( \tau' \), we define

\[
\mathbf{A}_{\tau, \tau'} = \mathbf{A}(I_\tau, I_{\tau'})
\]

and require that every such matrix have rank of at most \( k \). Additionally, for each leaf node \( \tau \) there must exist basis matrices \( \mathbf{U}_\tau \) and \( \mathbf{V}_\tau \) such that for every leaf node \( \tau' \neq \tau \) we have

\[
\mathbf{A}_{\tau, \tau'} = \mathbf{U}_\tau \tilde{\mathbf{A}}_{\tau, \tau'} \mathbf{V}_{\tau'}^*.
\]

(2) Assumptions on the ranks of off-diagonal blocks of levels \( \ell = L-1, L-2, \ldots, 1 \). The following conditions must hold for each level \( \ell = L-1, L-2, \ldots, 1 \). For every
Fig. 2: Tessellation of an HBS matrix with depth 3. Low-rank blocks are shown in gray, and blocks that are not necessarily low-rank are shown in pink.

pair of distinct nodes \( \tau \) and \( \tau' \) on level \( \ell \) with children \((\alpha, \beta)\) and \((\alpha', \beta')\), respectively, we define

\[
\mathbf{A}_{\tau, \tau'} = \begin{bmatrix}
\tilde{\mathbf{A}}_{\alpha, \alpha'} & \tilde{\mathbf{A}}_{\alpha, \beta'} \\
\tilde{\mathbf{A}}_{\beta, \alpha'} & \tilde{\mathbf{A}}_{\beta, \beta'}
\end{bmatrix}
\]

and require that every such matrix have rank of at most \( k \). Additionally, for each node \( \tau \) on level \( \ell \) there must exist basis matrices \( \mathbf{U}_\tau \) and \( \mathbf{V}_\tau \) such that for every node \( \tau' \neq \tau \) on level \( \ell \), we have

\[
\mathbf{A}_{\tau, \tau'} = \mathbf{U}_\tau \tilde{\mathbf{A}}_{\tau, \tau'} \mathbf{V}_{\tau'}^*.
\]

Notably, no assumptions are made on the ranks of the on-diagonal blocks of level \( L \), and those blocks may have full rank. An example tessellation of an HBS matrix showing compressible and incompressible blocks is given in Figure 2.
3.3. Telescoping factorizations. We define the following block-diagonal basis matrices.

\[
U^{(\ell)} = \text{diag}(U_\tau : \tau \text{ is a node on level } \ell), \quad \ell = 1, \ldots, L
\]

\[
V^{(\ell)} = \text{diag}(V_\tau : \tau \text{ is a node on level } \ell), \quad \ell = 1, \ldots, L
\]

Then we obtain a factorization of level \( L \) of the form

\[
A = U^{(L)} \tilde{A}^{(L)} (V^{(L)})^* + D^{(L)},
\]

where

\[
\tilde{A}^{(L)} = (U^{(L)})^* A V^{(L)}
\]

\[
D^{(L)} = A - U^{(L)} \tilde{A}^{(L)} (V^{(L)})^*.
\]

Equation (3.2) can be viewed as a decomposition of \( A \) into a term that “fits” into the low-rank approximation using basis matrices \( U^{(L)} \) and \( V^{(L)} \) and a discrepancy term \( D^{(L)} \) that does not.

For successively coarser levels \( \ell = L-1, L-2, \ldots, 1 \), we similarly have

\[
\tilde{A}^{(\ell+1)} = U^{(\ell)} \tilde{A}^{(\ell)} (V^{(\ell)})^* + D^{(\ell)},
\]

where

\[
\tilde{A}^{(\ell)} = (U^{(\ell)})^* \tilde{A}^{(\ell+1)} V^{(\ell)}
\]

\[
D^{(\ell)} = \tilde{A}^{(\ell+1)} - U^{(\ell)} \tilde{A}^{(\ell)} (V^{(\ell)})^*.
\]

For the root level, we define

\[
D^{(0)} = \tilde{A}^{(1)}.
\]

Equations (3.2) and (3.3) define a telescoping factorization of \( A \). For example, a factorization with \( L = 3 \) takes the form

\[
A = U^{(3)} (U^{(2)} (U^{(1)} D^{(0)} (V^{(1)})^* + D^{(1)}) (V^{(2)})^* + D^{(2)}) (V^{(3)})^* + D^{(3)}.
\]

Algorithm 3.1 describes the process of efficiently applying the telescoping factorization to a vector.

