FAST SYMMETRIC FACTORIZATION OF HIERARCHICAL MATRICES WITH APPLICATIONS[*]

SIVARAM AMBIKASARAN[†] AND MICHAEL O'NEIL[†]

Abstract. We present a fast direct algorithm for computing symmetric factorizations, i.e. $A = WW^T$, of symmetric positive-definite hierarchical matrices with weak-admissibility conditions. The computational cost for the symmetric factorization scales as $\mathcal{O}(n \log^2 n)$ for hierarchically off-diagonal low-rank matrices. Once this factorization is obtained, the cost for inversion, application, and determinant computation scales as $\mathcal{O}(n \log n)$. In particular, this allows for the near optimal generation of correlated random variates in the case where A is a covariance matrix. This symmetric factorization algorithm depends on two key ingredients. First, we present a novel symmetric factorization formula for low-rank updates to the identity of the form $I + UKU^T$. This factorization can be computed in $\mathcal{O}(n)$ time, if the rank of the perturbation is sufficiently small. Second, combining this formula with a recursive divide-and-conquer strategy, near linear complexity symmetric factorizations for hierarchically structured matrices can be obtained. We present numerical results for matrices relevant to problems in probability & statistics (Gaussian processes), interpolation (Radial basis functions), and Brownian dynamics calculations in fluid mechanics (the Rotne-Prager-Yamakawa tensor).

Key words. Symmetric factorization, Hierarchical matrix, Fast algorithms, Covariance matrices, Direct solvers, Low-rank, Gaussian processes, Multivariate random variable generation, Mobility matrix, Rotne-Prager-Yamakawa tensor.

AMS subject classifications. 15A23, 15A15, 15A09

1. Introduction. This article describes a computationally efficient method for constructing symmetric factorization of large dense matrices. The symmetric factorization of large dense matrices is important in several fields, including, among others, data analysis [13, 28, 35], geostatistics [27, 34], and hydrodynamics [15, 23]. For instance, several schemes for multi-dimensional Monte Carlo simulations require drawing covariant realizations of multi-dimensional random variables. In particular, in the case where the marginal distribution of each random variable is normal, the covariant samples can be obtained by applying the *symmetric factor* of the corresponding covariance matrix to independent normal random variates. The symmetric factorization of a symmetric positive definite matrix can be computed as the factor W in $A = W^T W$. One of the major computational issues in dealing with these large covariance matrices is that they are often dense. Conventional methods of obtaining a symmetric factorization based on the Cholesky decomposition are expensive, since the computational cost scales as $\mathcal{O}(n^3)$ for a $n \times n$ matrix. Relatively recently, however, it has been observed that large dense (full-rank) covariance matrices can be efficiently represented using hierarchical decompositions [4, 5, 6, 12, 25, 30]. Taking advantage of this underlying structure, we derive a novel symmetric factorization for large dense Hierarchical Off-Diagonal Low-Rank (HODLR) matrices that scales as $\mathcal{O}(n \log^2 n)$. i.e., for a given $n \times n$ matrix A, we decompose it as $A = WW^T$. A major difference of our scheme versus the Cholesky decomposition is the fact that the matrix W is no longer a triangular matrix. In fact, the matrix W is a product of matrices that are block low-rank updates of the identity matrix, and the cost of applying the factor W to a vector scales as $\mathcal{O}(n \log n)$.

Hierarchical matrices were first introduced in the context of integral equations [19, 21] arising out of elliptic partial differential equations and potential theory. Since then, it has been observed that a large class of dense matrices arising out of boundary integral equations [24, 39], dense fill-ins in finite element matrices [7, 36], radial basis function interpolation [3], kernel density estimation in machine learning, co-variance structure in statistic models [12], Bayesian inversion [3, 5, 6], Kalman filtering [25], and Gaussian processes [4] can be efficiently represented as data-sparse hierarchical matrices. After a suitable ordering of columns and rows, these matrices can be recursively sub-divided using a tree structure and certain sub-matrices at each level in the tree can be well-represented by low-rank matrices. We refer the readers to [2, 9, 10, 11, 17, 19, 20, 21] for more details on these matrices. Depending on the tree structure and low-rank approximation technique, different hierarchical decompositions exist. For example, the original fast multipole method [18] accelerates the calculation of long-range gravitational forces for n-body problems by hierarchically compressing (via a quad- or oct-tree) certain interactions in the associated matrix operator using analytical low-rank considerations. The low-rank sparsity structure of these hierarchical matrices can be

[†]Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, N.Y. 10012, `sivaram@cims.nyu.edu`, `oneil@cims.nyu.edu`.

exploited to construct fast dense linear algebra schemes, including direct inversion, determinant computation, symmetric factorization, etc.

Most of the existing results relevant to symmetric factorization of low-rank modifications to the identity are based on rank 1 or rank r modifications to the Cholesky factorization, which are computationally expensive, i.e., their scaling is at least $\mathcal{O}(rn^2)$. We do not seek to review the entire literature here, except to direct the readers to a few references [8, 16, 22, 31]. To our knowledge, the scheme presented in this paper is the first symmetric factorization for hierarchical matrices that scales nearly linearly. In fact, replacing the HODLR structure with other (more stringent) hierarchical structures would yield linear schemes. This extension is currently under investigation. It is worth pointing out that Xia and Gu [37] discuss a Cholesky factorization for $n \times n$ Hierarchically Semi-Separable (HSS) matrices that scales as $\mathcal{O}(n^2)$.

The paper is organized as follows: Section 2 contains the key idea behind the algorithm discussed in this paper: a fast, symmetric factorization for low-rank updates to the identity. Section 3 extends the formula of Section 2 to a nested product of block low-rank updates to the identity. The details of the compatibility of this structure with HODLR matrices is discussed. Section 4 contains numerical results, accuracy and complexity scaling, of applying the factorization algorithms to matrices relevant to problems in statistics, interpolation and hydrodynamics. Section 5 summarizes the previous results and discusses further extensions and areas of ongoing research.

2. Symmetric Factorization of low-rank update. Almost all of the hierarchical factorizations are typically based on incorporating low-rank perturbations in a hierarchical manner. In this section, we briefly discuss some well-known identities which allow for the rapid inversion and determinant computation of low-rank updates to the identity matrix.

2.1. The Sherman-Morrison-Woodbury formula. If the inverse of a matrix $A \in \mathbb{R}^{n \times n}$ is already known, then the inverse of subsequent low-rank updates, for $U, V \in \mathbb{R}^{n \times p}$ and $C \in \mathbb{R}^{p \times p}$, can be calculated as

$$(2.1) \qquad \left(A + UCV^T\right)^{-1} = A^{-1} - A^{-1}U\left(C^{-1} + V^TU\right)^{-1}V^TA^{-1},$$

where we should point out that the quantity V^TU is only a $p \times p$ matrix. This formula is known as the Sherman-Morrison-Woodbury (SMW) formula. Further simplifying, in the case where $A = I$, we have

$$(2.2) \qquad \left(I + UCV^T\right)^{-1} = I - U(C^{-1} + V^TU)^{-1}V^T.$$

Note that the SMW formula shows that the inverse of a low-rank perturbation to the identity matrix is also a low-rank perturbation to the identity matrix. Furthermore, the row-space and column-space of the low-rank perturbation and its inverse are the same. The main advantage of equation (2.2) is that if $p \ll n$, we can obtain the inverse (or equivalently solve a linear system) of a rank p perturbation of an $n \times n$ identity matrix at a computational cost of $\mathcal{O}(p^2n)$. In general, if $B \in \mathbb{R}^{n \times n}$ is a low-rank perturbation of $A \in \mathbb{R}^{n \times n}$, then the inverse of B is also a low-rank perturbation of the inverse of A.

