

MODIFIED INCOMPLETE CHOLESKY FACTORIZATION PRECONDITIONERS FOR A SYMMETRIC POSITIVE DEFINITE MATRIX

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ABSTRACT. We propose variants of the modified incomplete Cholesky factorization preconditioner for a symmetric positive definite (SPD) matrix. Spectral properties of these preconditioners are discussed, and then numerical results of the preconditioned CG (PCG) method using these preconditioners are provided to see the effectiveness of the preconditioners.

1. Introduction

In this paper, we consider a linear system of equations

$$(1) \quad Ax = b, \quad x, b \in \mathbb{R}^n,$$

where $A \in \mathbb{R}^{n \times n}$ is a large sparse symmetric positive definite (SPD) matrix. Since A is a large sparse matrix, direct methods such as Gaussian elimination become prohibitively expensive because of a lot of fill-in elements. As an alternative, the preconditioned CG (PCG) iterative method [2] is widely used for the purpose of finding an approximate solution of the problem (1). Given an initial guess x_0 , the PCG method computes iteratively new approximations x_k to the true solution $x^* = A^{-1}b$. The iterate x_k is accepted as a solution if the residual $r_k = b - Ax_k$ satisfies $\frac{\|r_k\|_2}{\|b\|_2} \leq tol$.

The convergence rate and robustness of the PCG largely depend on how well the preconditioner approximates A . One of the powerful preconditioning methods in terms of reducing the number of iterations is

Received February 5, 2002. Revised April 24, 2002.

2000 Mathematics Subject Classification: 65F10, 65F50.

Key words and phrases: modified incomplete Cholesky factorization, P-regular splitting, preconditioner, PCG method.

This research was supported by the Chungbuk National University Basic Science Research Fund BSRI-01-6.

the incomplete Cholesky factorization method studied by Meijerink and van der Vorst [4] and Yun [8]. It was shown in [4] that for every zero pattern set, there exists an incomplete Cholesky factorization of a symmetric M -matrix. However, the incomplete Cholesky factorization for a symmetric positive definite matrix does not always exist. To this end, Robert [7] introduced the modified incomplete Cholesky factorization which exists for any symmetric positive definite matrix. The purpose of this paper is to study variants of the modified incomplete Cholesky factorization for a symmetric positive definite matrix. This paper is organized as follows. In Section 2, we consider some properties of P -regular splittings. In Section 3, we consider variants of the modified incomplete Cholesky factorization. In Section 4, we provide numerical results. In Section 5, some conclusions are drawn.

2. Properties of P -regular splitting

For two matrices $A = (a_{ij})$ and $B = (b_{ij})$, $A \leq B$ denotes $a_{ij} \leq b_{ij}$ for all i and j , and $A \geq B$ denotes $a_{ij} \geq b_{ij}$ for all i and j . We say that a real matrix A is *monotone* if $Ax \geq 0$ implies $x \geq 0$. It is well known that A is monotone if and only if $A^{-1} \geq 0$. A real square matrix $A = (a_{ij})$ is called an *M -matrix* if $a_{ij} \leq 0$ for $i \neq j$ and it is monotone. A real matrix A is *positive definite* (*positive semi-definite*) if $\operatorname{Re}(x^H Ax) > 0$ ($\operatorname{Re}(x^H Ax) \geq 0$) for every nonzero vector $x \in \mathbb{C}^n$, or equivalently $x^T Ax > 0$ ($x^T Ax \geq 0$) for every nonzero vector $x \in \mathbb{R}^n$, where $\operatorname{Re}(x^H Ax)$ refers to the real part of $x^H Ax$.

The *spectral radius* $\rho(A)$ of a matrix A is $\rho(A) = \max\{|\lambda| \mid \lambda \in \sigma(A)\}$, where $\sigma(A)$ denotes the *spectrum* of A , that is, the set of eigenvalues of A . A representation $A = M - N$ is called a *splitting* of A when M is nonsingular. A splitting $A = M - N$ is a *convergent splitting* of A if $\rho(M^{-1}N) < 1$. A splitting $A = M - N$ is a *P -regular splitting* if $M + N$ is positive definite. Obviously, the matrix $M + N$ is positive definite if and only if $M^T + N$ is positive definite. Throughout the paper, we use the notation $M \succ 0$ ($M \succeq 0$) for a matrix to be symmetric positive definite (symmetric positive semi-definite), and $M_1 \succ M_2$ ($M_1 \succeq M_2$) denotes that $M_1 - M_2 \succ 0$ ($M_1 - M_2 \succeq 0$).