It follows from (3.1) that matrices \( D^{(\ell)}, \ell = 0, 1, \ldots, L \), are also block-diagonal. Matrix \( D^{(\ell)} \) can be described in terms of its on-diagonal blocks as

\[
D^{(\ell)} = \text{diag}(D_\tau : \tau \text{ is a node on level } \ell),
\]

where

\[
D_\tau = A_{\tau,\tau} - U_\tau U^*_\tau A_{\tau,\tau} V_\tau V^*_\tau.
\]

Remark 3.1. A common practice is to define the telescoping factorization with \( D^{(L)} \) as the block-diagonal part of \( A \) and with \( \tilde{A}^{(L)} \) as all but the block-diagonal part of \( A \), and to define \( D^{(\ell)} \) and \( \tilde{A}^{(\ell)} \) similarly for \( \ell = 0, 1, \ldots, L-1 \). That approach, which is taken by [19], necessitates directly accessing entries of the matrix to form the matrices \( D^{(\ell)} \). Our definition of the telescoping factorization facilitates compressing the matrix while accessing it only through randomized sampling, as will become clear in later sections.
Algorithm 3.1 Apply a compressed HBS matrix to a vector: \( u = Aq \).

**Upward pass**

for level \( \ell = L, L - 1, \ldots, 1 \) do
  for node \( \tau \) in level \( L \) do
    if \( \tau \) is a leaf node then
      \( \hat{q}_\tau = V^*_{\tau} q(I_\tau) \)
    else
      Let \( \alpha \) and \( \beta \) be the children of \( \tau \).
      \( \hat{q}_\tau = V^*_{\tau} \begin{bmatrix} q_\alpha \\ q_\beta \end{bmatrix} \)
    end if
  end for
end for

**Downward pass**

for levels \( \ell = 0, 1, \ldots, L \) do
  if \( \tau \) is the root node then
    Let \( \alpha \) and \( \beta \) be the children of \( \tau \).
    \( \begin{bmatrix} \hat{u}_\alpha \\ \hat{u}_\beta \end{bmatrix} = D_\tau \begin{bmatrix} q_\alpha \\ q_\beta \end{bmatrix} \)
  else if \( \tau \) is a parent node then
    Let \( \alpha \) and \( \beta \) be the children of \( \tau \).
    \( \begin{bmatrix} \hat{u}_\alpha \\ \hat{u}_\beta \end{bmatrix} = U_\tau \hat{u}_\tau + D_\tau \begin{bmatrix} q_\alpha \\ q_\beta \end{bmatrix} \)
  else
    \( u(I_\tau) = U_\tau \hat{u}_\tau + D_\tau q(I_\tau) \)
  end if
end for

4. An algorithm for compressing HBS matrices. In this section we present the main algorithm for compressing an HBS matrix. Let \( A \) be an \( N \times N \) HBS matrix with block rank \( k \), and let \( r = k+p \), where \( p \) represents a small amount of oversampling (\( p = 5 \) or \( p = 10 \) are often sufficient). Let \( \Omega \) and \( \Psi \) be \( N \times s \) Gaussian test matrices, where \( s \geq \max(r + m, 3r) \), and define sample matrices \( Y = A\Omega \) and \( Z = A^*\Psi \). Our objective is to use the information contained in the test and sample matrices to construct a telescoping factorization of \( A \), as defined in subsection 3.3.