It is also worth noting that if A and B are well-conditioned, then the Sherman-Morrison-Woodbury formula is numerically stable [40]. The SMW formula has found applications in, to name a few, Kalman filters [26], recursive least-squares [14], and fast direct solvers for hierarchical matrices [3].

2.2. Sylvester's determinant theorem. Calculating the determinant of an $n \times n$ matrix A, classically, using a cofactor expansions requires $\mathcal{O}(n!)$ operations. However, if the LU or eigenvalue decomposition is obtained, this cost is reduced to $\mathcal{O}(n^3)$. Recently [4], it was shown that the determinant of HODLR matrices could be calculated in $\mathcal{O}(n \log n)$ time using Sylvester's determinant theorem [1], a formula relating the determinant of a low-rank update of the identity to the determinant of a smaller matrix. Determinants of matrices are very important in probability and statistics, in particular in Bayesian inference, as they often serve as the normalizing factor in likelihood calculations and in the evaluation of the conditional evidence.

Sylvester's determinant theorem states that for $A, B \in \mathbb{R}^{n \times p}$,

$$(2.3) \qquad \det\left(I + AB^T\right) = \det\left(I + B^TA\right),$$

where the determinant on the right hand side is only of a $p \times p$ matrix. Hence, the determinant of a rank p perturbation to an $n \times n$ identity matrix, where $p \ll n$, can be computed at a computational cost of

$\mathcal{O}(p^2 n)$. This formula has recently found applications in Bayesian statistics for computing precise values of Gaussian likelihood functions (which depend on the determinant of the corresponding covariance matrix) [4] and computing the determinant of large matrices in random matrix theory [33].

2.3. Symmetric factorization of a low-rank update. In the spirit of the Sherman-Morrison-Woodbury formula and Sylvester's determinant theorem, we obtain a formula that enables the symmetric factorization of a rank p perturbation to the $n \times n$ identity at a computational cost of $\mathcal{O}(p^2 n)$. In particular, for a symmetric positive definite (from now on abbreviated as SPD) matrix of the form $I + UKU^T$, where I is an $n \times n$ identity matrix, $U \in \mathbb{R}^{n \times p}$, $K \in \mathbb{R}^{p \times p}$, and $p \ll n$, we obtain the factorization

$$(2.4) \qquad I + UKU^T = WW^T.$$

We now state this as the following theorem.

THEOREM 2.1. *For rank p matrices $U \in \mathbb{R}^{n \times p}$ and $K \in \mathbb{R}^{p \times p}$, if the matrix $I + UKU^T$ is SPD then it can be symmetrically factored as*

$$(2.5) \qquad I + UKU^T = \left(I + UXU^T\right)\left(I + UXU^T\right)^T$$

where X is obtained as

$$(2.6) \qquad X = L^{-T}\left(M - I\right)L^{-1},$$

the matrix L is the symmetric factor of $U^T U$, and M is the symmetric factor of $I + L^T KL$, i.e.,

$$(2.7) \qquad LL^T = U^T U,$$
$$(2.8) \qquad MM^T = I + L^T KL.$$

We first prove two lemmas related to the construction of X in equation (2.6), which directly lead to the proof of Theorem 2.1. In the subsequent discussion, we will assume the following unless otherwise stated:
1. I is the identity matrix.
2. $p \ll n$.
3. $U \in \mathbb{R}^{n \times p}$ is of rank p.
4. $K \in \mathbb{R}^{p \times p}$ is of rank p.
5. $I + UKU^T$ is SPD.

It is easy to show that the last item implies that the matrix K is symmetric. The first lemma we prove relates the positivity of the smaller matrix $I + L^T KL \in \mathbb{R}^{p \times p}$ to the positivity of the larger $n \times n$ matrix, $I + UKU^T$.

LEMMA 2.2. *Let LL^T denote a symmetric factorization of $U^T U$, where $L \in \mathbb{R}^{p \times p}$. If the matrix $I + UKU^T$ is SPD (semi-definite), then $I + L^T KL$ is also SPD (semi-definite).*

Proof. To prove that $I + L^T KL$ is SPD, it suffices to prove that given any non-zero $\boldsymbol{y} \in \mathbb{R}^p$, we have $\boldsymbol{y}^T(I + L^T KL)\boldsymbol{y} > 0$. Note that since U is full rank, the matrix $U^T U$ is invertible. We now show that given any $\boldsymbol{y} \in \mathbb{R}^p$, there exists an $\boldsymbol{x} \in \mathbb{R}^n$ such that $\boldsymbol{y}^T(I + L^T KL)\boldsymbol{y} = \boldsymbol{x}^T(I + UKU^T)\boldsymbol{x}$. This will enable us to conclude that $I + L^T KL$ is positive definite since $I + UKU^T$ is positive definite. In fact, we will directly construct $\boldsymbol{x} \in \mathbb{R}^n$ such that $\boldsymbol{y}^T(I + L^T KL)\boldsymbol{y} = \boldsymbol{x}^T(I + UKU^T)\boldsymbol{x}$.

Let us begin by choosing $\boldsymbol{x} = U(U^T U)^{-1}L\boldsymbol{y}$. Then, the following two criteria are met:
(i) $\|\boldsymbol{x}\|_2 = \|\boldsymbol{y}\|_2$
(ii) $\boldsymbol{x}^T UKU^T \boldsymbol{x} = \boldsymbol{y}^T L^T KL\boldsymbol{y}$
Expanding the norm of $\boldsymbol{x}$ we have:

$$(2.9) \qquad \|\boldsymbol{x}\|_2^2 = \boldsymbol{y}^T L^T (U^T U)^{-T} \overbrace{U^T U(U^T U)^{-1}}^{I} L\boldsymbol{y}$$
$$(2.10) \qquad = \boldsymbol{y}^T L^T (U^T U)^{-T} L\boldsymbol{y}$$
$$(2.11) \qquad = \boldsymbol{y}^T L^T (LL^T)^{-T} L\boldsymbol{y}$$
$$(2.12) \qquad = \boldsymbol{y}^T L^T (L^{-T}L^{-1}) L\boldsymbol{y}$$
$$(2.13) \qquad = \|\boldsymbol{y}\|_2^2.$$

This proves criteria (i). Furthermore, by our choice of $\boldsymbol{x}$, we also have that $U^T\boldsymbol{x} = L\boldsymbol{y}$. Therefore,

$$(2.14) \qquad \boldsymbol{x}^T UKU^T \boldsymbol{x} = (U^T\boldsymbol{x})^T K(U^T\boldsymbol{x})$$

$$(2.15) \qquad = (L\boldsymbol{y})^T K(L\boldsymbol{y})$$

$$(2.16) \qquad = \boldsymbol{y}^T L^T KL\boldsymbol{y}.$$

This proves criteria (ii). From the above, we can now conclude that

$$(2.17) \qquad \boldsymbol{y}^T(I + L^T KL)\boldsymbol{y} = \boldsymbol{x}^T(I + UKU^T)\boldsymbol{x}.$$

Hence, if $I + UKU^T$ is SPD, so is $I + L^T KL$. An identical calculation proves the positive semi-definite case. $\square$

We now state and prove a lemma required for solving a quadratic matrix equation that arises in the subsequent factorization scheme.

LEMMA 2.3. *A solution X to the quadratic matrix equation*

$$(2.18) \qquad XLL^T X^T + X + X^T = K$$

with $L, K \in \mathbb{R}^{p \times p}$ and L a full rank matrix is given by

$$(2.19) \qquad X = L^{-T}(M - I)L^{-1},$$

where $M \in \mathbb{R}^{p \times p}$ is a symmetric factorization of $I + L^T KL$, that is, $MM^T = I + L^T KL$.