THEOREM 2.1 ([3]). *Let A be a symmetric matrix and let $A = M - N$ be a P -regular splitting of A . Then $\rho(M^{-1}N) < 1$ if and only if A is positive definite.*

THEOREM 2.2 ([5]). *Let $A \succ 0$ and let $A = M_1 - N_1 = M_2 - N_2$ be two splittings of A . If $0 \preceq N_1 \preceq N_2$, then*

$$\rho(M_1^{-1}N_1) \leq \rho(M_2^{-1}N_2) < 1.$$

If $0 \preceq N_1 \prec N_2$, then

$$\rho(M_1^{-1}N_1) < \rho(M_2^{-1}N_2) < 1.$$

THEOREM 2.3 ([6]). *Let A be a symmetric matrix and let $A = M - N$ be a splitting of A . If $M \succ 0$ and $\rho(M^{-1}N) < 1$, then A is positive definite and $A = M - N$ is a P -regular splitting of A .*

THEOREM 2.4. *Let $A \succ 0$ and let $A = M - N$ be a splitting of A with $N \succeq 0$. Then $\rho(M^{-1}N) < 1$, $0 < \lambda_{M^{-1}A} \leq 1$, and $0 \leq \lambda_{M^{-1}N} < 1$, where $\lambda_{M^{-1}A}$ and $\lambda_{M^{-1}N}$ denote eigenvalues of $M^{-1}A$ and $M^{-1}N$, respectively.*

Proof. Suppose that λ is an eigenvalue of $M^{-1}N$. Then there exists a nonzero vector x such that $M^{-1}Nx = \lambda x$. Thus, $Nx = \lambda Mx$. It follows that

$$x^H Nx = \lambda x^H Mx = \lambda x^H Ax + \lambda x^H Nx.$$

Since $A \succ 0$ and $\lambda \neq 1$, $x^H Nx = \frac{\lambda}{1-\lambda} x^H Ax$. Since $x^H Ax > 0$ and $x^H Nx \geq 0$, $\frac{\lambda}{1-\lambda} \geq 0$. It follows that $0 \leq \lambda < 1$. Hence $0 \leq \lambda_{M^{-1}N} < 1$ is proved. From $M^{-1}A = I - M^{-1}N$, $\lambda_{M^{-1}A} = 1 - \lambda_{M^{-1}N}$. Thus, $0 < \lambda_{M^{-1}A} \leq 1$. For the proof of $\rho(M^{-1}N) < 1$, $N \succeq 0$ implies that $M = A + N \succ 0$. Hence, $A = M - N$ is a P -regular splitting of A . From Theorem 2.1, $\rho(M^{-1}N) < 1$ is obtained. \square

THEOREM 2.5. *Suppose that $A \succ 0$. Let $A = M - N$ be a splitting of A with M symmetric. Then $\rho(M^{-1}N) < 1$ if and only if $A = M - N$ is a P -regular splitting.*

Proof. Suppose that $A = M - N$ is a P -regular splitting. Then by Theorem 2.1, $\rho(M^{-1}N) < 1$ is immediately obtained. For the proof of the other direction, let's suppose that $\rho(M^{-1}N) < 1$. From the identity $M^{-1}A = I - M^{-1}N$, it can be seen that $M^{-1}A$ has eigenvalues with positive real parts. Notice that $M^{-1}A$ is similar to $A^{1/2}M^{-1}A^{1/2}$. Since $A^{1/2}M^{-1}A^{1/2}$ is symmetric, $M^{-1}A$ has real eigenvalues. It follows that $M^{-1}A$ has positive eigenvalues. Hence, $A^{1/2}M^{-1}A^{1/2} \succ 0$, from which $M \succ 0$. From Theorem 2.3, one obtains that $A = M - N$ is a P -regular splitting. \square

THEOREM 2.6 ([1]). *Let $A \succ 0$ and let $A = M - N$ be a splitting of A with M symmetric. Let $B_k^{-1} = \sum_{i=0}^{k-1} (M^{-1}N)^i M^{-1}$ ($k \geq 1$). Then*

- (a) B_k is symmetric.
- (b) For k odd, B_k is positive definite if and only if M is positive definite.
- (c) For k even, B_k is positive definite if and only if $M + N$ is positive definite.