We begin this section by describing the process of finding the level-\( L \) basis matrices \( U^{(L)} \) and \( V^{(L)} \) and the level-\( L \) discrepancy matrix \( D^{(L)} \). Next, we describe how to proceed to coarser levels of the tree. Finally, we analyze the asymptotic complexity of the compression algorithm.

4.1. Computing basis matrices \( U, V \). We start by describing the process of computing the basis matrix \( U^{(L)} \) of the finest level, which involves finding for each \( \tau \) on level \( L \) a basis matrix \( U_\tau \) that spans the range of \( \mathbf{A}(I_\tau, I'_\tau) \) for every node \( \tau' \neq \tau \) on level \( L \). We will compute \( U_\tau \) by applying the randomized algorithm described in subsection 2.3 to \( \mathbf{A}(I_\tau, I'_\tau) \), where \( I'_\tau = I \setminus I_\tau \) is the set of indices that are not in \( I_\tau \). Importantly, the procedure does not require the ability to apply \( \mathbf{A}(I_\tau, I'_\tau) \) to random vectors; rather we compute the randomized samples only using information contained
in $\Omega$ and $Y$.

We define the following blocks of size $m \times s$ associated with $\tau$.

$$\Omega_{\tau} = \Omega(I_{\tau,:})$$

$$Y_{\tau} = Y(I_{\tau,:})$$

Since $\Omega_{\tau}$ is of size $m \times s$, it has a nullspace of dimension at least $s - m \geq r$, so we can find a set of $r$ orthonormal vectors that belong to its nullspace

$$P_{\tau} = \text{null}(\Omega_{\tau}, r)$$

so that $\Omega_{\tau} P_{\tau} = 0$.

Then $\Omega P_{\tau}$ is of size $N \times r$ with $(\Omega P_{\tau})(I_{\tau,:), :) = \Omega_{\tau} P_{\tau} = 0$, and $(\Omega P_{\tau})(I_{\tau'}, :) = 0$ is a standard Gaussian random matrix of size $(N - m) \times r$. Considering the structure of $\Omega P_{\tau}$, the product $A \Omega P_{\tau}$ can be viewed as a randomized sample of $A$, excluding contributions from columns $A(:, I_{\tau'})$. Then the rows of $A \Omega P_{\tau}$ indexed by $I_{\tau}$ contain a randomized sample of $A(I_{\tau}, :)$ for each node $\tau$ on level $L$. Moreover, since $(A \Omega P_{\tau})(I_{\tau}, :) = (YP_{\tau})(I_{\tau}, :) = Y_{\tau} P_{\tau}$, we can obtain that sample inexpensively by simply multiplying $Y_{\tau} P_{\tau}$. Then we orthonormalize the sample to find basis matrix $U_{\tau}$,

$$U_{\tau} = qr(Y_{\tau} P_{\tau}, r).$$

We repeat the same procedure to find $U_{\tau}$ for each node $\tau$ on level $L$. A similar process using $\Psi$ and $Z$ yields basis matrices $V_{\tau}$,

$$Q_{\tau} = \text{null}(\Psi_{\tau}, r)$$

$$V_{\tau} = qr(Z, Q_{\tau}, r).$$

### 4.2. Computing discrepancy matrix $D$. Once we have computed $U^{(L)}$ and $V^{(L)}$, we next compute $D^{(L)}$. We proceed by rewriting (3.4) as

$$D_{\tau} = (I - U_{\tau} U_{\tau}^{*}) A_{\tau, \tau} + U_{\tau} U_{\tau}^{*} A_{\tau, \tau'} (I - V_{\tau} V_{\tau}^{*}),$$

and deriving formulas for computing $(I - U_{\tau} U_{\tau}^{*}) A_{\tau, \tau}$ and $U_{\tau} U_{\tau}^{*} A_{\tau, \tau'} (I - V_{\tau} V_{\tau}^{*})$ separately.

