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Some properties of generalized K-centrosymmetric H-matrices

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Abstract

Every $n \times n$ generalized K-centrosymmetric matrix A can be reduced into a 2×2 block diagonal matrix (see [Z. Liu, H. Cao, H. Chen, A note on computing matrix–vector products with generalized centrosymmetric (centrohermitian) matrices, Appl. Math. Comput. 169 (2) (2005) 1332–1345]). This block diagonal matrix is called the reduced form of the matrix A. In this paper we further investigate some properties of the reduced form of these matrices and discuss the square roots of these matrices. Finally exploiting these properties, the development of structure-preserving algorithms for certain computations for generalized K-centrosymmetric H-matrices is discussed.

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1. Introduction

A matrix A is said to be (*skew-*)*centrosymmetric* if $A = JAJ$ $(A = -JAJ)$, where J is the exchange matrix with ones on the anti-diagonal (lower left to upper right) and zeros elsewhere. This class of matrices find use, for example, in digital signal processing [3], in the numerical solution of certain differential equations [2], in Markov processes [25] and in various physics and engineering problems [9]. See [19] for some properties of centrosymmetric matrices.

Generalized versions of these matrices have been defined in [2,15,20,23].

Definition 1. A matrix $A \in \mathbb{R}^{n\times n}$ is said to be *generalized K-centrosymmetric* if $A = KAK$, and *generalized K-skew-centrosymmetric* if $A = -KAK$, where $K \in \mathbb{P}^{n\times n}$ can be any permutation matrix which is the product of disjoint transpositions (i.e., $K^2 = I$ and $K = K^{\mathrm{T}}$).

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Mirrorsymmetric matrices are a special subclass of generalized K-centrosymmetric matrices with

$$K = \begin{bmatrix} & & J_k \\ & I_p & \\ J_k & & \end{bmatrix}, \quad n = 2k + p,$$

where I_p is the $p \times p$ identity matrix and J_k is the $k \times k$ exchange matrix. They play a role in the analysis of multiconductor transmission line equations [16].

The blurring matrices arising in image reconstruction [7,17] are also a special subclass of generalized K-centrosymmetric matrices with

$$K = \begin{bmatrix} J_l & & & & \\ & \cdot & & & \\ & & J_l & & \\ & & & \cdot & \\ & & & & J_l \end{bmatrix}. \tag{1.1}$$

Symmetric block Toeplitz matrices form another important subclass of generalized K-centrosymmetric matrices with

$$K = \begin{bmatrix} & & & & I_l \\ & & & \cdot & \\ & & I_l & & \\ & \cdot & & & \\ I_l & & & & \end{bmatrix}.$$

They appear in signal processing, trigonometric moment problems, integral equations and elliptic partial differential equations with boundary conditions, solved by means of finite differences, see for instance [6,11,12,24].

This paper focuses on generalized K-centrosymmetric H-matrices. In next section we review the definitions of H-matrices, and some basic properties of these matrices, as well as a reduced form of generalized K-centrosymmetric matrices. Some properties of the reduced form of generalized K-centrosymmetric H-matrices will be investigated in Section 3 and the square root of a generalized K-centrosymmetric is discussed in Section 4. Finally, exploiting these properties discussed in preceding two sections, we develop effective algorithms for different computational tasks: for constructing an incomplete LU factorization of a generalized K-centrosymmetric H-matrix with positive diagonal entries, for iteratively solving linear systems with a generalized K-centrosymmetric H-matrix as coefficient matrix, and for computing the principal square root of a generalized K-centrosymmetric H-matrix with positive diagonal entries.

2. Preliminaries

In this section we begin with some basic notation frequently used in the sequel (see, e.g., [4]). For definiteness, matrices throughout this paper are assumed to be real, and the matrix K denotes a fixed permutation matrix of order n consisting of the product of disjoint transpositions.

Definition 2. A matrix $A = (a_{ij})$ is called: a *Z-matrix* if $a_{ij} \leqslant 0$ for $i \neq j$; an *M-matrix* if A is a Z-matrix and $A^{-1} \geqslant 0$; an *H-matrix* if its comparison matrix $\langle A \rangle$ is an M-matrix, where $\langle A \rangle = (\alpha_{ij})$ with $\alpha_{ii} = |a_{ii}|$ for $i = j$, $\alpha_{ij} = -|a_{ij}|$ for $i \neq j$.

Definition 3. An $n \times n$ matrix A is called a generalized K-centrosymmetric H-matrix if it is an H-matrix and also generalized K-centrosymmetric.

Generalized K-centrosymmetric H-matrices are of interest in, e.g., image reconstruction [7,17]: the problem of high-resolution image reconstruction usually reduces to solving the following linear system:

$$Ex = \hat{b}, \tag{2.1}$$

where E is the blurring matrix which is a generalized K-centrosymmetric matrix with $K = \mathrm{Bdiag}(J_l, \ldots, J_l)$ as in (1.1). The system in (2.1) is ill-conditioned and susceptible to noise. The common scheme to remedy this is to use the

Tikhonov regularization which solves the system

$$Fx = b, \tag{2.2}$$

where $F = E^{\mathrm{T}}E + \beta R$, $b = E^{\mathrm{T}}\hat{b}$, R is a regularization operator (usually chosen to be the identity operator or some differential operators) and $\beta > 0$ is the regularization parameter, see [7]. The coefficient matrix F in (2.2) is a generalized K-centrosymmetric matrix for periodic or symmetric boundary condition, where $K = \mathrm{Bdiag}(J_l, \dots, J_l)$ as in (1.1). Furthermore, if β is chosen to be large enough, then F is a generalized K-centrosymmetric H-matrix with positive diagonal entries.