If the B_k defined in Theorem 2.6 is symmetric positive definite, then it can be used as a preconditioner for the PCG method and it is called *k-step polynomial preconditioner* corresponding to the splitting $A = M - N$. It is easy to see that $\lim_{k \rightarrow \infty} B_k^{-1} = A^{-1}$ if $\rho(M^{-1}N) < 1$. It is well-known that the convergence rate of the PCG method with a preconditioner M for solving $Ax = b$ depends on how small $\frac{\lambda_{\max}(M^{-1}A)}{\lambda_{\min}(M^{-1}A)}$ is, where $\lambda_{\max}(M^{-1}A)$ and $\lambda_{\min}(M^{-1}A)$ denote the maximum and minimum eigenvalues of $M^{-1}A$, respectively. More specifically, if $A = M - N$ is a splitting of A with M being SPD, then the convergence rate of the PCG with the preconditioner M may depend on how small $\rho(M^{-1}N)$ is. Thus, if $\rho(M^{-1}N) < 1$ and $M \succ 0$ is easily invertible, then the M may be considered as a good preconditioner for the PCG.

3. Modified incomplete Cholesky factorizations

Let $P_n = \{(i, j) \mid i \neq j, 1 \leq i, j \leq n\}$. Then, it was shown in [4] that for every symmetric zero pattern set $Z \subset P_n$ (i.e. $(i, j) \in Z$ implies $(j, i) \in Z$), there exists an incomplete Cholesky factorization of a symmetric M -matrix A such that $A = U^T D U - R$ is a regular splitting of A , where U is an upper triangular M -matrix and D is a diagonal matrix whose i th diagonal element is an inverse of the i th diagonal element of U .

It is clear that $U^T D U$ in the above factorization is positive definite since D is positive definite. Thus, the $U^T D U$ obtained from the incomplete Cholesky factorization of a symmetric M -matrix can be used as a preconditioner for the PCG method. However, next example shows that the incomplete Cholesky factorization for a symmetric positive definite matrix A which is not an M -matrix does not always exist. That is, there exists a diagonal matrix D with a nonpositive diagonal element such that $A = U^T D U - R$.

EXAMPLE 3.1. Let

$$A = \begin{pmatrix} 1 & -1 & 0 & 0.1 \\ -1 & 3 & 0.4 & 0 \\ 0 & 0.4 & 1.08 & 2 \\ 0.1 & 0 & 2 & 3.97 \end{pmatrix}.$$

Since all eigenvalues of A are positive, $A \succ 0$. It is clear that A is not an M -matrix. For the zero pattern set $Z = \{(1, 3), (2, 4), (3, 1), (4, 2)\}$, the incomplete factorization of A such that $A = U^T D U - R$ is

$$U^T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 2 & 0 & 0 \\ 0 & 0.4 & 1 & 0 \\ 0.1 & 0 & 2 & -0.04 \end{pmatrix}, \quad D = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -25 \end{pmatrix}, \quad R = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -0.1 \\ 0 & 0 & 0 & 0 \\ 0 & -0.1 & 0 & 0 \end{pmatrix}.$$

Since D contains a negative diagonal element -25 , $U^T D U$ is not positive definite and hence it can not be used as a preconditioner of the PCG iterative method. Also note that $A = U^T D U - R$ is not a regular splitting of A .

The incomplete factorization of A proposed in [6] such that $A = U^T D U - R$ requires that all diagonal elements of the matrix R are zero. By suppressing this requirement, Robert [10] proposed a modified incomplete Cholesky factorization which always exists for any symmetric positive definite matrix A .

THEOREM 3.2 ([7]). *Let $A \succ 0$. Then for every symmetric zero pattern set $Z \subset P_n$ there exists a modified incomplete Cholesky factorization of A such that $A = U^T D U - R$, where U is an upper triangular matrix with positive diagonal elements, D is a diagonal matrix whose i th diagonal element is an inverse of the i th diagonal element of U , and R is positive semi-definite.*

The modified incomplete Cholesky factorization (MICF) in [7] is described in a theoretical way, so the MICF algorithm which can be easily implemented is provided below. Let a_{ij} denote the (i, j) component of A and let Z be a zero pattern set. Since A is symmetric, only the lower triangular part of A is used and updated.