For $(I - U_{\tau} U_{\tau}^{*}) A_{\tau, \tau}$, we first express $Y_{\tau}$ as a blocked matrix product

$$Y_{\tau} = \sum_{\tau'} A_{\tau', \tau} \Omega_{\tau', :}.$$

Multiplying $(I - U_{\tau} U_{\tau}^{*})$ and applying (3.1) gives

$$(I - U_{\tau} U_{\tau}^{*}) Y_{\tau} = (I - U_{\tau} U_{\tau}^{*}) A_{\tau, \tau} \Omega_{\tau}.$$

Solving a least-squares problem with $\Omega_{\tau}$ gives

$$A_{\tau, \tau'} (I - V_{\tau} V_{\tau}^{*}) = ((I - V_{\tau} V_{\tau}^{*}) Z_{\tau} \Psi_{\tau}^{*})^{*}.$$
4.3. Compressing levels $\ell = L - 1, L - 2, \ldots, 0$. After compressing level $L$, we proceed to the next coarser level $L - 1$. That is, we seek $U^{(L-1)}, V^{(L-1)}$, and $D^{(L-1)}$ that satisfy (3.3). We do so by first obtaining randomized samples of $\tilde{A}^{(L)}$, and then finding $U^{(L-1)}, V^{(L-1)}$, and $D^{(L-1)}$ using the same procedure as for level $L$.

To compute randomized samples of $\tilde{A}^{(L)}$, we multiply $\Omega$ and rearrange to obtain

$$Y = A\Omega = (U^{(L)} \tilde{A}^{(L)} (V^{(L)})^* + D^{(L)})\Omega$$

Then $(U^{(L)})^*(Y - D^{(L)}\Omega)$ contains $s$ randomized samples of $\tilde{A}^{(L)}$ with test matrix $(V^{(L)})^*\Omega$. Then for each node $\tau$ on level $L - 1$, we define

$$\Omega_\tau = \begin{bmatrix} V_\alpha^*\Omega_\alpha \\ V_\beta^*\Omega_\beta \end{bmatrix}$$
$$Y_\tau = \begin{bmatrix} U_\alpha^*(Y_\alpha - D_\alpha\Omega_\alpha) \\ U_\beta^*(Y_\beta - D_\beta\Omega_\beta) \end{bmatrix},$$

where $\alpha$ and $\beta$ are the children of $\tau$. We define $\Psi_\tau$ and $Z_\tau$ analogously. Once we have $\Omega_\tau, \Psi_\tau, Y_\tau, Z_\tau$ for each $\tau$ on level $L - 1$, we compute $U_\tau, V_\tau, \text{ and } D_\tau$ for each node $\tau$ on level $L - 1$ exactly as before using (4.1), (4.2), and (4.6).

This process is applied to successively coarser levels of the tree until the root node is reached. For the root node $\tau$, we have $Y_\tau = D^{(0)}\Omega_\tau$, so we simply solve $D^{(0)} = Y_\tau, \Omega_\tau^\dagger$. The full compression procedure is summarized in Algorithm 4.1.

**Remark 4.1.** The computation of $D_\tau$ involves solving least squares problems with Gaussian matrices $\Omega_\tau$ and $\Psi_\tau$ of size $m \times s$ or $2r \times s$. Gaussian matrices with nearly square shapes have non-negligible probabilities of being ill-conditioned, but the probabilities quickly become negligible even for slightly rectangular matrices [6, 7]. Such concerns can be alleviated by choosing $s$ to be sufficiently large. For the numerical experiments in section 5, we simply use $s = r + m = 3r$.

**Remark 4.2.** For levels $l = L - 1, L - 2, \ldots, 1$, $V^{(l)}$ depends on the draw of $\Omega$, and therefore the test matrices defined in subsection 4.3 may not exactly be standard Gaussian matrices. However, we observe empirically that the dependence is very weak, and the new test matrices behave like Gaussian test matrices.