Proof. First note that from Lemma 2.2, since $I + L^T KL$ is positive definite, the symmetric factorization $I + L^T KL = MM^T$ exists. Now the easiest way to check if equation (2.19) satisfies equation (2.18) is to plug in the value of X from equation (2.19) in equation (2.18). This yields:

$$(2.20) \qquad XLL^T X^T = L^{-T}(M - I) \overbrace{L^{-1}L}^{I} L^T(L^{-T}(M - I)L^{-1})^T$$

$$(2.21) \qquad = L^{-T}(M - I) \underbrace{L^T L^{-T}}_{I}(M - I)^T L^{-1}.$$

Further simplifying the expression, we have:

$$(2.22) \qquad XLL^T X^T = L^{-T}(M - I)(M^T - I)L^{-1}$$

$$(2.23) \qquad = L^{-T}(MM^T - M - M^T + I)L^{-1}$$

$$(2.24) \qquad = L^{-T}(2I - M - M^T + L^T KL)L^{-1}$$

$$(2.25) \qquad = L^{-T}(I - M)L^{-1} + L^{-T}(I - M^T)L^{-1} + K$$

$$(2.26) \qquad = -X - X^T + K.$$

Therefore, we have that $XLL^T X^T + X + X^T = K$ $\square$

We are now ready to prove the main result, Theorem 2.1.

Proof. (Proof of Theorem 2.1) The proof follows immediately from the previous two lemmas. With X and L as previously defined as in equation (2.6), we have

$$(2.27) \qquad (I + UXU^T)(I + UXU^T)^T = I + U(X + X^T + XU^T UX^T)U^T$$

$$(2.28) \qquad = I + U(X + X^T + XLL^T X^T)U^T.$$

Since $X = L^{-T}(M - I)L^{-1}$ and $MM^T = I + L^T KL$, from Lemma 2.3 we have that $X + X^T + XLL^T X^T = K$. Substituting in the previous equation, we get

$$(2.29) \qquad (I + UXU^T)(I + UXU^T)^T = I + UKU^T.$$

This proves the symmetric factorization. $\blacksquare$

REMARK 2.4. *A slightly more numerically stable variant of factorization* (2.5) *is:*

$$(2.30) \qquad I + UKU^T = \left(I + Q\tilde{X}Q^T\right)\left(I + Q\tilde{X}Q^T\right)^T,$$

where Q is a unitary matrix such that $U = QR$.

REMARK 2.5. *Even though the previous theorem only addresses the symmetric factorization problem with no restrictions on the symmetric of the factors, we can also easily obtain a* square-root factorization *in a similar manner. By this we mean that for a given symmetric positive definite matrix A, one can obtain a symmetric matrix G such that $G^2 = A$. The key ingredient is obtaining a square-root factorization of a low-rank update to the identity:*

$$(2.31) \qquad I + UKU^T = (I + UXU^T)^2,$$

where X is a symmetric matrix and satisfies

$$(2.32) \qquad K = X(UU^T)X + 2X$$

The solution to equation (2.32) *is given by*

$$(2.33) \qquad X = L^{-1}(M - I)L^{-1}$$

where L and M are symmetric square-roots of U^TU and $I + LKL$:

$$(2.34) \qquad L^2 = U^TU.$$

$$(2.35) \qquad M^2 = I + LKL.$$

These factorizations can easily be obtained via a singular value or eigenvalue decomposition. This can then be combined with the recursive divide-and-conquer strategy discussed in the next section to yield an $\mathcal{O}(n\log^2 n)$ algorithm for computing square-roots of HODLR matrices.

Theorem 2.1 has the two following useful corollaries.

COROLLARY 2.6. *If $p = 1$, i.e., the perturbation to the identity in equation* (2.5) *is of rank 1, then*

$$(2.36) \qquad I + \boldsymbol{u}\boldsymbol{u}^T = (I + \alpha\boldsymbol{u}\boldsymbol{u}^T)(I + \alpha\boldsymbol{u}\boldsymbol{u}^T),$$

where $\alpha = \dfrac{\sqrt{1 + \|\boldsymbol{u}\|_2^2} - 1}{\|\boldsymbol{u}\|_2^2}$.

This result can also be found in [16]. Corollary 2.7 extends low-rank updates to SPD matrices *other* than the identity.

COROLLARY 2.7. *Given a symmetric factorization of the form WW^T, where the inverse of W can be applied fast (i.e., the linear system $W\boldsymbol{x} = \boldsymbol{y}$ can be solved fast), then a symmetric factorization of a SPD matrix of the form $WW^T + UKU^T$, where $U \in \mathbb{R}^{n\times p}$ and $p \ll n$, can also be obtained fast. For instance, if the linear system $W\boldsymbol{x} = \boldsymbol{y}$ can be solved at a computational cost of $\mathcal{O}(n)$, then the symmetric factorization $W(I + \tilde{U}X\tilde{U}^T)(I + \tilde{U}X\tilde{U}^T)^TW^T$ can also be obtained at a computational cost of $\mathcal{O}(n)$.*

A numerical example demonstrating Corollary 2.7 is contained in Section 4.1.

Note that the factorizations in equations (2.5) and (2.30) are similar to the Sherman-Morrison-Woodbury formula; in each case, the symmetric factor is a low-rank perturbation to the identity. Furthermore, the row-space and column-space of the perturbed matrix are the same as the row-space and column-space of the symmetric factors. Another advantage of the factorization in equations (2.5) and (2.30) is that the storage cost and the computational cost of applying the factor to a vector, which is of significant interest as indicated in the introduction, scales as $\mathcal{O}(pn)$.

We now describe a computational algorithm for finding the symmetric factorization described in Theorem 2.1. Algorithm 1 lists the individual steps in computing the symmetric factorization and their associated computational cost. The only computational cost is the in the computation of the matrix X in equation (2.5). Note that the dominant cost is the matrix-matrix product of an $p \times n$ matrix with a $n \times p$ matrix. The rest of the steps are performed on a lower p-dimensional space.

Algorithm 1 Symmetric factorization of $I + UKU^T$.

Step	Computation	Cost
1	Calculate $A = U^T U \in \mathbb{R}^{p \times p}$	$\mathcal{O}(p^2 n)$
2	Factor A as LL^T, where $L \in \mathbb{R}^{p \times p}$	$\mathcal{O}(p^3)$
3	Calculate $T = I + L^T K L \in \mathbb{R}^{p \times p}$	$\mathcal{O}(p^3)$
4	Factorize T as MM^T, where $M \in \mathbb{R}^{p \times p}$	$\mathcal{O}(p^3)$
5	Calculate $X = L^{-T}(M - I_p)L^{-1} \in \mathbb{R}^{p \times p}$	$\mathcal{O}(p^3)$

Algorithm 1 can be made more stable by first performing a QR decomposition of the matrix U as indicated in Equation (2.30). Here, the dominant cost is in obtaining the QR factorization of the matrix U. This is described in Algorithm 2.

Algorithm 2 Stable version of symmetric factorization of $I + UKU^T$.

Step	Computation	Cost
1	QR decompose $U = QR$, where $Q \in \mathbb{R}^{n \times p}$ and $R \in \mathbb{R}^{p \times p}$	$\mathcal{O}(p^2 n)$
2	Calculate $T = I + RKR^T \in \mathbb{R}^{p \times p}$	$\mathcal{O}(p^3)$
3	Factorize T as MM^T, where $M \in \mathbb{R}^{p \times p}$	$\mathcal{O}(p^3)$
4	Calculate $X = M - I \in \mathbb{R}^{p \times p}$	$\mathcal{O}(p)$

REMARK 2.8. *If U is rank deficient, then the reduced-rank QR decomposition must be computed. Algorithm 2 proceeds accordingly with a smaller internal rank $\tilde{p}$.*

3. Symmetric Factorization of HODLR matrices. In this section, we extend the symmetric factorization formula of the previous section to a class of hierarchically structured matrices, known as Hierarchical Off-Diagonal Low-Rank matrices.