Another example is the well-known block tridiagonal matrix $T = \mathrm{Btridiag}\,(-I, D, -I)$, which is a symmetric block Toeplitz matrix obtained from the second-order elliptic partial differential equation via a difference scheme, where $D = \mathrm{tridiag}(-1, 4, -1)$ is a tridiagonal centrosymmetric matrix of order l. Obviously, such a matrix T is a generalized centrosymmetric H-matrix.

Some basic results for M-matrices (see for instance [4]) used in the sequel are given next.

Lemma 1. 1. *Let A be a Z-matrix, then A is an M-matrix if and only if there exists a nonnegative vector x such that* $Ax > 0$.

2. *Let B and C be two M-matrices. If $B \leqslant A \leqslant C$, then A is an M-matrix.*

3. *Let A be an M-matrix, then all the principal submatrices of any order are M-matrices.*

Some useful facts about generalized K-centrosymmetric matrices can be found in [20]. We will briefly recall those needed here.

Lemma 2. *Let K be a fixed permutation matrix as in Definition* 1.

1. *If C is an $n \times n$ generalized K-centrosymmetric matrix, then its comparison matrix $\langle C \rangle$ and its transpose C^{T} are generalized K-centrosymmetric. Also, if C is nonsingular, then C^{-1} is generalized K-centrosymmetric.*
2. *If E and $F \in \mathbb{R}^{n\times n}$ are generalized K-centrosymmetric matrices, then $E \pm F$ and EF are generalized K-centrosymmetric matrices respectively too.*

In particular, in [20] it is shown that every $n \times n$ generalized K-centrosymmetric matrix can be reduced to a 2×2 block diagonal matrix by a simple similarity transformation. As we will make use of the reduction later on, we restate the derivation in the following:

The matrix K is a permutation matrix consisting of the product of disjoint transpositions. Hence, without loss of generality, we can assume that

$$K = P_{j_1,\kappa(j_1)} P_{j_2,\kappa(j_2)} \cdots P_{j_l,\kappa(j_l)}, \quad l \leqslant n,$$

where P_{ij} is the transposition which interchanges the rows i and j and $j_i \neq \kappa(j_i)$ for $i = 1, \dots, l$ (that is we do not allow for $P_{u,\kappa(u)} = I$, when $u = \kappa(u)$).

Define $Q^{(j_i,\kappa(j_i))}$ as the matrix that differs from the identity in the four entries

$$\begin{bmatrix} Q_{j_i,j_i} & Q_{j_i,\kappa(j_i)} \\ Q_{\kappa(j_i),j_i} & Q_{\kappa(j_i),\kappa(j_i)} \end{bmatrix} = \begin{bmatrix} \dfrac{\sqrt{2}}{2} & \dfrac{\sqrt{2}}{2} \\ \dfrac{\sqrt{2}}{2} & -\dfrac{\sqrt{2}}{2} \end{bmatrix}. \tag{2.3}$$

$Q^{(j_i,\kappa(j_i))}$ is an orthogonal matrix and for $i, s = 1, \dots, l$,

$$Q^{(j_i,\kappa(j_i))} Q^{(j_s,\kappa(j_s))} = Q^{(j_s,\kappa(j_s))} Q^{(j_i,\kappa(j_i))}.$$

The product of all these rank-2 modifications of the identity

$$\tilde{Q} = Q^{(j_1,\kappa(j_1))} Q^{(j_2,\kappa(j_2))} \cdots Q^{(j_l,\kappa(j_l))} \tag{2.4}$$

yields an orthogonal matrix $\tilde{Q}$. Let $\tilde{P}$ be a permutation matrix such that in $Q=\tilde{Q}\tilde{P}$ the columns of $\tilde{Q}$ are interchanged such that the columns $\kappa(j_1), \kappa(j_2), \ldots, \kappa(j_l)$ of $\tilde{Q}$ become the columns $n-l+1, n-l+2, \ldots, n$ of a new matrix Q. Partition Q as

$$Q=\tilde{Q}\tilde{P}=[Q_1, Q_2], \tag{2.5}$$

where Q_1 denotes the matrix consisting of the first $n-l$ columns of Q and Q_2 denotes the matrix consisting of the last l columns of Q.

Define

$$K_1=\tfrac{1}{2}(I+K), \quad K_2=\tfrac{1}{2}(I-K). \tag{2.6}$$

It is easy to check that the matrices Q_1 and Q_2 are the maximum rank factorizations of the matrices K_1 with $\operatorname{rank}(K_1)=n-l$ and K_2 with $\operatorname{rank}(K_2)=l$ in (2.6), respectively; $Q_1Q_1^{\mathrm{T}}=K_1$ and $Q_2Q_2^{\mathrm{T}}=K_2$.

Lemma 3 ([20, Theorem 1]). *Let K be a fixed permutation matrix of order n and Q be defined as in* (2.5). *Then $A\in\mathbb{R}^{n\times n}$ is a generalized K-centrosymmetric matrix if and only if*

$$Q^{\mathrm{T}}AQ=\begin{bmatrix} B & \\ & C \end{bmatrix}, \tag{2.7}$$

where $B\in\mathbb{R}^{(n-l)\times(n-l)}$ and $C\in\mathbb{R}^{l\times l}$ with $l=\operatorname{rank}(K_2)$ and K_2 is defined as in (2.6).

