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A Note on Preconditioned Conjugate Gradients for Solving Singular Systems*

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The polynomial accelerations are very efficient methods for solving large sparse linear systems. In [2] we discussed the general polynomial acceleration methods based on basic iteration methods for solving singular systems, especially, the Chebyshev semi-iteration and the preconditioned conjugate gradient acceleration. In [4] E. F. Kaasschieter discussed the preconditioned conjugate gradients for solving singular systems of which the coefficient matrices are singular Stieljes matrices by using incomplete Cholesky decomposition as preconditioners. But the proof of the main result in [4] (Theorem 3.2) is incorrect. In this note we study the incomplete decomposition of the general singular M-matrix, when the matrix is a Stieljes one our result corrects the error in [4].

Let $\Theta \in R^{n\times n}$, whose entries $0 \leq \theta_{ij} \leq 1$, $i, j = 1, \cdots, n$, are called ignoration factors. The most general form of an incomplete Doolittle decomposition of $A \in R^{n\times n}$: $A + R = LU$ can be expressed as follows:

For $i = 1, \cdots, n$

$$\begin{aligned} u_{ij} &:= a_{ij} - \theta_{ij} \sum_{k=1}^{i-1} l_{ik} u_{kj}, \quad j = i, i+1, \cdots, n, \\ l_{ji} &:= (a_{ji} - \theta_{ji} \sum_{k=1}^{i-1} l_{jk} u_{ki}) / u_{ii}, \quad j = i+1, \cdots, n, \end{aligned} \tag{1}$$

when $\theta_{ij} \equiv 1$, we have the full Doolittle decomposition: $A = \tilde{L}\tilde{U}$. If $R \neq 0$, then $A + R = LU$ is called a proper incomplete Doolittle decomposition (PIDD).

If A is a symmetric positive semi-definite matrix (SPSD), let $\Theta \in R^{n\times n}$ ($0 \leq \theta_{ij} \leq 1$, $i, j = 1, \cdots, n$) be a symmetric ignoration matrix. The most general form of an incomplete Cholesky decomposition of A: $A + B = CC^T$, can be exprassed as follows:

For $i = 1, \cdots, n$

For $j = 1, \cdots, i-1$

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$$c_{ij} = (a_{ij} - \theta_{ij} \sum_{k=1}^{j-1} c_{ik}c_{jk})/c_{jj}, \quad (2)$$

$$c_{ii} = (a_{ii} - \theta_{ii} \sum_{k=1}^{i-1} c_{ik}^2)^{1/2},$$

when $\theta_{ij} \equiv 1$, we have the full Cholesky decomposition: $A = \widetilde{C}\widetilde{C}^T$. If $R \neq 0$ then $A + R = CC^T$ is called a proper incomplete Cholesky decomposition (PICD).

We define $0/0 = 0$ in (1), (2), because the matrix A may be singular.

In what follows in this note we follow closely the notation presented in [1] without explanation.

Theorem 1 Let $A \in R^{n \times n}$ be a singular, irreducible Stieljes matrix, then the Cholesky decomposition of A exists: $A = \widetilde{C}\widetilde{C}^T$. The entries of the triangular matrix $\widetilde{C}$ satisfy the following relations:

$$\widetilde{c}_{ii} > 0 \ (i = 1, \cdots, n-1), \ \widetilde{c}_{nn} = 0, \quad \widetilde{c}_{ij} \leq 0 \ (i > j), \ \widetilde{c}_{ij} = 0 \ (i < j), \quad (3)$$

and for each j ($j = 1, \cdots, n-1$) we have:

There is at least one i ($> j$) such that $\widetilde{c}_{ij} < 0$. (4)

Proof The existence of the decomposition follows straight from [1] (Corollary (4.17)); (3) follows from (2) (where $\theta_{ij} \equiv 1$) and the properties of matrix A. Now we prove (4). From the assumption of the theorem we know that there exists a vector $x \gg 0$ such that $Ax = 0$, i.e. $\widetilde{C}\widetilde{C}^T x = 0$. Thus, we have

$$\widetilde{C}^T x = 0. \quad (5)$$

Expanding (5), we get successively:

$$\widetilde{c}_{nn} = 0, \ \widetilde{c}_{n,n-1} < 0,$$

and for each j ($j = n-2, \cdots, 1$): there exists at least one i ($> j$) such that $\widetilde{c}_{ij} < 0$.

Theorem 2 Let A be a singular, irreducible Stieljes matrix, then for any symmetric ignoration matrix Θ exists the corresponding incomplete Cholesky decomposition: $A + R = CC^T$. If this decomposition is a PICD, then we have the following inequalities:

$$c_{ii} > 0 \ (i = 1, \cdots, n), \ c_{ij} \leq 0 \ (i > j), \ c_{ij} = 0 \ (i < j).$$

Proof The existence of incomplete Cholesky decomposition can be proof easily (c.f. [4] or Theorem 6 below).