3.1. Hierarchical Off-Diagonal Low Rank matrices. There exists a variety of hierarchically structured matrices depending on the particular matrix, choice of recursive sub-division (inherent tree structure), and low-rank sub-block compression technique (refer to Chapter 3 of [2] for more details). In this article, we will focus on a specific class of matrices known as Hierarchical Off-Diagonal Low-Rank (HODLR) matrices. Furthermore, since this article deals with SPD matrices, we shall restrict our attention to SPD-HODLR matrices. We first briefly review the HODLR matrix structure.

A matrix $A \in \mathbb{R}^{n \times n}$ is termed a 2-level HODLR matrix if it can be written in the form:

$$(3.1) \qquad A = \begin{bmatrix} A_1^{(1)} & U_1^{(1)} K_{1,2}^{(1)} V_2^{(1)^T} \\ U_2^{(1)} K_{2,1}^{(1)} V_1^{(1)^T} & A_2^{(1)} \end{bmatrix}$$

$$(3.2) \qquad = \begin{bmatrix} \begin{bmatrix} A_1^{(2)} & U_1^{(2)} K_{1,2}^{(2)} V_2^{(2)^T} \\ U_2^{(2)} K_{2,1}^{(2)} V_1^{(2)^T} & A_2^{(2)} \end{bmatrix} & U_1^{(1)} K_{1,2}^{(1)} V_2^{(1)^T} \\ U_2^{(1)} K_{2,1}^{(1)} V_1^{(1)^T} & \begin{bmatrix} A_3^{(2)} & U_3^{(2)} K_{3,4}^{(2)} V_4^{(2)^T} \\ U_4^{(2)} K_{4,3}^{(2)} V_3^{(2)^T} & A_4^{(2)} \end{bmatrix} \end{bmatrix},$$

where the off-diagonal blocks are of low-rank. Throughout this section, for pedagogical purposes, we shall assume that the rank of these off-diagonal blocks are the same at all levels. However, in practice the ranks of different blocks on different levels is determined numerically, and are frequently non-constant.

In general, for a κ-level HODLR matrix A, the ith diagonal block at level k, where $1 \le i \le 2^k$ and $0 \le k < \kappa$, denoted as $A_i^{(k)}$, can be written as

$$(3.3) \qquad A_i^{(k)} = \begin{bmatrix} A_{2i-1}^{(k+1)} & U_{2i-1}^{(k+1)} K_{2i-1,2i}^{(k+1)} V_{2i}^{(k+1)^T} \\ U_{2i}^{(k+1)} K_{2i,2i-1}^{(k+1)} V_{2i-1}^{(k+1)^T} & A_{2i}^{(k+1)} \end{bmatrix}$$
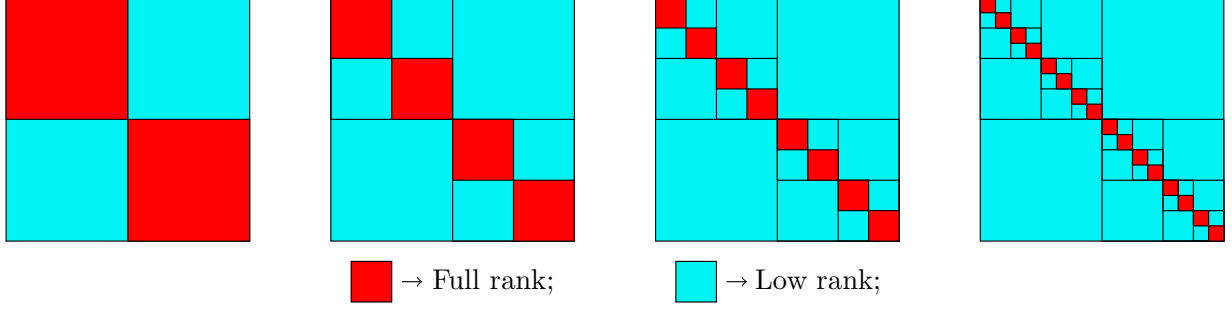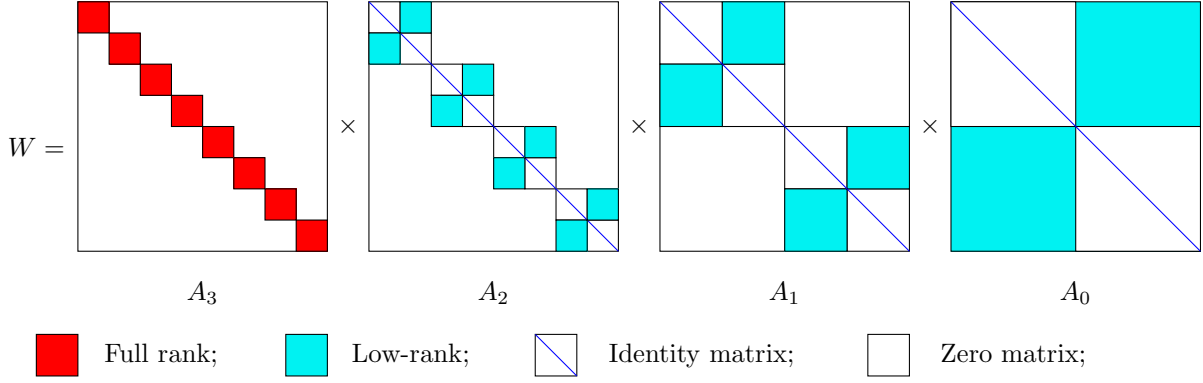
FIG. 3.1. *A HODLR matrix at different levels.*

$$W = \quad A_3 \quad \times \quad A_2 \quad \times \quad A_1 \quad \times \quad A_0$$

Full rank;   Low-rank;   Identity matrix;   Zero matrix;

FIG. 3.2. *Pictorial factorization of the W factor in equation* (3.7) *when* $\kappa = 3$.

where

$$A_i^{(k)} \in \mathbb{R}^{n/2^k \times n/2^k}, \tag{3.4}$$

$$U_{2i-1}^{(k)}, U_{2i}^{(k)}, V_{2i-1}^{(k)}, V_{2i}^{(k)} \in \mathbb{R}^{n/2^k \times p}, \tag{3.5}$$

$$K_{2i-1,2i}^{(k)}, K_{2i,2i-1}^{(k)} \in \mathbb{R}^{p \times p}, \tag{3.6}$$

and $p \ll n$. The maximum number of levels, κ, is $\lfloor \log_2(n/2p) \rfloor$. Figure 3.1 depicts the typical structure of a HODLR matrix at different levels. See [3] for details on the actual numerical decomposition of a matrix into HODLR form.

3.2. The symmetric factorization of a SPD-HODLR matrix. Given a SPD-HODLR matrix $A \in \mathbb{R}^{n \times n}$, we wish to obtain a symmetric factorization into $2\kappa + 2$ block diagonal matrices, that is we will factor A as:

$$A = \underbrace{A_\kappa A_{\kappa-1} A_{\kappa-2} \cdots A_0}_{W} \overbrace{A_0^T \cdots A_{\kappa-2}^T A_{\kappa-1}^T A_\kappa^T}^{W^T}, \tag{3.7}$$

where $A_k \in \mathbb{R}^{n \times n}$ is a block diagonal matrix with 2^k diagonal blocks each of size $\frac{n}{2^k} \times \frac{n}{2^k}$. The important feature of this factorization is that each of the diagonal blocks on all levels is a low-rank update to an identity matrix. Also, since A is symmetric, we will assume that $U_i^{(k)} = V_i^{(k)}$ and $K_{i,j}^{(k)} = K_{j,i}^{(k)}{}^T$ in Equation (3.3) for the remainder of the article. A graphical description of the W factor for a three-level SPD-HODLR matrix is shown in figure 3.2.