Algorithm 3.1 (MICF).

$$d_1 = 1/a_{11}$$

For $i = 2..n$

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For  $j = 1, i - 1$ 
  For  $k = i, n$ 
     $a_{ki} = a_{ki} - a_{kj} \cdot a_{ij} \cdot d_j$ 
  end
end
For  $k = i + 1, n$ 
  if  $(k, i) \in Z$ , then
     $a_{ii} = a_{ii} + |a_{ki}|$ 
     $a_{kk} = a_{kk} + |a_{ki}|$ 
     $a_{ki} = 0$ 
  end if
end
 $d_i = 1/a_{ii}$ 
end

```

From Algorithm 3.1, the modified incomplete Cholesky factorization of the matrix A given in Example 3.1 such that $A = U^T D U - R$ is

$$U^T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & \frac{21}{10} & 0 & 0 \\ 0 & \frac{2}{5} & \frac{527}{525} & 0 \\ \frac{1}{10} & 0 & 0 & \frac{1981}{26350} \end{pmatrix}, D = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{10}{21} & 0 & 0 \\ 0 & 0 & \frac{525}{527} & 0 \\ 0 & 0 & 0 & \frac{26350}{1981} \end{pmatrix}, R = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{10} & 0 & -\frac{1}{10} \\ 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{10} & 0 & \frac{1}{10} \end{pmatrix}.$$

Notice that the lower triangular matrix U^T and the diagonal matrix D are obtained directly from Algorithm 3.1, while the matrix R is computed from the identity $R = U^T D U - A$. Since we are only interested in the matrix $U^T D U$ which can be used as a preconditioner of the PCG method, all algorithms in this paper do not contain the computational step for the matrix R . From now on, the $U^T D U \succ 0$ obtained from Algorithm 3.1 is called the MICF preconditioner.

Below we propose a variant of the modified incomplete Cholesky factorization (VMICF) algorithm which is more efficient than Algorithm 3.1 (see Tables 1 and 3). This variant also yields a splitting $A = \hat{U}^T \hat{D} \hat{U} - \hat{R}$ such that $\hat{U}^T \hat{D} \hat{U} \succ 0$ and $\hat{R} \succeq 0$. From now on, the $\hat{U}^T \hat{D} \hat{U} \succ 0$ is called the VMICF preconditioner.

Algorithm 3.2 (VMICF).

```

For  $i = 1, n$ 
   $d_i = 1/a_{ii}$ 
  For  $j = i + 1, n$ 
     $d_j = a_{ji} \cdot d_i$ 
  end
end

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For  $j = i + 1, n$ 
  For  $k = j, n$ 
    if  $(k, j) \in Z$ , then
       $a_{kj} = a_{kj} - d_k \cdot a_{ji}$ 
       $a_{kk} = a_{kk} + |a_{kj}|$ 
       $a_{jj} = a_{jj} + |a_{kj}|$ 
       $a_{kj} = 0$ 
    else
       $a_{kj} = a_{kj} - d_k \cdot a_{ji}$ 
    end if
  end
end
end
    