From (2) we have:

$$c_{ii} \geq \widetilde{c}_{ii} > 0 \ (i = 1, \cdots, n-1), \ c_{nn} \geq \widetilde{c}_{nn} = 0, \quad 0 \geq c_{ij} \geq \widetilde{c}_{ij} \ (i \neq j) \quad (6)$$

If the decomposition is a PICD then $C \neq \widetilde{C}$ and there exsists at least one $c_{i_0 j_0}$ ($i_0 \geq j_0$) such that $c_{i_0 j_0} > \widetilde{c}_{i_0 j_0}$. From (2) and (6) we have $c_{i_0 i_0} > \widetilde{c}_{i_0 i_0}$. We can assume $i_0<n$ (otherwise the proof is completed). From Theorem 1 we know that there exists at least one i_1 ($>i_0$) sueh that $\tilde{c}_{i_1, i_0}\neq 0$, then from (2), (6) and the inequality $c_{i_0 i_0}>\tilde{c}_{i_0 i_0}$ we have $0\geq c_{i_1 i_0}>\tilde{c}_{i_1 i_0}$. Hence, we have, again from (2) and (6), $c_{i_1 i_1}>\tilde{c}_{i_1 i_1}$. Continue this process, we get, finally, $c_{nn}>\tilde{c}_{nn}=0$.

The proof of Theorem 2 provides a correct proof for Theorem 3.2 in [4].

Now we consider nonsymmetric singular systems.

Theorem 3 Let $A\in R^{n\times n}$ be a singular, irreducible M-matrix, then there exists a unit lower triangular M-matrix $\tilde{L}$ and an upper triangular M-matrix $\tilde{U}$ such that $A=\tilde{L}\tilde{U}$, i.e. A has a Doolittle decomposition. Furthermore, holds the following argument: For each j ($j=1,\cdots,n-1$) there exists at least one i_l ($>j$) and one i_u ($>j$) such that $\tilde{l}_{i_l j}<0$ and $\tilde{u}_{j i_u}<0$.

Proof Since the leading principal submatrix of order ($n-1$) of A is a nonsingular M-matrix of order $n-1$, the $n-1$ leading principal minore of A are all positive. From the unique LDU decomposition theorem[3] we have $A=\tilde{L}D\hat{U}\equiv\tilde{L}\tilde{U}$, where $\tilde{L}$ and $\hat{U}$ are unit lower and unit upper triangular nonsingular M-matrix, respectively, $D=\mathrm{diag}(d_{ii})$ is a nonnegative diagonal matrix with $d_{ii}>0$ ($i=1,\cdots,n-1$), hence, $\tilde{U}\equiv D\hat{U}$ is a M-matrix.

Since A is a singular, irreducible matrix, there exists a vector $y\gg 0$ such that $Ay=0$, i.e. $\tilde{L}\tilde{U}y=0$. Since $\tilde{L}$ is nonsingular we have

$$Uy=0. \qquad (7)$$

By expanding (7) and considering $\tilde{u}_{ii}>0$ ($i=1,\cdots,n-1$) we have successively:

$u_{nn}=0$, $u_{n-1,n}<0$ and for each j ($j=n-2,\cdots,1$) there exists at least one i_u ($>j$) such that $\tilde{u}_{j i_u}<0$.

Sincc $A^T=\hat{U}^T D\tilde{L}^T$ is also a singular, irreducible M-matrix, there exists a vector $\hat{y}\gg 0$ such that $\hat{U}^T D\tilde{L}^T\hat{y}=0$. Thus we have

$$D\tilde{L}^T\hat{y}=0. \qquad (8)$$

By expanding (8) and considering $d_{ii}>0$ ($i=1,\cdots,n-1$), we have successively:

$\tilde{l}_{n,n-1}<0$, and for each j ($j=n-2,\cdots,1$) there exists at least one i_l ($>j$) such tkat $\tilde{l}_{i_l j}<0$.

Corollary 4 Let A be a nonsingular M-matrix or a singular, irreducible M-matrix, $B\in Z^{n\times n}$ and $A\leq B$, then B has a Doolittle decomposition.

Proof From [6] or Theorem 3 we know that A has a Doolittle decomposition $A=\tilde{L}\tilde{U}$. From (1) and the assumption on B one can easily get that B

has a Doolittle decomposition $B=\hat{L}\hat{U}$ and hold the following inequalities:

$$\tilde{L}\leq\hat{L} \text{ and } \tilde{U}\leq\hat{U}.$$

Crrollary 5 Let A be a singular, irreducible M-matrix, $B\in Z^{n\times n}$ and $A<B$, then B is a nonsingular M-matrix.