3.3. The algorithm. We now, in detail, describe an algorithm for computing a symmetric factorization of a SPD-HODLR matrix.

STEP 1: The first step in the algorithm is to factor out the block diagonal matrix on the leaf level, i.e., obtain any symmetric factorization of the form:

$$(3.8) \qquad \begin{bmatrix} A_{11}^{(\kappa)} & 0 & 0 & \cdots & 0 \\ 0 & A_{22}^{(\kappa)} & 0 & \cdots & 0 \\ 0 & 0 & A_{33}^{(\kappa)} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & A_{2^\kappa,2^\kappa}^{(\kappa)} \end{bmatrix} = A_\kappa A_\kappa^T$$

where

$$(3.9) \qquad A_\kappa = \begin{bmatrix} W_{11}^{(\kappa)} & 0 & 0 & \cdots & 0 \\ 0 & W_{22}^{(\kappa)} & 0 & \cdots & 0 \\ 0 & 0 & W_{33}^{(\kappa)} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & W_{2^\kappa,2^\kappa}^{(\kappa)} \end{bmatrix}$$

and $A_{ii}^{(\kappa)} = W_{ii}^{(\kappa)} W_{ii}^{(\kappa)^T}$. The computational cost of this step is $\mathcal{O}(n)$.

REMARK 3.1. *Throughout this algorithm, it is worth recalling the fact that any diagonal sub-block of a SPD matrix is also SPD.*

STEP 2: The next step is to factor out A_κ and A_κ^T from the left and right respectively, i.e., write

$$A = A_\kappa \tilde{A}_\kappa A_\kappa^T.$$

Note that when factoring out A_κ we only need to apply the inverse of $W_{ii}^{(\kappa)}$ to each of the $U_i^{(k)}$ at all levels k. Hence, we need to apply the inverse of $W_{ii}^{(\kappa)}$ to $p\kappa$ column vectors. Since the size of $W_{ii}^{(\kappa)}$ is $\mathcal{O}(p)$ and there are 2^κ such matrices, the cost of this step is $\mathcal{O}(\kappa n)$.

REMARK 3.2. *Since the matrix is symmetric, no additional work needs to be done for factoring out A_κ^T on the right.*

STEP 3: Now note that the matrix $\tilde{A}_\kappa$ can be written as

$$(3.10) \qquad \tilde{A}_\kappa = \begin{bmatrix} A_{11}^{(\kappa-1,1)} & U_1^{(\kappa-1,1)} K_{1,2}^{(\kappa-1)} U_2^{(\kappa-1,1)^T} & \cdots & \cdots \\ U_2^{(\kappa-1,1)} K_{2,1}^{(\kappa-1)} U_1^{(\kappa-1,1)^T} & A_{22}^{(\kappa-1,1)} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \cdots \\ \vdots & \vdots & \vdots & A_{2^{\kappa-1},2^{\kappa-1}}^{(\kappa-1,1)} \end{bmatrix}$$

where

$$(3.11) \qquad A_{ii}^{(\kappa-1,1)} = \begin{bmatrix} I & U_{2i-1}^{(\kappa,1)} K_{2i-1,2i}^{(\kappa)} U_{2i}^{(\kappa,1)^T} \\ U_{2i}^{(\kappa,1)} K_{2i,2i-1}^{(\kappa)} U_{2i-1}^{(\kappa,1)^T} & I \end{bmatrix}$$

and $U_j^{(k,1)}$ indicates that $U_j^{(k)}$ has been updated when factoring out A_κ. Using Theorem 2.1, we can now obtain the symmetric factorization of the diagonal blocks:

$$(3.12) \qquad \begin{bmatrix} A_{11}^{(\kappa-1,1)} & 0 & 0 & \cdots & 0 \\ 0 & A_{22}^{(\kappa-1,1)} & 0 & \cdots & 0 \\ 0 & 0 & A_{33}^{(\kappa-1,1)} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & A_{2^{\kappa-1},2^{\kappa-1}}^{(\kappa-1,1)} \end{bmatrix} = A_{\kappa-1} A_{\kappa-1}^T$$

where

$$(3.13) \qquad A_{\kappa-1} = \begin{bmatrix} W_{11}^{(\kappa-1)} & 0 & 0 & \cdots & 0 \\ 0 & W_{22}^{(\kappa-1)} & 0 & \cdots & 0 \\ 0 & 0 & W_{33}^{(\kappa-1)} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & W_{2^{\kappa-1},2^{\kappa-1}}^{(\kappa-1)} \end{bmatrix}$$

and

$$(3.14) \qquad W_{ii}^{(\kappa-1)} W_{ii}^{(\kappa-1)^T} = A_{ii}^{(\kappa-1,1)}.$$

with

$$(3.15) \qquad A_{ii}^{(\kappa-1,1)} = I + \begin{bmatrix} U_{2i-1}^{(\kappa-1,1)} & 0 \\ 0 & U_{2i}^{(\kappa-1,1)} \end{bmatrix} \begin{bmatrix} 0 & K_{2i-1,2i}^{(\kappa-1)} \\ K_{2i,2i-1}^{(\kappa-1)} & 0 \end{bmatrix} \begin{bmatrix} U_{2i-1}^{(\kappa-1,1)} & 0 \\ 0 & U_{2i}^{(\kappa-1,1)} \end{bmatrix}^T.$$

Hence, the cost of obtaining $A_{\kappa-1}$ is $\mathcal{O}(n)$.

STEP 4: As before, the next step is to factor out $A_{\kappa-1}$ and $A_{\kappa-1}^T$ from the left and right sides, respectively, i.e., write

$$(3.16) \qquad \tilde{A}_\kappa = A_{\kappa-1} \tilde{A}_{\kappa-1} A_{\kappa-1}^T$$

Indeed, we now have:

$$(3.17) \qquad A = A_\kappa A_{\kappa-1} \tilde{A}_{\kappa-1} A_{\kappa-1}^T A_\kappa^T$$

From Theorem 2.1, since $W_{ii}^{(\kappa-1)}$ is a low-rank perturbation to identity, the computational cost of applying the inverse of $W_{ii}^{(\kappa-1)}$ (using the Sherman-Morrison-Woodbury formula) to all of the $U_i^{(k,1)}$, where k ranges from 1 to $\kappa-1$, is $\mathcal{O}((\kappa-1)n/2^{\kappa-1})$. Since there are $2^{\kappa-1}$ such matrices $W_{ii}^{(\kappa-1)}$, the net cost of factoring out $A_{\kappa-1}$ is $\mathcal{O}((\kappa-1)n)$.

STEP 5: Steps 2 through 4 are repeated until we reach level 0, yielding a total computational cost of

$$(3.18) \qquad \sum_{k=0}^{\kappa} \mathcal{O}((k+1)n) = \mathcal{O}(\kappa^2 n) = \mathcal{O}(n \log^2 n),$$

where we have used the fact that $\kappa = \mathcal{O}(\log n)$.

REMARK 3.3. *If a nested low-rank structure exists for the off-diagonal blocks, i.e., if the HODLR matrix can in fact be represented as a Hierarchically Semi-Separable matrix, then the computational cost of obtaining the factorization is $\mathcal{O}(n)$.*

4. Numerical benchmarks. We first present some numerical benchmarks for the symmetric factorization of a low-rank update to a banded matrix, and then demonstrate the performance of our symmetric factorization scheme on HODLR matrices.

4.1. Fast symmetric factorization of low-rank updates to banded matrices. To highlight the computational speedup gained by this new factorization, we compare the time taken for our algorithm with the time taken for Cholesky-based factorizations for low-rank updates [32].