We will refer to the matrix on the right-hand side of Eq. (2.7) as the reduced form of the matrix A, under the orthogonal similarity transformation with the orthogonal matrix Q (2.5).

3. Some properties of the reduced form

In this section we will investigate some properties of the reduced form of generalized K-centrosymmetric matrices. Note that if a generalized K-centrosymmetric matrix A is nonsingular, symmetric or positive definite respectively, then due to the orthogonal similarity, the reduced form (2.7) has the same structure, that is, these properties are preserved in the reduced form. In particular, we will see that the reduced form (2.7) of a generalized K-centrosymmetric H-matrix is an H-matrix.

Theorem 1. *Assume that $A\in\mathbb{R}^{n\times n}$ is a generalized K-centrosymmetric H-matrix and the orthogonal matrix Q is as defined in* (2.5). *Then the reduced form* (2.7) *of the matrix A is an H-matrix.*

Proof. As $A=(a_{ij})_{i,j=1,\ldots,n}$ is a generalized K-centrosymmetric H-matrix, by Lemma 2 and by the definition of an H-matrix, we have that the comparison matrix $\langle A\rangle=(\alpha_{ij})$ of the matrix A is a generalized K-centrosymmetric M-matrix and thus Lemma 3 yields

$$Q^{\mathrm{T}}\langle A\rangle Q=\begin{bmatrix} \hat{B} & \\ & \hat{C} \end{bmatrix}, \tag{3.1}$$

where $\hat{B}=Q_1^{\mathrm{T}}\langle A\rangle Q_1\in\mathbb{R}^{(n-l)\times(n-l)}$ and $\hat{C}=Q_2^{\mathrm{T}}\langle A\rangle Q_2\in\mathbb{R}^{l\times l}$ with Q_1, Q_2 as in (2.5) and $l=\operatorname{rank}(I-K)$.

Next we show that $\hat{B}=(\hat{b}_{uv})_{u,v=1,\ldots,n-l}$ is an M-matrix. By Lemma 1, there exists a nonnegative vector y such that $\langle A\rangle y>0$. From the construction of the matrix Q (2.5) we have that the matrix Q_1 is a nonnegative matrix and that there is at least one nonzero entry in each of its columns. Therefore we obtain that $Q_1^{\mathrm{T}}\langle A\rangle y>0$, and hence, $\hat{B}z>0$, where $z=Q_1^{\mathrm{T}}y\geqslant 0$. Again, by Lemma 1, $\hat{B}$ is an M-matrix if $\hat{B}$ has the sign pattern of a Z-matrix.

Note that the (u, v)th entry $\hat{b}_{uv}$ of the matrix $\hat{B}$ can be expressed as follows:

$$\hat{b}_{uv} = \begin{cases} \alpha_{uv}, & u = \kappa(u), \quad v = \kappa(v), \\ \dfrac{\sqrt{2}}{2}[\alpha_{uv} + \alpha_{u,\kappa(v)}], & u = \kappa(u), \quad v \neq \kappa(v), \\ \dfrac{\sqrt{2}}{2}[\alpha_{uv} + \alpha_{\kappa(u),v}], & u \neq \kappa(u), \quad v = \kappa(v), \\ \alpha_{uv} + \alpha_{\kappa(u),v}, & u \neq \kappa(u), \quad v \neq \kappa(v), \end{cases} \tag{3.2}$$

where α_{uv} denotes the (u, v)th entry of the comparison matrix $\langle A \rangle$ of the matrix A. We now consider the signs of the off-diagonal elements in $\hat{B}$ (3.2). If $u = \kappa(u)$ and $v = \kappa(v)$, we have $\hat{b}_{uv} = \alpha_{uv} \leqslant 0$. If $u = \kappa(u)$ and $v \neq \kappa(v)$, then from $KAK = A$ we get $\alpha_{uv} = \alpha_{\kappa(u),\kappa(v)}$, and, hence, $\hat{b}_{uv} = \sqrt{2}\alpha_{uv} \leqslant 0$. Similarly, if $u \neq \kappa(u)$ and $v = \kappa(v)$, we obtain that $\hat{b}_{uv} = \sqrt{2}\alpha_{uv} \leqslant 0$. If $u \neq \kappa(u)$ and $v \neq \kappa(v)$, using the fact that $u \neq v$ and $\kappa(u) \neq v$ (since the transpositions $\{\kappa_i\}_{i=1}^{l}$ are disjoint), we have that $\hat{b}_{uv} = \alpha_{uv} + \alpha_{\kappa(u),v} \leqslant 0$. That is to say that $\hat{B}$ is a Z-matrix. Thus we have proved that $\hat{B}$ is an M-matrix.