```

The main difference between Algorithms 3.1 and 3.2 is as follows. At the i th step, Algorithm 3.1 updates the i th column using the first $(i - 1)$ columns and then modifies diagonal elements according to a zero pattern set Z , while Algorithm 3.2 updates the last $(n - i)$ columns using the i th column and then modifies diagonal elements according to the zero pattern set Z . Here, we provide an example which shows the difference between Algorithms 3.1 and 3.2.

EXAMPLE 3.3. Let

$$A = \begin{pmatrix} 4 & 0 & -1 & -1 \\ 0 & 2 & 1 & -1 \\ -1 & 1 & 2 & 0 \\ -1 & -1 & 0 & 2 \end{pmatrix}.$$

Let $Z = \{(1, 2), (2, 1), (3, 4), (4, 3)\}$. Since A is an irreducibly diagonally dominant matrix with positive diagonal elements, $A \succ 0$. From Algorithm 3.1, one obtains $A = U^T D U - R$ with

$$U^T = \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ -1 & 1 & \frac{3}{2} & 0 \\ -1 & -1 & 0 & \frac{3}{2} \end{pmatrix}, \quad D = \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & \frac{2}{3} \end{pmatrix}, \quad R = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4} & -\frac{1}{4} \\ 0 & 0 & -\frac{1}{4} & \frac{1}{4} \end{pmatrix}.$$

From Algorithm 3.2, one obtains $A = \hat{U}^T \hat{D} \hat{U} - \hat{R}$ with

$$\hat{U}^T = \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ -1 & 1 & 2 & 0 \\ -1 & -1 & 0 & 2 \end{pmatrix}, \hat{D} = \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{2} \end{pmatrix}, \hat{R} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{3}{4} & -\frac{1}{4} \\ 0 & 0 & -\frac{1}{4} & \frac{3}{4} \end{pmatrix}.$$

The spectral condition numbers of A , $U^T D U$, and $\hat{U}^T \hat{D} \hat{U}$ are

$$\kappa_2(A) = \|A\|_2 \cdot \|A^{-1}\|_2 \approx 8.80781$$

$$\kappa_2(U^T D U) = \|U^T D U\|_2 \cdot \|(U^T D U)^{-1}\|_2 \approx 5.8143$$

$$\kappa_2(\hat{U}^T \hat{D} \hat{U}) = \|\hat{U}^T \hat{D} \hat{U}\|_2 \cdot \|(\hat{U}^T \hat{D} \hat{U})^{-1}\|_2 \approx 4.8508.$$

It is easy to show that $0 \preceq R \preceq \hat{R}$. From Theorem 2.2, one obtains

$$\rho((U^T D U)^{-1} R) \leq \rho((\hat{U}^T \hat{D} \hat{U})^{-1} \hat{R}) < 1.$$

Note that direct calculations yield

$$\rho((U^T D U)^{-1} R) = 1/3$$

$$\rho((\hat{U}^T \hat{D} \hat{U})^{-1} \hat{R}) = 1/2.$$

Suppose that $A = U^T D U - R$ and $A = \hat{U}^T \hat{D} \hat{U} - \hat{R}$ are splittings of A obtained from Algorithms 3.1 and 3.2, respectively. Since $U^T D U \succ 0$, $\hat{U}^T \hat{D} \hat{U} \succ 0$, $R \succeq 0$ and $\hat{R} \succeq 0$, from Theorem 2.5 $\rho((U^T D U)^{-1} R) < 1$ and $\rho((\hat{U}^T \hat{D} \hat{U})^{-1} \hat{R}) < 1$. In addition, Theorem 2.6 implies that for any $k \geq 1$

$$M_k^{-1} = \sum_{i=0}^{k-1} ((U^T D U)^{-1} R)^i (U^T D U)^{-1}$$

$$\hat{M}_k^{-1} = \sum_{i=0}^{k-1} ((\hat{U}^T \hat{D} \hat{U})^{-1} \hat{R})^i (\hat{U}^T \hat{D} \hat{U})^{-1}$$

are symmetric positive definite. Hence, the M_k and \hat{M}_k can be used as preconditioners for the PCG method. The M_k and \hat{M}_k are called k -step MICF and k -step VMICF polynomial preconditioners, respectively. Notice that for $k = 1$, the M_k and \hat{M}_k reduce to the standard MICF and VMICF preconditioners, respectively. It can be shown that $0 \preceq R \preceq \hat{R}$ and thus $\rho((U^T D U)^{-1} R) \leq \rho((\hat{U}^T \hat{D} \hat{U})^{-1} \hat{R})$. From this point of view, the MICF preconditioner obtained from Algorithm 3.1 may provide better convergence rate of the PCG than the VMICF preconditioner obtained from Algorithm 3.2. Numerical experiments in Section 4 show that the convergence rate of the PCG with MICF preconditioner is as

good as or slightly better than that with VMICF preconditioner, but the construction time for MICF preconditioner is much larger than that for VMICF preconditioner (see Tables 1 and 3). So, the VMICF is more efficient preconditioner than the MICF on the Cray T3E supercomputer.

Next we consider other variants of the modified incomplete Cholesky factorization preconditioner. Let A be a symmetric positive definite 2×2 block matrix of the form