4.1.1. Example 1. Consider a set of n points randomly distributed in the interval $[-1,1]$. Let the i,j entry of the matrix A be given as $A(i,j) = \sigma^2 \delta_{ij} + x_i x_j$, where x_i denotes the location of the ith point. Note that the matrix A is a rank 1 update to a scaled identity matrix and can be written as $A = \sigma^2 I + \boldsymbol{x}\boldsymbol{x}^T$, where $\boldsymbol{x} = \begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix}^T$. It is easy to check that the matrix A is SPD. In fact, in the context of Gaussian processes, this is the covariance matrix that arises when using a linear covariance function given by $K(x_i, x_j) = x_i x_j$. Taking $\sigma = 1$, we have $A = I + \boldsymbol{x}\boldsymbol{x}^T$.
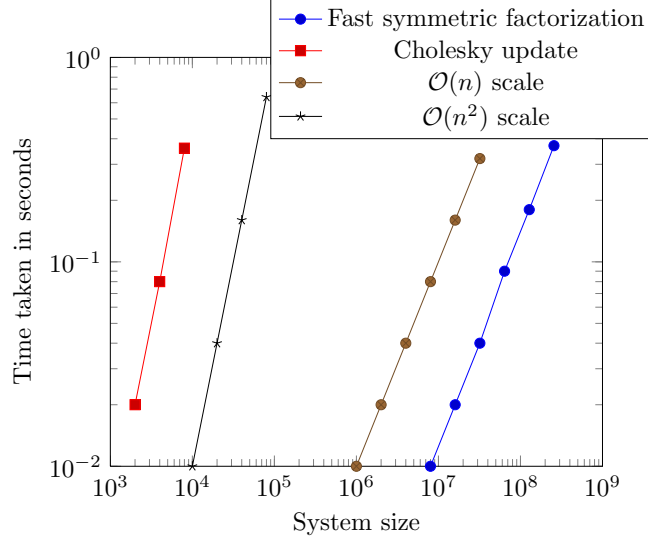
From Corollary 2.6, the only quantity we need to compute is $\alpha = \left(\sqrt{1 + \|\boldsymbol{x}\|_2^2} - 1 \right) / \|\boldsymbol{x}\|_2^2$. Figure 4.1 compares the time taken to obtain the fast symmetric factorization versus the Cholesky factorization of A.

4.1.2. Example 2. Next, we consider a rank r update to a SPD tridiagonal matrix:

$$(4.1) \qquad\qquad\qquad\qquad A = T + UU^T$$

where $U \in \mathbb{R}^{n \times r}$ and $T \in \mathbb{R}^{n \times n}$ is a tridiagonal matrix with entries given as:

$$(4.2) \qquad\qquad\qquad T(i,j) = \begin{cases} 1 & \text{if } i = j = 1 \\ 2 & \text{if } i = j > 1 \\ -1 & \text{if } |i - j| = 1 \\ 0 & \text{otherwise.} \end{cases}$$

Note that the Cholesky factorization of $T = LL^T$ is

$$(4.3) \qquad\qquad\qquad L(i,j) = \begin{cases} 1 & \text{if } i = j \\ -1 & \text{if } i - j = 1 \\ 0 & \text{otherwise,} \end{cases}$$

where $L \in \mathbb{R}^{n \times n}$. The first step to obtain the symmetric factorization of $LL^T + UU^T$ is to first factor out L to obtain

$$(4.4) \qquad\qquad\qquad LL^T + UU^T = L(I + \tilde{U}\tilde{U}^T)L^T,$$

$$(4.5) \qquad\qquad\qquad\qquad L\tilde{U} = U.$$

The next step is to obtain the symmetric factorization of $I + \tilde{U}\tilde{U}^T$ as $(I + \tilde{U}X\tilde{U}^T)(I + \tilde{U}X^T\tilde{U}^T)$. Now the symmetric factorization of $T + UU^T$ is given as

$$(4.6) \qquad\qquad\qquad T + UU^T = (I + \tilde{U}X\tilde{U}^T)(I + \tilde{U}X\tilde{U}^T)^T L^T.$$

Figure 4.2 compares the time taken versus system size for different low-rank perturbation, while Figure 4.3 fixes the system size and plots the time taken to obtain the symmetric factorization versus the rank of the low-rank perturbation.
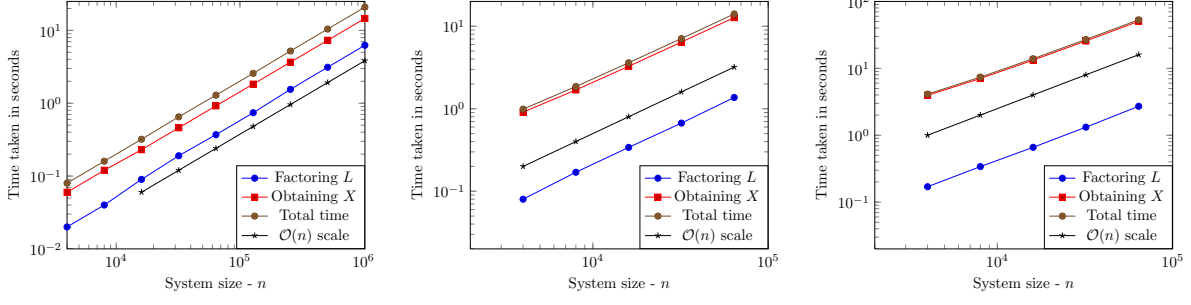
FIG. 4.2. *Time taken (in secs) by the algorithm for Example 4.1.2 with different ranks r. Left: $r = 25$, Middle: $r = 100$, Right: $r = 200$.*
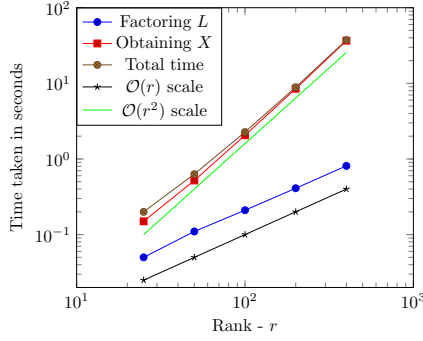

FIG. 4.3. *Time taken (in secs) by the algorithm for Example 4.1.2 with $n = 10000$.*

4.2. Fast symmetric factorization of HODLR matrices. We now present numerical benchmarks for applying our symmetric factorization algorithm to Hierarchical Off-Diagonal Low-Rank Matrices. In particular, we show results for symmetrically factorizing covariance matrices and the *mobility matrix* encountered in hydrodynamic fluctuations.

Section 4.2.1 contains results for applying the algorithm to a covariance matrix whose entires are obtained by evaluating a Gaussian covariance kernel acting on data-points in three dimensions. The following section, Section 4.2.2 contains analogous results for the covariance matrix obtained from a biharmonic covariance kernel evaluated on data-points in one and two dimensions. In fact, this matrix also occurs when performing second-order radial basis function interpolation. Finally, in Section 4.2.3 we apply the algorithm of this paper to the Rotne-Prager-Yamakawa (RPY) tensor. This tensor serves as a model for the hydrodynamic forces between spheres of constant radii. We distribute sphere locations along one-, two-, and three-dimensional manifolds all embedded in three dimensions.

In all numerical examples, the error provided is the approximate relative l_2 precision in the solution to a test problem $K\boldsymbol{x} = \boldsymbol{y}$, where $\boldsymbol{y}$ was generated *a priori* by applying the matrix K to a known vector $\boldsymbol{x}$. The points in all dimensions are ordered based on a k-d tree. The low-rank decomposition of the off-diagonal blocks is obtained using a slight modification of the adaptive cross approximation [29, 41] algorithm, which is essentially a variant of the partially pivoted LU algorithm.