Next we show that $B = (b_{uv})$ in (2.7) is an H-matrix. Note that the (u, v)th entry b_{uv} of the matrix B can be expressed as follows:

$$b_{uv} = \begin{cases} a_{uv}, & u = \kappa(u), \quad v = \kappa(v), \\ \dfrac{\sqrt{2}}{2}[a_{uv} + a_{u,\kappa(v)}], & u = \kappa(u), \quad v \neq \kappa(v), \\ \dfrac{\sqrt{2}}{2}[a_{uv} + a_{\kappa(u),v}], & u \neq \kappa(u), \quad v = \kappa(v), \\ a_{uv} + a_{\kappa(u),v}, & u \neq \kappa(u), \quad v \neq \kappa(v), \end{cases} \tag{3.3}$$

where a_{uv} denotes the (u, v)th entry of the matrix A. Now consider the comparison matrix $\langle B \rangle = (\beta_{uv})$ of the matrix B, that is $\beta_{uu} = |b_{uu}|$ if $u = v$ or $\beta_{uv} = -|b_{uv}|$ if $u \neq v$. Comparing the (u, v)th entry of $\langle B \rangle$ with the corresponding one in the matrix $\hat{B}$ in (3.2), we find that

$$\beta_{uv} \geqslant \hat{b}_{uv},$$

which implies

$$\hat{B} \leqslant \langle B \rangle \leqslant D_{\langle B \rangle},$$

where $D_{\langle B \rangle} = \mathrm{diag}(\beta_{11}, \ldots, \beta_{rr})$. By Lemma 1, $\langle B \rangle$ is an M-matrix. Hence, B in (2.7) is an H-matrix.

We finally show that $C = (c_{uv})$ in (2.7) is an H-matrix too. Using the assumptions, it is easy to show that

$$c_{uv} = a_{uv} - a_{\kappa(u),v},$$

where $u \neq \kappa(u)$ and $v \neq \kappa(v)$ and $\kappa(u) \neq v$. We denote the comparison matrix of the matrix C by $\langle C \rangle = (\gamma_{uv})$ with $\gamma_{uu} = |c_{uu}|$ for $u = v$ and $\gamma_{uv} = -|c_{uv}|$ for $u \neq v$. Denote by $\tilde{Q}[j_1, \ldots, j_l]$ the matrix which consists of column $j_1, \ldots,$ column j_l of the matrix $\tilde{Q}$ in (2.4), respectively, and let $\breve{B} = \tilde{Q}^{\mathrm{T}}[j_1, \ldots, j_l]\langle A \rangle \tilde{Q}[j_1, \ldots, j_l]$. Comparing the (u, v)-entry $\breve{b}_{uv}$ of $\breve{B}$ with the corresponding one of the matrix $\langle C \rangle$, we find that

$$\breve{b}_{uv} \leqslant \gamma_{uv}.$$

That is to say that

$$\breve{B} \leqslant \langle C \rangle. \tag{3.4}$$

In fact, the matrix $\breve{B}$ is an $l \times l$ principal submatrix of the matrix $\hat{B}$ in (3.2). Since $\hat{B}$ is an M-matrix, the matrix $\breve{B}$ is also an M-matrix by Lemma 1. Combining (3.4) with the inequality $\langle C \rangle \leqslant D_{\langle C \rangle}$ where $D_{\langle C \rangle} = \mathrm{diag}(\gamma_{11}, \ldots, \gamma_{ll})$, we obtain that $\langle C \rangle$ is an M-matrix by Lemma 1. This proves the theorem. $\square$

Furthermore, if a generalized K-centrosymmetric matrix A is an H-matrix with positive diagonal entries, then its reduced form (2.7) inherits this property.

Corollary 1. *If A is an $n \times n$ generalized K-centrosymmetric H-matrix with positive diagonal entries, then the matrices B and C in the reduced form* (2.7) *are also H-matrices with positive diagonal entries.*

Proof. It suffices to show that the diagonal entries of the matrices B and C are positive. Note that $\hat{B}$ in (3.1) is an M-matrix. Hence its diagonal entries are all positive. For $u = 1, \ldots, n$, we have

$$
\begin{aligned}
0 < \hat{b}_{uu} &= \begin{cases} \alpha_{uu}, & u = \kappa(u), \\ \alpha_{uu} + \alpha_{\kappa(u),u}, & u \neq \kappa(u), \end{cases} \\
&= \begin{cases} |a_{uu}|, & u = \kappa(u), \\ |a_{uu}| - |a_{\kappa(u),u}|, & u \neq \kappa(u). \end{cases}
\end{aligned}
$$

The diagonal entries $\{b_{uu}\}_{u=1}^{n}$ of the matrix B in (2.7) are given by

$$
b_{uu} = \begin{cases} a_{uu}, & u = \kappa(u), \\ a_{uu} + a_{\kappa(u),u}, & u \neq \kappa(u), \end{cases}
$$

while the diagonal entries $\{c_{uu}\}_{u=1}^{n}$ of the matrix C in (2.7) are given by

$$
c_{uu} = a_{uu} - a_{\kappa(u),u}, \quad u \neq \kappa(u).
$$

Since $a_{uu} > 0$, we have $a_{uu} \geqslant |a_{uu}| > 0$ for $u = \kappa(u)$ and $a_{uu} \pm a_{\kappa(u),u} \geqslant |a_{uu}| - |a_{\kappa(u),u}| > 0$ for $u \neq \kappa(u)$. That is, the diagonal entries of the matrices B and C are all positive. □

In general, the converse of Theorem 1 does not hold. Some additional restrictions on the original matrix A are necessary.