Proof From Theorem 3 and Corollary 4 we know that A and B have Doolittle decompositions $A=\tilde{L}\tilde{U}$ and $B=\hat{L}\hat{U}$, respectively. Since $A<B$, at least one of the following inequalities holds:

$$\tilde{L}<\hat{L} \text{ and } \tilde{U}<\hat{U}.$$

From Theorem 3 and (1)(c.f. the proof of Theorem 2) we know that the entries of $\hat{L}$ or $\hat{U}$ which are strictly larger than the corresponding ones in $\tilde{L}$ or $\tilde{U}$ move down or rightwards to the rightdown corner of the matrix. Therefore, we get, finally, $\hat{u}_{nn}>\tilde{u}_{nn}=0$. Thus, $\hat{L}$ and $\hat{U}$ are all nonsingular M-matrices, therefore, $B=\hat{L}\hat{U}$ is a nonsingular M-matrix.

Theorem 6 Let A be a singular, irreducible M-matrix, then A has an incomplete Doolittle decomposition:

$$A+R=LU. \tag{9}$$

If this is a PIDD then the decomposition (9) yields a regular splitting of A.

Proof From Theorem 3 we know that A has full Doolittle decomposition $A=\tilde{L}\tilde{U}$. Since A be a singular, irreducible M-matrix, the leading principal submartix of order n-1 of A is a nonsingular M-matrix, whose incomplete Doolittle decomposition exists (c.f. [6]) and (1) (replace n with n-1) can be used to compute u_{ij} and l_{ji} and the following inequalities hold:

$$u_{ij}\geq\tilde{u}_{ij},\ l_{ji}\geq\tilde{l}_{ji}\ (i,\ j=1,\cdots,\ n-1). \tag{10}$$

Obviously, the expressions in (1) when $i=n$ are meaningfull and hold the following inequalities:

$$u_{kn}\geq\tilde{u}_{kn}\ (k=1,\cdots,n),\quad l_{nk}\geq\tilde{l}_{nk}\ (k=1,\cdots,\ n-1). \tag{11}$$

Hence, A has an incomplete decomposition which yields a splitting of A:

$$A=LU-R, \tag{12}$$

where $R\geq0$ because of the fact that the entries of the ignoration matrix Θ satisfy the inequalities; $0\leq\theta_{ij}\leq1$ $(i,\ j=1,\cdots,\ n)$. If the decomposition (9) of A is a PIDD then $R>0$. Hence, $LU>A$. It is easy to show (c.f. the proof of Corollary 5) that L and U are nonsingular M-matrices. Since $(LU)^{-1}=U^{-1}L^{-1}\geq0$, hence (12) is a regular splitting of A.

Finally, we study the case when A is a singular H-matrix.

Theorem 7 Let A be a singular, irreducible H-matrix, then A has an incomplete Doolittle decomposition with respect to any ignoration matrix Θ: $A+R=LU$. If this decomposition is a PIDD, then LU is nonsingular.

Proof At first, we assume the diagonals of A are all nonnegative. Let $\hat{A}$ be the comparision matrix for A. Obviously, $\hat{A}$ is a singular, irreducible M-matrix, so that $\hat{A}$ has an incomplete Doolittle decomposition $\hat{A}+\hat{R}=\hat{L}\hat{U}$. By induction on i in (1) it is easy to show[5] that A has an incomplete Doolittle decompsition $A+R=LU$ and the following inequalities hold:

$$u_{ii}\geq\hat{u}_{ii}\ (i=1,\cdots,\ n),\quad 0\geq-|l_{ji}|\geq\hat{l}_{ji}$$
$$0\geq-|u_{ij}|\geq\hat{u}_{ij}\ (j=i+1,\ \cdots,\ n)\ . \tag{13}$$

If the decomposition is a PIDD, then from Theorem 6 we know that $\hat{L}$ and $\hat{U}$ are nonsingular M-matrices. Therefore, from (13) we know that U is a nonsingular upper triangular matrix.

For a general singular, irreducible H-matrix A let $D=\text{diag}\ (\text{sign}\ (a_{ii}))$, where the function sign (a) is defined as follows:

$$\text{sign}(a)=\begin{cases}1, & \text{if } a\geq 0,\\ -1, & \text{if } a<0.\end{cases}$$

Let $\check{A}=AD$, obviously, $\check{A}$ is a singular, irreducible H-matrix with nonnegative diagonals and $\check{A}$ and A have the same comparision matrix. Since $\check{A}$ has an incomplete Doolittle decomposition $\check{A}+\check{R}=\check{L}\check{U}$, it implies that A has decomposition $A+\check{R}D=\check{L}(\check{U}D)\equiv LU$. If the decomposition is a PIDD, i.e. $\check{R}D\neq 0$, then $\check{R}\neq 0$, hence, $\check{L}\check{U}$ is nonsingular. finally, we get that LU is nonsingular.

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