4.2.1. A Gaussian covariance kernel. Covariance matrices constructed using positive definite parametric covariance kernels arise frequently when performing nonparametric regression using Gaussian processes. Related results for similar algorithms can be found in [4]. The entries of covariance matrices corresponding to a Gaussian covariance kernel are calculated as

$$(4.7) \qquad\qquad K(i,j) = \sigma^2 \delta_{ij} + \exp\left(-\|r_i - r_j\|^2\right),$$

where σ^2 is proportional to the inherent measurement noise in the underlying regression model. In our numerical experiments, we set $\sigma = 1$ and distribute the points r_i randomly in the cube $[-3,3] \times [-3,3] \times [-3,3]$. The timings relevant to this matrix are presented in Table 4.1.

System size	Time (in secs)	Error
10000	19.4	10^{-11}
20000	39.9	10^{-10}
50000	91.3	10^{-8}
100000	193.2	10^{-8}

4.2.2. A biharmonic covariance kernel. As in the previous section, a covariance matrices arising in Gaussian processes can be modeled using the biharmonic covariance kernel, where the i, j entry is given as

$$(4.8) \qquad\qquad K(i,j) = \sigma^2 \delta_{ij} + \frac{r_{ij}^2}{a^2} \log\left(\frac{r_{ij}}{a}\right),$$

where the parameters σ and a are chosen so that the matrix is positive definite. For $\sigma = a = 1$, Table 4.2 summarizes the results.

4.2.3. The Rotne-Prager-Yamakawa tensor. The RPY diffusion tensor is frequently used to model the hydrodynamic interactions in simulations of Brownian dynamics. The RPY tensor is defined as

$$(4.9) \qquad D_{ij} = \begin{cases} \dfrac{k_B T}{6\pi\eta a}\left[\left(1 - \dfrac{9}{32}\dfrac{r_{ij}}{a}\right)\mathbf{I} + \dfrac{3}{32a}\dfrac{\mathbf{r}_{ij}\otimes\mathbf{r}_{ij}}{r_{ij}}\right] & r < 2a, \\[3ex] \dfrac{k_B T}{8\pi\eta r_{ij}}\left[\mathbf{I} + \dfrac{\mathbf{r}_{ij}\otimes\mathbf{r}_{ij}}{r_{ij}^2} + \dfrac{2a^2}{3r_{ij}^2}\left(\mathbf{I} - 3\dfrac{\mathbf{r}_{ij}\otimes\mathbf{r}_{ij}}{r_{ij}^2}\right)\right] & r \geq 2a, \end{cases}$$

where k_B is the Boltzmann constant, T is the absolute temperature, η is the viscosity of the fluid a is the hydrodynamic radius of the particles, r_{ij} is the distance between the ith and j^{th} particle and $\mathbf{r}_{ij}$ is the vector connecting the ith and j^{th} particles. The tensor is obtained as an approximation to the Stokes flow around two spheres by neglecting the hydrodynamic rotation-rotation and rotation-translation coupling. The resulting matrix is often referred to as the mobility matrix. It has been shown in [38] that this tensor is positive definite for all particle configurations. Fast symmetric factorizations of the RPY tensor are crucial in Brownian dynamics simulations. Geyer and Winter [15] discuss an $\mathcal{O}(n^2)$ algorithm for approximating the square-root of the RPY tensor. Jiang et al. [23] discuss an approximate algorithm, which relies on a Chebyshev spectral approximation of the matrix square-root coupled with a fast multipole method. Their method scales as $\mathcal{O}(\sqrt{\kappa}n)$, where κ is the condition number of the RPY tensor. Our algorithm scales as $\mathcal{O}(n\log^2 n)$ if the particles are located along a line, $\mathcal{O}(n^2)$ if the particles are distributed on a surface, and as $\mathcal{O}(n^{7/3})$, if the particles are distributed in a three-dimensional volume.

REMARK 4.1. *Note that since the RPY tensor is singular, on* 2*D and* 3*D manifolds the ranks of the off-diagonal blocks would grow as* $\mathcal{O}(n^{1/2})$ *and* $\mathcal{O}(n^{2/3})$, *respectively. Since the computational cost of the symmetric factorization scales as* $\mathcal{O}(p^2 n)$, *the computational cost for the symmetric factorization to scale as* $\mathcal{O}(n^2)$ *and* $\mathcal{O}(n^{7/3})$ *on* 2*D and* 3*D manifolds, respectively. The numerical benchmarks also validate this scaling of our algorithm in all three configurations.*

5. Conclusion. The article discusses a fast symmetric factorization for a class of symmetric positive definite hierarchically structured matrices. Our symmetric factorization algorithm is based on two ingredients: a novel formula for the symmetric factorization of a low-rank update to the identity, and a recursive divide-and-conquer strategy compatible with hierarchically structures matrices.

In the case where the hierarchical structure present is that of Hierarchically Off-Diagonal Low-Rank matrices, the algorithm scales as $\mathcal{O}(n\log^2 n)$. The numerical benchmarks for dense covariance matrix examples validate the scaling. Furthermore, we also applied the algorithm to the mobility matrix encountered in Brownian-hydrodynamics, elements of which are computed from the Rotne-Prager-Yamakawa tensor. In this case, since the ranks of off-diagonal blocks scale as $\mathcal{O}(n^{2/3})$, when the particles are on a three-dimensional manifold, the algorithm scales as $\mathcal{O}(n^{7/3})$. Obtaining an $\mathcal{O}(n)$ symmetric factorization for the mobility matrix is a subject of ongoing research within our group.

TABLE 4.2

Biharmonic kernel: In $1D$ the points are distributed in interval $[-1, 1]$ and in $2D$ the points are distributed in $[-1, 1]^2$.

System size	1D		2D	
	Time (in secs)	Error	Time (in secs)	Error
10000	0.15	10^{-12}	5.5	10^{-11}
20000	0.34	10^{-13}	11.98	10^{-9}
50000	0.98	10^{-11}	31.22	10^{-10}
100000	2.24	10^{-10}	81.48	10^{-8}
200000	5.02	–	193.23	–
500000	18.34	–	545.98	–
1000000	42.34	–	1312.87	–

TABLE 4.3

RPY tensor. Particles are distributed along $1D$, $2D$ and $3D$ manifolds. Note that the system size is $n \times n$, $2n \times 2n$ and $3n \times 3n$ respectively. The time taken to obtain the symmetric factorization along with the relative error is reported in the table.

# particles	1D		2D		3D	
	Time (in secs)	Error	Time (in secs)	Error	Time (in secs)	Error
10000	0.19	10^{-12}	15.22	10^{-11}	117.34	10^{-9}
20000	0.44	10^{-10}	50.44	10^{-9}	566.32	10^{-8}
50000	1.51	10^{-9}	305.21	10^{-9}	2701.92	10^{-7}
100000	3.36	10^{-8}	1152.73	10^{-8}	–	–
200000	7.23	–	–	–	–	–
500000	23.45	–	–	–	–	–
1000000	54.67	–	–	–	–	–

It is also worth noting that with nested low-rank basis of the off-diagonal blocks, i.e., if the HODLR matrices are assumed to have an Hierarchical Semi-Separable structure instead, then the computational cost of the algorithm would scale as $\mathcal{O}(p^2 n)$. Extension to this case is relatively straightforward.

References.

[1] Alkiviadis G Akritas, Evgenia K Akritas, and Genadii I Malaschonok. Various proofs of Sylvester's (determinant) identity. *Mathematics and Computers in Simulation*, 42(4):585–593, 1996.

[2] Sivaram Ambikasaran. *Fast Algorithms for Dense Numerical Linear Algebra*. PhD thesis, Stanford University, August 2013.