Theorem 2. *Let A be an $n \times n$ generalized K-centrosymmetric matrix and let the orthogonal matrix Q be as in* (2.5). *If the matrix $\hat{B}$ defined in* (3.1) *is an M-matrix, then A is a generalized K-centrosymmetric H-matrix.*

Proof. From the hypothesis, $\hat{B}$ is an M-matrix. By Lemma 1, there exists an nonnegative vector $y \in \mathbb{R}^{n-l}$ such that $\hat{B}y > 0$. From the construction of $Q = [Q_1, Q_2]$ in (2.5) it follows that Q_1 is a nonnegative matrix, the positions of nonzero entries are disjoint and the number of nonzero entries in each of its columns is either 1 or 2. We arbitrarily choose a nonnegative vector x satisfying $y = Q^{\mathrm{T}}x$. For example, if there is only one nonzero entry in the uth column of the matrix Q_1, that is, $u = \kappa(u)$, we select $x_u = y_u$. Otherwise, that is in case $u \neq \kappa(u)$, we take $x_u = \sqrt{2}y_u$ and $x_{\kappa(u)} = 0$. Note from (3.1) that

$$
\langle A \rangle = Q \begin{bmatrix} \hat{B} & \\ & \hat{C} \end{bmatrix} Q^{\mathrm{T}}
$$

with $Q = [Q_1, Q_2]$ in (2.5), $Q_1^{\mathrm{T}} Q_1 = I_r$ and $Q_2^{\mathrm{T}} Q_1 = 0$. Right-multiplying $\langle A \rangle$ by $K_1 x$ with K_1 as in (2.6) shows that

$$
\begin{aligned}
\langle A \rangle K_1 x &= [Q_1, Q_2] \begin{bmatrix} \hat{B} & \\ & \hat{C} \end{bmatrix} \begin{bmatrix} Q_1^{\mathrm{T}} \\ Q_2^{\mathrm{T}} \end{bmatrix} K_1 x \\
&= [Q_1, Q_2] \begin{bmatrix} \hat{B} & \\ & \hat{C} \end{bmatrix} \begin{bmatrix} Q_1^{\mathrm{T}} x \\ 0 \end{bmatrix} \\
&= Q_1 \hat{B} Q_1^{\mathrm{T}} x \\
&= Q_1 \hat{B} y > 0.
\end{aligned}
$$

As $K_1 x \geqslant 0$, by Lemma 1 we obtain that $\langle A \rangle$ is an M-matrix. This completes the proof of Theorem 2. □

4. Square roots of generalized K-centrosymmetric matrices

In this section we present some new results on the square roots of nonsingular matrices with generalized central symmetry.

Recall that an $n \times n$ matrix X is said to be a square root of a square matrix A of order n, if $X^2 = A$. It is shown in [8, Lemma 1] that any nonsingular matrix always has a square root. Note by Lemma 2 that the product of two generalized K-centrosymmetric matrices is generalized K-centrosymmetric. In fact, if the square $X = A^2$ is a generalized K-centrosymmetric matrix $KXK = X$, then so is A as $A = X^2$ implies $KAK = A$. Here we will first answer the question whether the converse is true as well, that is whether a generalized K-centrosymmetric matrix has square roots which are also generalized K-centrosymmetric.

Theorem 3. *Let A be an $n \times n$ generalized K-centrosymmetric matrix. Then, A has a generalized K-centrosymmetric square root if and only if each of B and C in* (2.7) *admits a square root.*

Proof. Let A be generalized K-centrosymmetric. Then, by Lemma 3, A has the reduced form (2.7).

$\Longrightarrow$ Assume that A has a generalized K-centrosymmetric square root, denoted by $\tilde{X}$. From Lemma 3, we have

$$Q^{\mathrm{T}} \tilde{X} Q = X = \mathrm{diag}(X_1, X_2),$$

where Q is defined as in (2.5). Note that $\tilde{X}^2 = A$ implies that $X_1^2 = B$ and $X_2^2 = C$ hold simultaneously, i.e., X_1 and X_2 are square roots of B and C, respectively.

$\Longleftarrow$ If B and C in (2.7) have square roots X_1 and X_2, respectively, then $X = \mathrm{diag}(X_1, X_2)$ is a square root of the matrix $\mathrm{diag}(B, C)$. By Lemma 3, $\tilde{X} = QXQ^{\mathrm{T}}$ is a generalized K-centrosymmetric square root of A. Hence A always has a generalized K-centrosymmetric square root $\tilde{X}$. $\square$

Corollary 2. *For any nonsingular generalized K-centrosymmetric matrix A of order n there exists a generalized K-centrosymmetric square root.*

Proof. As A is generalized K-centrosymmetric and nonsingular, the matrices B and C in the reduced form (2.7) of A are nonsingular. Then, each of B and C has a square root. Therefore, by Theorem 3, we know that A always has a generalized K-centrosymmetric square root. $\square$

In the remaining part of this section we will discuss the square roots of a generalized K-centrosymmetric matrix A, which are functions of A. For the reader's convenience, we now recall the definition of matrix function of a nonsingular matrix A:

Definition 4 (*[13]*). For a given function f and a matrix $A \in \mathbb{C}^{n \times n}$, $f(A)$ can be defined as $g(A)$; where g is a polynomial of minimal degree that interpolates f on the spectrum of A, i.e.,

$$g^{(j)}(\lambda_k) = f^{(j)}(\lambda_k), \quad 0 \leqslant j \leqslant n_k - 1, \quad 1 \leqslant k \leqslant s,$$

where A has s distinct eigenvalues λ_k and n_k is the largest Jordan block in which λ_k appears.

Obviously, the function $f(\lambda) = \lambda^{1/2}$ is clearly defined on the spectrum of a nonsingular matrix A.