$$(2) \quad A = \begin{pmatrix} A_1 & C_1 \\ C_1^T & A_2 \end{pmatrix},$$

where A_1 and A_2 are square matrices. Since $A \succ 0$, $A_1 \succ 0$ and $A_2 \succ 0$. Thus, there exist modified incomplete Cholesky factorizations for A_1 and A_2 .

LEMMA 3.4. *Suppose that A is a symmetric positive definite matrix of the form (2). Then for every nonzero vector $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$*

$$\begin{aligned} x_1^T A_1 x_1 + x_2^T A_2 x_2 + 2x_1^T C_1 x_2 &> 0 \\ x_1^T A_1 x_1 + x_2^T A_2 x_2 - 2x_1^T C_1 x_2 &> 0. \end{aligned}$$

Proof. Since A is a symmetric positive definite matrix of the form (2), for any nonzero vector $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$

$$(-x_1^T, x_2^T)A \begin{pmatrix} -x_1 \\ x_2 \end{pmatrix} = (-x_1^T, x_2^T) \begin{pmatrix} A_1 & C_1 \\ C_1^T & A_2 \end{pmatrix} \begin{pmatrix} -x_1 \\ x_2 \end{pmatrix} > 0.$$

Therefore, $x_1^T A_1 x_1 - 2x_1^T C_1 x_2 + x_2^T A_2 x_2 > 0$. Since

$$x^T A x = (x_1^T, x_2^T) \begin{pmatrix} A_1 & C_1 \\ C_1^T & A_2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} > 0,$$

the second inequality is obtained. □

THEOREM 3.5. *Suppose that A is a symmetric positive definite matrix of the form (2). Let $A_1 = U_1^T D_1 U_1 - R_1$ and $A_2 = U_2^T D_2 U_2 - R_2$ be splittings obtained from Algorithms 3.1 or 3.2. Let*

$$U = \begin{pmatrix} U_1 & 0 \\ 0 & U_2 \end{pmatrix}, D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix}, U_* = \begin{pmatrix} U_1 & (U_1^T D_1)^{-1} C_1 \\ 0 & U_2 \end{pmatrix}.$$

Let $M = U^T D U$, $M_* = U_*^T D U_*$, $N = M - A$, and $N_* = M_* - A$. Then $A = M - N$ and $A = M_* - N_*$ are P -regular splitting of A .

Proof. Note that

$$M + N = 2M - A = \begin{pmatrix} U_1^T D_1 U_1 + R_1 & -C_1 \\ -C_1^T & U_2^T D_2 U_2 + R_2 \end{pmatrix}.$$

Let $x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ be a nonzero vector. Then

$$\begin{aligned} x^T (M + N)x &= x_1^T (U_1^T D_1 U_1 + R_1)x_1 + x_2^T (U_2^T D_2 U_2 + R_2)x_2 - 2x_1^T C_1 x_2 \\ &= 2x_1^T R_1 x_1 + 2x_2^T R_2 x_2 + x_1^T A_1 x_1 + x_2^T A_2 x_2 - 2x_1^T C_1 x_2. \end{aligned}$$

Since R_1 and R_2 are positive semi-definite, Lemma 3.4 implies that $x^T (M + N)x > 0$. Hence, $A = M - N$ is a P -regular splitting of A . Next we will show that $A = M_* - N_*$ is a P -regular splitting of A . Note that

$$\begin{aligned} M_* + N_* &= 2M_* - A \\ &= 2 \begin{pmatrix} U_1^T D_1 U_1 & C_1 \\ C_1^T & U_2^T D_2 U_2 + C_1^T (U_1^T D_1)^{-T} D_1 (U_1^T D_1)^{-1} C_1 \end{pmatrix} - A \\ &= \begin{pmatrix} A_1 + 2R_1 & C_1 \\ C_1^T & 2C_1^T (U_1^T D_1)^{-T} D_1 (U_1^T D_1)^{-1} C_1 + A_2 + 2R_2 \end{pmatrix}. \end{aligned}$$

If we let $V_1 = (U_1^T D_1)^{-1} C_1$, then

$$M_* + N_* = \begin{pmatrix} A_1 + 2R_1 & C_1 \\ C_1^T & 2V_1^T D_1 V_1 + A_2 + 2R_2 \end{pmatrix}.$$

Thus for each nonzero vector x , one obtains

$$\begin{aligned} x^T (M_* + N_*)x &= x_1^T (A_1 + 2R_1)x_1 + 2x_1^T C_1 x_2 \\ &\quad + x_2^T (A_2 + 2R_2)x_2 + 2x_2^T V_1^T D_1 V_1 x_2 \\ &= x_1^T A_1 x_1 + 2x_1^T C_1 x_2 + x_2^T A_2 x_2 + 2x_1^T R_1 x_1 \\ &\quad + 2x_2^T R_2 x_2 + 2x_2^T V_1^T D_1 V_1 x_2. \end{aligned}$$

By assumption, $R_1 \succeq 0$, $R_2 \succeq 0$ and $D_1 \succ 0$. Hence, Lemma 3.4 implies that $x^T (M_* + N_*)x > 0$. It follows that $A = M_* - N_*$ is a P -regular splitting of A . \square

Since the two splittings $A = M - N$ and $A = M_* - N_*$ introduced in Theorem 3.5 are P -regular splittings, from Theorem 2.1 $\rho(M^{-1}N) < 1$ and $\rho(M_*^{-1}N_*) < 1$. Hence, the $M \succ 0$ and $M_* \succ 0$ can be used as preconditioners for the PCG method. Theorem 2.6 also shows that

$$B_k^{-1} = \sum_{i=0}^{k-1} (M^{-1}N)^i M^{-1} \quad \text{and} \quad \hat{B}_k^{-1} = \sum_{i=0}^{k-1} (M_*^{-1}N_*)^i M_*^{-1}$$

are symmetric positive definite and thus they can be used as k -step polynomial preconditioners for the PCG method. Below we provide an efficient algorithm for computing $B_k^{-1}r$ which is one of the basic time-consuming computational kernels of the PCG, where r is a given vector.

Algorithm 3.3 (PRESOL(k)).