[3] Sivaram Ambikasaran and Eric Darve. An $\mathcal{O}(n \log n)$ fast direct solver for partial hierarchically semi-separable matrices. *Journal of Scientific Computing*, pages 1–25, 2013.

[4] Sivaram Ambikasaran, Daniel Foreman-Mackey, Leslie Greengard, David W Hogg, and Michael O'Neil. Fast direct methods for Gaussian processes and the analysis of NASA *Kepler* mission data. *arXiv preprint arXiv:1403.6015*, 2014.

[5] Sivaram Ambikasaran, Judith Yue Li, Peter K Kitanidis, and Eric Darve. Large-scale stochastic linear inversion using hierarchical matrices. *Computational Geosciences*, 17(6):913–927, 2013.

[6] Sivaram Ambikasaran, Arvind Krishna Saibaba, Eric F Darve, and Peter K Kitanidis. Fast algorithms for Bayesian inversion. In *Computational Challenges in the Geosciences*, pages 101–142. Springer, 2013.

[7] Amirhossein Aminfar, Sivaram Ambikasaran, and Eric Darve. A fast block low-rank dense solver with applications to finite-element matrices. *arXiv preprint arXiv:1403.5337*, 2014.

[8] Åke Björck and Sven Hammarling. A Schur method for the square root of a matrix. *Linear algebra and its applications*, 52:127–140, 1983.

[9] Steffen Börm, Lars Grasedyck, and Wolfgang Hackbusch. Hierarchical matrices. *Lecture notes*, 21, 2003.

[10] Shivkumar Chandrasekaran, Patrick Dewilde, Ming Gu, William Lyons, and Timothy Pals. A fast solver for HSS representations via sparse matrices. *SIAM Journal on Matrix Analysis and Applications*, 29(1):67–81, 2006.

[11] Shivkumar Chandrasekaran, Ming Gu, and Timothy Pals. A fast ULV decomposition solver for hierarchi-

cally semiseparable representations. *SIAM Journal on Matrix Analysis and Applications*, 28(3):603–622, 2006.

[12] Jie Chen. Data structure and algorithms for recursively low-rank compressed matrices. *Argonne National Laboratory*, 2014.

[13] Andrzej Cichocki, Rafal Zdunek, Anh Huy Phan, and Shunichi Amari. *Nonnegative matrix and tensor factorizations: applications to exploratory multi-way data analysis and blind source separation.* John Wiley & Sons, 2009.

[14] Matthieu Geist and Olivier Pietquin. Statistically linearized recursive least squares. In *Machine Learning for Signal Processing (MLSP), 2010 IEEE International Workshop on*, pages 272–276. IEEE, 2010.

[15] Tihamér Geyer and Uwe Winter. An $\mathcal{O}(n^2)$ approximation for hydrodynamic interactions in brownian dynamics simulations. *The Journal of chemical physics*, 130(11):114905, 2009.

[16] Philip E Gill, Gene H Golub, Walter Murray, and Michael A Saunders. Methods for modifying matrix factorizations. *Mathematics of Computation*, 28(126):505–535, 1974.

[17] Lars Grasedyck and Wolfgang Hackbusch. Construction and arithmetics of $\mathcal{H}$-matrices. *Computing*, 70(4):295–334, 2003.

[18] Leslie Greengard and Vladimir Rokhlin. A fast algorithm for particle simulations. *Journal of Computational Physics*, 73(2):325–348, 1987.

[19] Wolfgang Hackbusch. A sparse matrix arithmetic based on $\mathcal{H}$-matrices. Part I: Introduction to $\mathcal{H}$-matrices. *Computing*, 62(2):89–108, 1999.

[20] Wolfgang Hackbusch and Steffen Börm. Data-sparse approximation by adaptive $\mathcal{H}^2$-matrices. *Computing*, 69(1):1–35, 2002.

[21] Wolfgang Hackbusch and Boris N Khoromskij. A sparse $\mathcal{H}$-matrix arithmetic. *Computing*, 64(1):21–47, 2000.

[22] Nicholas J Higham. Newton's method for the matrix square root. *Mathematics of Computation*, 46(174):537–549, 1986.

[23] Shidong Jiang, Zhi Liang, and Jingfang Huang. A fast algorithm for brownian dynamics simulation with hydrodynamic interactions. *Mathematics of Computation*, 82(283):1631–1645, 2013.

[24] Lai Jun, Sivaram Ambikasaran, and Leslie F Greengard. A fast direct solver for high frequency scattering from a large cavity in two dimensions. *arXiv preprint arXiv:1404.3451*, 2014.

[25] Judith Y Li, Sivaram Ambikasaran, Eric F Darve, and Peter K Kitanidis. A Kalman filter powered by $\mathcal{H}^2$-matrices for quasi-continuous data assimilation problems. *arXiv preprint arXiv:1403.5337*, 2014.

[26] Jan Mandel. *Efficient implementation of the ensemble Kalman filter.* University of Colorado at Denver and Health Sciences Center, Center for Computational Mathematics, 2006.

[27] Georges Matheron. Principles of geostatistics. *Economic geology*, 58(8):1246–1266, 1963.

[28] V Paul Pauca, Jon Piper, and Robert J Plemmons. Nonnegative matrix factorization for spectral data analysis. *Linear algebra and its applications*, 416(1):29–47, 2006.

[29] Sergej Rjasanow. Adaptive cross approximation of dense matrices. *IABEM 2002, International Association for Boundary Element Methods*, 2002.

[30] Arvind Krishna Saibaba, Sivaram Ambikasaran, Judith Yue Li, Peter K Kitanidis, and Eric F Darve. Application of hierarchical matrices to linear inverse problems in geostatistics. *Oil and Gas Science and Technology-Revue de l'IFP-Institut Francais du Petrole*, 67(5):857, 2012.

[31] Matthias Seeger et al. Low rank updates for the Cholesky decomposition. *University of California at Berkeley, Tech. Rep*, 2007.

[32] G. W. Stewart. *Matrix Algorithms, Volume 1: Basic Decompositions*, SIAM, Philadelphia, PA, 1998.

[33] Terence Tao. *Topics in random matrix theory*, volume 132. American Mathematical Soc., 2012.

[34] Hans Wackernagel. *Multivariate geostatistics.* Springer, 2003.

[35] Dingding Wang, Tao Li, Shenghuo Zhu, and Chris Ding. Multi-document summarization via sentence-level semantic analysis and symmetric matrix factorization. In *Proceedings of the 31st annual international ACM SIGIR conference on Research and development in information retrieval*, pages 307–314. ACM, 2008.

[36] Jianlin Xia, Shivkumar Chandrasekaran, Ming Gu, and Xiaoye S Li. Superfast multifrontal method for large structured linear systems of equations. *SIAM Journal on Matrix Analysis and Applications*, 31(3):1382–1411, 2009.

[37] Jianlin Xia and Ming Gu. Robust approximate Cholesky factorization of rank-structured symmetric

positive definite matrices. *SIAM Journal on Matrix Analysis and Applications*, 31(5):2899–2920, 2010.

[38] Hiromi Yamakawa. Transport properties of polymer chains in dilute solution: hydrodynamic interaction. *The Journal of Chemical Physics*, 53(1):436–443, 2003.

[39] Lexing Ying. Fast algorithms for boundary integral equations. In *Multiscale Modeling and Simulation in Science*, pages 139–193. Springer, 2009.

[40] EL Yip. A note on the stability of solving a rank-p modification of a linear system by the Sherman-Morrison-Woodbury formula. *SIAM Journal on Scientific and Statistical Computing*, 7(2):507–513, 1986.

[41] Kezhong Zhao, Marinos N Vouvakis, and J-F Lee. The adaptive cross approximation algorithm for accelerated method of moments computations of emc problems. *Electromagnetic Compatibility, IEEE Transactions on*, 47(4):763–773, 2005.