Theorem 4. *If $A \in \mathbb{C}^{n \times n}$ is a nonsingular generalized K-centrosymmetric matrix, then all square roots of A which are functions of A are generalized K-centrosymmetric.*

Proof. Assume that $\tilde{X}$ is a square root of A which is a function of A, that is, $\tilde{X}^2 = A$ and $\tilde{X} = f(A)$. By Lemma 2, we have that the sum and product of two generalized K-centrosymmetric matrices are also generalized K-centrosymmetric, therefore any polynomial p in A is generalized K-centrosymmetric. As a function $f(A)$ is defined as its interpolating polynomial g in the sense of Definition 4, we have that $\tilde{X} = g(A)$ is obviously generalized K-centrosymmetric. $\square$

It is known that any matrix A having no nonpositive real eigenvalues has a unique square root for which every eigenvalue has positive real part, denoted by $A^{1/2}$ and called the principal square root; that is, $(A^{1/2})^2 = A$ and $\mathrm{Re}(\lambda_k) > 0$ for all k, where $\lambda_k(A)$ denotes an eigenvalue of A. By Theorem 4, the following corollary holds immediately.

Corollary 3. *Let A be a nonsingular generalized K-centrosymmetric matrix of order n. If A has no eigenvalues on the nonpositive real axis, then the principal square root $A^{1/2}$ is generalized K-centrosymmetric.*

Theorem 5. *If A is an $n \times n$ generalized K-centrosymmetric H-matrix with positive diagonal entries, then its principal square root $A^{1/2}$ is a generalized K-centrosymmetric H-matrix with positive diagonal entries and unique.*

Proof. Because A is an H-matrix with positive diagonal entries, we have by Lemma 14 in [18], that all eigenvalues of A have positive real part. Hence, the principal square root $A^{1/2}$ exists and unique. $A^{1/2}$ is a generalized K-centrosymmetric matrix by Corollary 3.

An H-matrix with positive diagonal entries has a unique square root which is also an H-matrix with positive diagonal entries [18], we therefore conclude that $A^{1/2}$ is a generalized K-centrosymmetric H-matrix with positive diagonal entries and unique. $\square$

This result is not surprising as it is already known that for an H-matrices with positive diagonal elements there exists one and only one square root which is also an H-matrix with positive diagonal elements [18]. The principal square root of a centrosymmetric H-matrix with positive diagonal elements is a unique centrosymmetric H-matrix with positive diagonal entries [21].

5. Structured algorithms

In the preceding two sections we investigated some properties of generalized K-centrosymmetric (H-) matrices. In this section we exploit those properties to develop several structured algorithms for some potential applications. It is shown that under certain conditions our structured algorithms ensure significant saving, as compared to the corresponding nonstructured algorithms.

As any $n \times n$ generalized K-centrosymmetric matrix can be reduced into a 2×2 block diagonal matrix, it may seem that all computational problems for a generalized K-centrosymmetric matrix can be reduced to ones for two smaller matrices. This is true for some problems, but not for all as not all properties of a generalized K-centrosymmetric matrix are preserved in its reduced form (2.7). For example, the reduced form of a centrosymmetric M-matrix A is not necessarily an M-matrix. In this case, the effective computational methods for M-matrices cannot be directly applied to the reduced form of A.

5.1. Incomplete LU factorization

In this subsection we consider the incomplete LU factorization of an $n \times n$ generalized K-centrosymmetric H-matrix A with positive diagonal entries, which is one of the most important preconditioning strategies for conjugate gradient method and other Krylov subspace methods.

It is known that if A is positive definite, then A always has an LU factorization; that is there exists an unit lower triangular matrix $L = (l_{ij})$ and an upper triangular matrix $U = (u_{ij})$ such that

$$A = LU. \tag{5.1}$$

The incomplete LU factorization of the positive definite matrix A is an LU factorization of a modified matrix of A. That is

$$A = \hat{L}\hat{U} - R, \tag{5.2}$$

where $\hat{L} = (\hat{l}_{ij})$ and $\hat{U} = (\hat{u}_{ij})$ are unit lower triangular and upper triangular, R is the residual matrix.

As shown in [22], if A is an H-matrix with positive diagonal entries, then the incomplete LU factorization exists for any predetermined sparsity pattern $\mathbb{S}$. That is to say that given set $\mathbb{S}$ of ordered pairs of integers (i, j), $1 \leqslant i, j \leqslant n$, one can construct $\hat{L}$ and $\hat{U}$ such that $\hat{l}_{ij} \neq 0$ $(i > j)$, $\hat{u}_{ij} \neq 0$ $(i < j)$ for $(i, j) \in \mathbb{S}$.

Let us consider the solution of linear system

$$Ax = b \tag{5.3}$$

by Gaussian elimination, where A is an $n \times n$ generalized K-centrosymmetric H-matrix with positive diagonal entries. From (2.7), we know that solving (5.3) is equivalent to solving the following two smaller linear systems:

$$By_1 = c_1, \tag{5.4}$$

$$Cy_2 = c_2, \tag{5.5}$$

where $y_1, c_1 \in \mathbb{R}^{n-l}$, $y_2, c_2 \in \mathbb{R}^l$, $(y_1^{\mathrm{T}}, y_2^{\mathrm{T}})^{\mathrm{T}} = Q^{\mathrm{T}}x$ and $(c_1^{\mathrm{T}}, c_2^{\mathrm{T}})^{\mathrm{T}} = Q^{\mathrm{T}}b$.