```

 $x_0 = 0$ 
For  $i = 1, k$ 
     $x_i = x_{i-1} + M^{-1}(r - Ax_{i-1})$ 
end

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From Algorithm 3.3, it can be seen that $x_k = B_k^{-1}r$. Notice that Algorithm 3.3 computes $B_k^{-1}r$ without using the matrix N . If we replace M in Algorithm 3.3 with M_* , then $\hat{B}_k^{-1}r$ is computed. Since U_i 's and D_i 's in Theorem 3.5 can be computed independently for different i , the M and M_* can be constructed in parallel based on matrix blocks. The idea provided in Theorem 3.5 can be easily extended to a general $m \times m$ block-tridigonal matrix A which is symmetric positive definite.

4. Numerical results

The test PDE problem we are considering in this paper is

$$(3) \quad -(a(x, y)u_x(x, y))_x - (b(x, y)u_y(x, y))_y + c(x, y)u(x, y) = f(x, y)$$

with $a(x, y) > 0$, $b(x, y) > 0$, $c(x, y) \geq 0$, and $(x, y) \in \Omega$, where Ω is a square region, and with suitable boundary conditions on $\partial\Omega$ which denotes the boundary of Ω . All numerical results have been obtained using the PCG method. The MICF and VMICF preconditioners we have used for numerical experiments were obtained without fill-ins. In all cases, the PCG was started with an initial vector $x_0 = 0$ and it was stopped when $\frac{\|r_i\|_2}{\|b\|_2} < 10^{-8}$, where r_i refers to the i th residual $b - Ax_i$. All numerical experiments have been carried out using 64-bit arithmetic on the Cray T3E at the KISTI supercomputing center. In Tables 1 to 4, $ITER$ stands for the number of iterations satisfying the stopping criterion mentioned

above, *Prec* stands for the preconditioner to be used, *P-time* and *I-time* stand for the CPU time required for constructing preconditioners and the CPU time required for the PCG with these preconditioners, respectively. All timing results are reported in seconds using one processor of the Cray T3E. For all test problems, only the matrix A , which is constructed from five-point finite difference discretization of the given PDE, is of importance, so the right-hand side vector b is created artificially. Hence, the right-hand side function f in Examples 4.1 and 4.2 is not relevant.

EXAMPLE 4.1. We consider Equation (3) over the square region $\Omega = (0, 1) \times (0, 1)$ with $a(x, y) = b(x, y) = \cos x$, $c(x, y) = 0$, and Dirichlet boundary condition $u = 0$ on $\partial\Omega$. That is, the following PDE problem is considered:

$$\begin{cases} -\nabla \cdot (\cos x \nabla u) = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases}$$

We have used two uniform meshes of $\Delta x = \Delta y = \frac{1}{101}$ and $\Delta x = \Delta y = \frac{1}{201}$ which lead to two matrices of order $n = 100 \times 100$ and $n = 200 \times 200$, where Δx and Δy refer to the mesh sizes in the x -direction and y -direction, respectively. We have used both the natural row-wise ordering and the Red-Black ordering of the mesh grid. The matrix A generated from this discretization is a symmetric M -matrix and hence it is also a SPD matrix. To generate a SPD matrix which is not an M -matrix, all off-diagonal elements of the matrix A are made positive by taking their absolute values. Once the matrix A is constructed, the right-hand side vector b is chosen so that the exact solution is the discretization of $10xy(1-x)(1-y)e^{x^{4.5}}$. Numerical results for this problem are listed in Tables 1 and 2.

EXAMPLE 4.2. We consider Equation (3) over the square region $\Omega = (0, 1) \times (0, 1)$ with $a(x, y) = b(x, y) = 1$, $c(x, y) = 0$, and Dirichlet boundary condition $u = 0$ on $\partial\Omega$. That is, the following PDE problem is considered:

$$\begin{cases} -\Delta u = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases}$$

We have used the same uniform meshes as in Example 4.1. Once the matrix A is constructed as in Example 4.1, the right-hand side vector b is chosen so that $b = A[1, 1, \dots, 1]^T$. Numerical results for this problem are listed in Tables 3 and 4.