4.4. Asymptotic complexity. We assume for simplicity that $m = 2r$ and $s = 3r$. Algorithm 4.1 requires $s$ matrix-vector products of $A$ and $A^*$, and an additional $O(r^3)$ operations for each node in the tree, of which there are approximately $2N/m$. Therefore, the total compression time is

$$T_{\text{compress}} = 6r N \times T_{\text{rand}} + 6r \times T_{\text{mult}} + O(r^2 N) \times T_{\text{flop}},$$

where $T_{\text{rand}}$ denotes the time to sample a value from the standard Gaussian distribution, $T_{\text{mult}}$ denotes the time to apply $A$ or $A^*$ to a vector, and $T_{\text{flop}}$ denotes the time to carry out a floating point arithmetic operation.

**Remark 4.3** (Comparison of information efficiency). If we view each randomized sample as carrying $N$ values worth of information about $A$, and still assume $m = 2r$ and $s = 3r$, we find that the compression algorithm requires a total of $6r N$ values to...
Algorithm 4.1 Compressing an HBS matrix

Compute randomized samples of $A$ and $A^*$. Form Gaussian random test matrices $\Omega$ and $\Psi$ of size $N \times s$. Multiply $Y = A\Omega$ and $Z = A^*\Psi$.

Compress level by level from finest to coarsest.

for level $\ell = L, L - 1, \ldots, 0$ do
    for node $\tau$ in level $\ell$ do
        if $\tau$ is a leaf node then
            $\Omega_\tau = \Omega(I_{\tau}, :)$, $\Psi_\tau = \Psi(I_{\tau}, :)$
            $Y_\tau = Y(I_{\tau}, :)$, $Z_\tau = Z(I_{\tau}, :)$
        else
            Let $\alpha$ and $\beta$ denote the children of $\tau$.
            $\Omega_\tau = \begin{bmatrix} V_\alpha^* \Omega_\alpha \\ V_\beta^* \Omega_\beta \end{bmatrix}$, $\Psi_\tau = \begin{bmatrix} U_\alpha^* \Psi_\alpha \\ U_\beta^* \Psi_\beta \end{bmatrix}$
            $Y_\tau = \begin{bmatrix} U_\alpha^* (Y_\alpha - D_\alpha \Omega_\alpha) \\ U_\beta^* (Y_\beta - D_\beta \Omega_\beta) \end{bmatrix}$, $Z_\tau = \begin{bmatrix} V_\alpha^* (Z_\alpha - D_\alpha^* \Psi_\alpha) \\ V_\beta^* (Z_\beta - D_\beta^* \Psi_\beta) \end{bmatrix}$
        end if
    end for
end for

reconstruct the matrix. The algorithm of [19] requires only $r$ samples of $A$ and $A^*$, but it also requires access to $\sim mN$ matrix entries that form the block-diagonal part of $A$ as well as $\sim rN$ elements that appear in interpolative decompositions, for a total of $5rN$ values worth of information. Therefore, the algorithm in the present work requires only slightly more information to recover $A$, while having the advantage of being truly black-box.

5. Numerical experiments. In this section, we present a selection of numerical results. In subsections 5.1 to 5.4, we report the following quantities for a number of test problems and rank structure formats: (1) the time to compress the operator, (2) the time to apply the compressed representation to a vector, (3) the relative accuracy of the compressed representation, and (4) the storage requirements of the compressed representation measured as the number of values per degree of freedom. For compression time, we report both the total time taken for compression as well as the compression time excluding the time spent by the black-box multiplication routine for computing randomized samples. The algorithms for compressing matrices and applying compressed representations are written in Python, and the black-box multiplication routines are written in MATLAB. The experiments were carried out
Fig. 3: Contour $\Gamma$ on which the BIE (5.1) is defined.

on a workstation with an Intel Core i9-10900K processor with 10 cores and 128GB of memory.

We measure the accuracy of the compressed matrices using the relative error

$$\frac{\| \tilde{A} - A \|}{\| A \|}$$

computed via 20 iterations of the power method. We also report the maximum leaf node size $m$ and the number $r$ of random vectors per test matrix, which are inputs to the compression algorithm.