Hence, we can either solve (5.3) directly by Gaussian elimination (this process does not need pivoting, as A is an H-matrix with positive diagonal entries) or we can first reduce the system (5.3) (at almost no cost) to two subsystems (5.4) and (5.5), then solving them by Gaussian elimination. The first approach needs about $\frac{2}{3}n^3 + \mathrm{O}(n^2)$ flops, the second one takes about $\frac{2}{3}(n-l)^3 + \frac{2}{3}l^3 + \mathrm{O}(n^2)$ flops. If $l \approx n$ or $l \ll n$, then both flops counts are about the same, there is no need to first reduce (5.3) and then to work on the two smaller systems. However, if $l \approx n/2$, then the second choice ensures the savings of about $\frac{1}{2}n^3 + \mathrm{O}(n^2)$ flops.

Finally, we consider the solution of (5.3) by a preconditioned iterative methods based on an incomplete LU factorization. Because A is an H-matrix with positive diagonal entries, we can directly consider the incomplete LU factorization of A as its preconditioner for a given sparsity pattern $\mathbb{S}$ and then apply this preconditioner to the corresponding iterative method. On the other hand, by Theorem 1 and Corollary 1, we know that the coefficient matrices B and C in (5.4) and (5.5) are also H-matrices with positive diagonal entries. In this case the matrix B in (5.4) has an incomplete LU factorization based preconditioner for any predetermined sparsity pattern $\mathbb{S}_1$. So does C in (5.5) for any predetermined sparsity pattern $\mathbb{S}_2$. Therefore, we can get the solution of (5.3) by solving linear systems (5.4) and (5.5) by preconditioned iterative methods.

The computational costs of the above two approaches are rather complicated. If the computational costs of incomplete LU factorizations of A, B and C are negligible, then the second scheme (that is to solve (5.4) and (5.5) by preconditioned iterative methods) ensures significant savings if $l \approx n/2$, as compared to the first scheme (that is to directly solve (5.3) by the same preconditioned iterative method). For more details, see [20].

Based on the above analysis, it can be expected that the algorithm on page 162 in [17] as well as the corresponding preconditioned conjugate gradient method can be improved by exploiting the structured algorithm, which will be considered in our future work.

5.2. The classical iterative methods

The classical iterative methods including the Jacobi, Gauss–Seidel and successive over-relaxation (SOR) algorithms have been proved to be very effective for solving linear system (5.3) when A is an H-matrix. Assume that $A = M - N$ (M nonsingular) be a splitting of A. Then the classical iterative methods can be described as follows: Given an initial guess x^0, repeatedly compute $Mx^{j+1} = Nx^j + b$.

In order to illustrate the advantage of our structured algorithm, we only consider the Gauss–Seidel algorithm. For other iterative methods, such as two-stage iterative method in [10] and Schwarz iterative method in [5], etc., one can easily get similar results.

Let $A = D - L - U$ be a decomposition of A, where $D = \mathrm{diag}(a_{11}, \ldots, a_{nn})$, i.e., D consists of the diagonal elements of A, L and U consist of the lower triangular part and upper triangular part of A, respectively. Then the Gauss–Seidel iteration is as follows:

$$(D - L)x^{j+1} = Ux^j + b \quad \text{for } j = 1, \ldots, \text{until convergence.} \tag{5.6}$$

It is known that if A is an H-matrix, then the Gauss–Seidel iteration is convergent for any initial guess x^0.

Assume that A in (5.3) is a generalized K-centrosymmetric H-matrix. As before, we have two options to solve the linear system (5.3). The first option is directly to solve it by Gauss–Seidel iteration (5.6). It takes about $2n^2 + \mathrm{O}(n)$ flops to perform one iteration involving a upper triangular matrix–vector product, a vector–vector sum and a solution of a lower triangular linear system. The second option is first to reduce the system (5.3) to two subsystems (5.4) and (5.5).

By Theorem 1, B and C in (5.4) and (5.5) are two H-matrices. Thus the Gauss–Seidel iteration (5.6) can be applied to subsystems (5.4) and (5.5). The computational costs in each iteration step amount to about $2(n-l)^2+2l^2+\mathrm{O}(n)$ flops. Again, if $l \approx n$ or $l \ll n$, then both flops counts are about the same, there is no need to first reduce system (5.3) and then to work on the smaller subsystems (5.4) and (5.5). However, if $l \approx n/2$, then a structured iteration step ensures the savings of about $n^2 + \mathrm{O}(n)$ flops.

5.3. The computation of principal square roots

A stable algorithm (called the LL algorithm) for computing the principal square root of an H-matrix with positive diagonal entries was proposed by Lin and Liu in [18], which can be viewed as an extension of one developed in [1] (refereed to as AS iteration) for M-matrices, in which only nonnegative matrix additions and multiplications are involved. The AS iteration converges linearly (see [14]) and is stable. The LL iteration can be briefly outlined as follows.