TABLE 1. Numerical results of the PCG for Example 4.1

Ordering (Matrix type)	Prec	$n = 100 \times 100$			$n = 200 \times 200$		
		ITER	P-Time	I-Time	ITER	P-Time	I-Time
Natural (M -matrix)	MICF	121	5.52	1.84	239	98.4	14.1
	VMICF	121	0.01	1.83	239	0.05	14.1
Red-Black (M -matrix)	MICF	142	6.61	1.98	268	116.2	15.2
	VMICF	142	0.01	1.97	268	0.05	15.1
Natural (SPD matrix)	MICF	6	5.52	0.10	4	98.4	0.26
	VMICF	6	0.01	0.10	4	0.05	0.26
Red-Black (SPD matrix)	MICF	128	6.67	1.79	235	115.5	13.3
	VMICF	134	0.01	1.87	250	0.05	14.1

TABLE 2. Numerical results of the PCG with k -step VMICF polynomial preconditioner for Example 4.1

Ordering (Matrix type)	k	$n = 100 \times 100$			$n = 200 \times 200$		
		ITER	P-Time	I-Time	ITER	P-Time	I-Time
Natural (M -matrix)	1	121	0.01	1.83	239	0.05	14.1
	2	85		2.45	168		19.4
	3	68		2.89	136		23.1
	4	59		3.31	118		26.5
Natural (SPD matrix)	1	6	0.01	0.10	4	0.05	0.26
	2	3		0.09	3		0.37
	3	2		0.09	2		0.36
	4	2		0.12	2		0.47
Red-Black (M -matrix)	1	142	0.01	1.97	268	0.05	15.1
	2	154		4.08	255		27.8
	3	135		5.29	258		41.5
	4	122		6.32	233		49.5
Red-Black (SPD matrix)	1	134	0.01	1.87	250	0.05	14.1
	2	103		2.74	195		21.3
	3	86		3.38	161		25.9
	4	75		3.89	140		29.8

5. Conclusions

The construction time of the MICF preconditioner is much larger than that of the VMICF preconditioner, and the convergence rate of the PCG with the MICF preconditioner is as good as or slightly better than that with the VMICF preconditioner (see Tables 1 and 3). So, the VMICF preconditioner is recommended for use on the Cray T3E.

TABLE 3. Numerical results of the PCG for Example 4.2

Ordering (Matrix type)	Prec	$n = 100 \times 100$			$n = 200 \times 200$		
		ITER	P-Time	I-Time	ITER	P-Time	I-Time
Natural (M -matrix)	MICF	115	5.53	1.73	226	98.6	13.6
	VMICF	115	0.01	1.72	226	0.05	13.7
Red-Black (M -matrix)	MICF	130	6.67	1.80	244	115.6	13.9
	VMICF	130	0.01	1.80	243	0.05	13.9
Natural (SPD matrix)	MICF	6	5.53	0.09	4	98.7	0.26
	VMICF	6	0.01	0.09	4	0.05	0.26
Red-Black (SPD matrix)	MICF	122	6.67	1.69	226	115.7	12.8
	VMICF	123	0.01	1.71	225	0.05	12.8

TABLE 4. Numerical results of the PCG with k -step VMICF polynomial preconditioner for Example 4.2

Ordering (Matrix type)	k	$n = 100 \times 100$			$n = 200 \times 200$		
		ITER	P-Time	I-Time	ITER	P-Time	I-Time
Natural (M -matrix)	1	115	0.01	1.72	226	0.05	13.7
	2	81		2.33	159		18.4
	3	66		2.80	130		22.2
	4	57		3.20	112		25.4
Natural (SPD matrix)	1	6	0.01	0.09	4	0.05	0.26
	2	3		0.09	3		0.37
	3	2		0.09	2		0.36
	4	2		0.12	2		0.47
Red-Black (M -matrix)	1	130	0.01	1.80	234	0.05	13.8
	2	101		2.68	189		20.6
	3	85		3.33	157		25.2
	4	74		3.84	137		29.1
Red-Black (SPD matrix)	1	123	0.01	1.71	225	0.05	12.8
	2	93		2.47	175		19.0
	3	78		3.06	146		23.5
	4	70		3.63	130		27.6

The PCG with k -step VMICF polynomial preconditioner reduces the number of iterations as k increases (see Tables 2 and 4), but the computing time of the PCG with k -step VMICF polynomial preconditioner increases as k increases. This is because the reduction in the number of iterations is not enough to balance the increase in the computing time required for $\text{PRESOL}(k)$. Notice that 1-step VMICF polynomial preconditioner is the same as the VMICF preconditioner. Hence, k -step

VMICF polynomial preconditioner is recommended on the Cray T3E only for $k = 1$. That is, the PCG with VMICF preconditioner performs efficiently on the Cray T3E.

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