5.1. Boundary integral equation. We consider a matrix arising from the discretization of the Boundary Integral Equation (BIE)

$$\frac{1}{2} q(x) + \int_{\Gamma} \frac{(x - y) \cdot n(y)}{4\pi |x - y|^2} q(y) \, ds(y) = f(x), \quad x \in \Gamma,$$

where $\Gamma$ is the simple closed contour in the plane shown in Figure 3, and where $n(y)$ is the outwards pointing unit normal of $\Gamma$ at $y$. The BIE (5.1) is a standard integral equation formulation of the Laplace equation with boundary condition $f$ on the domain interior to $\Gamma$. The BIE (5.1) is discretized using the Nyström method on $N$ equispaced points on $\Gamma$, with the Trapezoidal rule as the quadrature (since the kernel in (5.1) is smooth, the Trapezoidal rule has exponential convergence).

The fast matrix-vector multiplication is in this case furnished by the recursive skeletonization (RS) procedure of [17]. To avoid spurious effects due to the rank structure inherent in RS, we compute the matrix-vector products at close to double precision accuracy, and with an entirely uncorrelated tree structure.

Results are given in Figure 4.

Remark 5.1. The problem under consideration here is artificial in the sense that there is no actual need to use more than a couple of hundred points to resolve (5.1) numerically to double precision accuracy. It is included merely to illustrate the asymptotic scaling of the proposed method.

5.2. Operator multiplication. We next investigate how the proposed technique performs on a matrix matrix multiplication problem. Specifically, we determine the Neumann-to-Dirichlet operator $T$ for the contour shown in Figure 3 using the well known formula

$$T = S \left( \frac{1}{2} I + D^* \right)^{-1},$$
where $S$ is the single layer operator $[S q](x) = \int_{\Gamma} \frac{1}{2\pi} \log |x - y| q(y) \, ds(y)$, and where $D^*$ is the adjoint of the double-layer operator $[D^* q](x) = \int_{\Gamma} \frac{n(x) \cdot (x - y)}{2\pi |x - y|^2} q(y) \, ds(y)$. The operators $S$ and $D$ are again discretized using a Nyström method on equispaced points (with sixth order Kapur-Rokhlin [15] corrections to handle the singularity in $S$), resulting in matrices $S$ and $D$. The $(0.5I + D^*)^{-1}$ is again applied using the recursive skeletonization procedure of [17].

Results are given in Figure 5.

5.3. Fast multipole method.

5.4. Frontal matrices in nested dissection. Our next example is a simple model problem that illustrates the behavior of the proposed method in the context of sparse direct solvers. The idea here is to use rank structure to compress the increasingly large Schur complements that arise in the LU factorization of a sparse matrix arising from the finite element or finite difference discretization of an elliptic PDE, cf. [22, Ch. 21]. As a model problem, we consider an $N \times N$ matrix $C$ that encodes the stiffness matrix for the standard five-point stencil finite difference approximation to the Poisson equation on a rectangle. We use a grid with $N \times 51$ nodes. We partition the grid into three sets $\{1, 2, 3\}$, as shown in Figure 6, and then tessellate $C$ accordingly,

$$C = \begin{bmatrix} C_{11} & 0 & C_{13} \\ 0 & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix}$$
5.5. Summary of observations.

- The results exhibit linear scaling of computation time for compressing the operators and for applying the compressed representations to vectors.
- The approximations achieve high accuracy in every case.
- The asymptotic storage cost, reported as number of floating point numbers
per degree of freedom, is depends on $r$ and $m$, but is independent of the problem size $N$.

6. Conclusions. This paper presents an algorithm for black-box randomized compression of Hierarchically Block Separable matrices. To compress an $N \times N$ matrix $A$, the algorithm requires only $O(k)$ samples of $A$ and $A^*$, where $k$ is the block rank of $A$. Numerical experiments demonstrate that the algorithms are accurate and very computationally efficient, with compression time scaling linearly in $N$ when the cost of applying $A$ and $A^*$ to a vector is $O(N)$.

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