Let $A=(a_{ij})$ be an H-matrix with positive diagonal entries. Let $\hat{N}=(\hat{n}_{ij})$ with $\hat{n}_{ij}=a_{ij}$ if $a_{ij}\geqslant 0$, $i \neq j$ and $\hat{n}_{ij}=0$ otherwise. Then the matrix A can be written as

$$A = sI - \hat{P} + \hat{N}$$

with $\hat{P}\geqslant 0$, $\hat{N}\geqslant 0$, where the scalar s is positive and satisfies the inequality $s\geqslant \max_{i=1}^{n} a_{ii}$. Denoting $P=\hat{P}/s$ and $N=\hat{N}/s$, we have that $A/s = I - P + N$. Hence, the square root problem of A is equivalent to that of A/s. Then the LL iteration is defined as follows for $X_0 = Y_0 = 0$:

$$\begin{aligned} X_{j+1} &= \tfrac{1}{2}(P + X_j^2 + Y_j^2), \quad j=0,1,2,\ldots, \\ Y_{j+1} &= \tfrac{1}{2}(N + X_jY_j + Y_jX_j). \end{aligned} \tag{5.7}$$

The sequences $\{X_j\}$ and $\{Y_j\}$ are convergent, i.e.,

$$X_j \to X, \quad Y_j \to Y \quad \text{as } j \to \infty,$$

and $I-X+Y$ is an H-matrix with positive diagonal entries and is the principal square root of the H-matrix $I-P+N$ with positive diagonal entries. The LL iteration inherits the linear converge rate from the AS iteration. For $N=0$, the matrix $I-P+N$ is an M-matrix and the LL iteration in (5.7) reduces to the AS iteration for computing the square root of an M-matrix.

As A is an H-matrix with positive diagonal entries, one could simply use the LL algorithm (5.7) from [18] to compute its root. But as A is also a generalized K-centrosymmetric matrix, it can be first transformed (at almost no cost) to its reduced form (2.7). As B and C in (2.7) are both H-matrices with positive diagonal entries, the LL algorithm can be directly applied to them to compute their roots. Let us say, the computed roots are E and F, respectively. Then

$$A^{1/2} = Q \begin{bmatrix} E & \\ & F \end{bmatrix} Q^{\mathrm{T}}. \tag{5.8}$$

If we compute the principal square root of an $n \times n$ generalized K-centrosymmetric H-matrix using the LL iteration (5.7), the main computational costs in each iteration step (that is the computation of X_{j+1} and Y_{j+1}) are roughly $8n^3 + \mathrm{O}(n^2)$ flops. Applying the LL iteration to the $(n-l)\times(n-l)$ matrix B and the $l \times l$ matrix C amounts to $8[(n-l)^3 + l^3] + \mathrm{O}((n-l)^2)$ flops. If $l \approx n$ or $l \ll n$, then both flops counts are about the same, there is no need to first transform A and then to work on the smaller matrices B and C (assuming that it is fair to say that both approaches will need the same number iterations in order to converge). However, if $l \approx n/2$, then the second algorithm ensures the savings of about $6n^3 + \mathrm{O}(n^2)$ flops in comparison with LL iteration, for each iteration.

A different option for computing the desired square root is the Schulz iteration [14] defined as follows for $Y_0 = A$, $Z_0 = I$:

$$\begin{aligned} Y_{j+1} &= \tfrac{1}{2}Y_j(3I - Z_jY_j), \quad j=0,1,2,\ldots \\ Z_{j+1} &= \tfrac{1}{2}(3I - Z_jY_j)Z_j. \end{aligned} \tag{5.9}$$

It possess quadratic convergence if $\|\mathrm{diag}(A-I, A-I)\| < 1$,

$$Y_j \to A^{1/2}, \quad Z_j \to A^{-1/2} \quad \text{as } j \to \infty.$$

Note that if $A = I - P + N$ is an H-matrix with positive diagonal entries, then $\langle A \rangle = I - (P + N)$ is an M-matrix with $\rho(P + N) < 1$, due to $|P - N| < P + N$, hence we have that $\rho(P - N) \leqslant \rho(|P - N|) < \rho(P + N) < 1$, which implies that $\|A - I\| < 1$ for a consistent norm. Therefore, the convergence condition of the Schulz iteration is satisfied.

As before, we have two different options here. We could either apply the Schulz iteration directly to A or we first transform A to its reduced form (2.7) and apply the Schulz iteration to B and C to compute their roots. Let us say, the computed roots are E and F, respectively. Then, as in (5.8), $A^{1/2}$ can be expressed via Q, E, F. If we compute the principal square root of an $n \times n$ generalized K-centrosymmetric H-matrix using the Schulz iteration (5.9), the main computational costs in each iteration step (that is the computation of X_{j+1} and Y_{j+1}) are roughly $6n^3 + \mathrm{O}(n^2)$ flops. Applying the Schulz iteration to the $(n-l) \times (n-l)$ matrix B and the $l \times l$ matrix C amounts to $6[(n-l)^3 + l^3] + \mathrm{O}((n-l)^2)$ flops. Again, if $l \approx n$ or $l \ll n$, then both flops counts are about the same, there is no need to first transform A and then to work on the smaller matrices B and C (assuming that it is fair to say that both approaches will need the same number iterations in order to converge). However, if $l \approx n/2$, then the second algorithm ensures the savings of about $\frac{9}{2}n^3 + \mathrm{O}(n^2)$ flops in comparison with Schulz iteration on A, for each iteration.

Both algorithms discussed here, the LL iteration and the Schulz iteration, encompass only matrix–matrix multiplications, an operation that can be done very efficiently on modern high performance computers. The convergence of the LL iteration is linear, while the convergence of the Schulz iteration is quadratic. However, we note that the LL iteration only uses nonnegative matrix–matrix multiplications and nonnegative matrix–matrix additions. That means that the LL iteration is potentially more stable than the Schulz iteration.

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