Nonsingularity Study of SAI Preconditioners for M-matrices

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Abstract

In this paper, we study the theoretical properties of sparse approximate inverse (SAI) preconditioners. Particularly, we show that for M-matrices, nonnegativeness is the key to compute the nonsingular SAI preconditioners.

1 Introduction

Consider a sparse linear system

$$Ax = b, \tag{1}$$

where A is a nonsingular general square matrix of order n. The convergence rate of a Krylov subspace solver applied directly to (1) may be slow if the matrix A is ill-conditioned. In order to speed up the convergence rate of such iterative methods, we transform (1) into an equivalent system

$$MAx = Mb, \tag{2}$$

where M, the preconditioner, is any nonsingular matrix of order n. Krylov subspace solver applied to the transformed system will converge faster than the original system if the condition number of MA is better than that of A.

A sparse approximate inverse (SAI) is simply a sparse matrix M which is a good approximation to A^{-1}. The major driving force behind the search for efficient sparse approximate inverse preconditioners is their potential advantages in parallel computing. The idea is that once computed, a sparse preconditioner matrix M can be applied via a simple matrix-vector product, which can be implemented efficiently on any parallel computer [12]. The ease and efficiency of this parallel operation compares favorably with the highly sequential nature of the triangular solution procedures used by incomplete LU factorization preconditioning techniques.

Many efforts have been made to improve the efficiency and robustness of standard SAI preconditioning techniques. Both multilevel and multistep preconditioning approaches [16, 18] were proposed, and they were shown to be more efficient and robust than the standard techniques. However, because the theoretical basis for high performance preconditioning is still not well understood, most of the achievements are based on experiential approaches, which restrict the development of robust preconditioning techniques. The theoretical analysis of the preconditioning process is a necessary for designing robust and efficient preconditioners.

One of the open theoretical problems in SAI preconditioning is the nonsingularity of the computed preconditioner. The SAI preconditioning attempts to transform the original linear system into a better-conditioned preconditioned system,

*The author's research work was funded by the U.S. National Science Foundation under grant ASC070018T and CNS-0739320, by the U.S. South Dakota Governor's Individual Research Seed Grant Award, by the South Dakota Brin Program of NIH/NCRR, and by the China National Science Foundation under grants 60673151 and 60403036. Email: Kai.Wang@usd.edu. URL:http://www.usd.edu/∼Kai.Wang.

†The author's research work was funded by the China National Science Foundation under grants 60673151 and 60403036.

which allows the Krylov subspace iterative solver converge faster. However, if the preconditioner M is singular, the preconitioned system will be singular. Thus, the following application of Krylov subspace solver will not yield correct solution even it converges successfully.

The nonsingularity justification is very important for the application of SAI preconditioner. Unfortunately, unlike the ILU type preconditioners, whose nonsingularity can be guaranteed by forcing the diagonal elements of the triangular matrices (L and U) to be nonzero, most of existing SAI preconditioning techniques, e.g., those based on Frobenius norm minimization, do not supply practically useful strategies to guarantee the nonsingularity during the computation. Even the factorized sparse approximate inverse preconditioners [4, 19] have the similar way as LU type preconditioners to guarantee the nonsingularity of the approximate inverse, their construction is inherently sequential, which makes them not suitable for parallel computing.

In this paper, we study the property of SAI preconditioners. We reveal the conditions for nonsingular SAI preconditioning. Particularly, for M-matrix, we find out that the nonnegativeness is the key to the nonsingularity of its SAI preconditioning matrix.

The paper is organized in the following way. Section 2 introduces background on sparse approximate inverse preconditioning techniques. Section 3 gives theoretical results from the analysis of the preconditioned system. Section 4 includes the nonsingularity justification of sparse approximate inverse preconditioning for general sparse matrices and M-Matrix. Section 5 contains some concluding remarks.

2 Sparse Approximate Inverse

The sparse approximate inverse technique that we study here is based on the idea of Frobenius norm minimization. This is also the one that initially motivated research in the sparse approximate inverse preconditioning [2, 3]. Its advantage over the other preconditioning methods lies in the high degree of parallelism in both the preconditioner construction and application phases.

Since we want M to be a good approximation to A^{-1}, it is ideal if $MA \approx I$ or $AM \approx I$. The $AM \approx I$ format is easier for us to illustrate the Frobenius norm minimization idea, which will be described in detail in the following paragraphs.

In order to have $AM \approx I$, we want to minimize the functional

$$f(M) = \min_{M} \|AM - I\| \tag{3}$$

for all possible nonsingular square matrices M of order n, with respect to a certain norm. Without any constraint on M, the minimization problem (3) has the obvious solution $M = A^{-1}$. This solution is undesirable because of its high computational and memory cost.

Thus, we are interested in a constrained minimization such that M has a certain sparsity pattern, or nonzero structure—that is, only certain entries of M are allowed to be nonzero. Given a sparsity pattern Ω (which could be fixed or depend on the original matrix), we minimize the functional

$$f(M) = \min_{M \in \Omega} \|AM - I\|. \tag{4}$$

Although any norm could be used in the above definition, a particularly convenient norm is the Frobenius norm, defined for a matrix $A = (a_{ij})_{n \times n}$ as $\|A\|_F = \sqrt{\sum_{i,j=1}^{n} a_{ij}^2}$ [14]. With the Frobenius norm, the minimization problem (4) can be decoupled into n independent subproblems and can proceed as (using square for convenience)

$$\|AM-I\|_F^2 = \sum_{k=1}^{n} \|(AM-I)e_k\|_2^2 = \sum_{k=1}^{n} \|Am_k-e_k\|_2^2, \tag{5}$$

where m_k and e_k are the kth columns of M and I, respectively. It follows that the minimization problem (4) is equivalent to minimizing the individual functions

$$\|Am_k - e_k\|_2, \qquad k = 1, 2, \ldots, n \tag{6}$$

with certain restrictions placed on the sparsity pattern of m_k. In other words, each column of M can be computed independently.

If the sparsity pattern of m_k allows, say, n_k nonzero entries, the rest of the entries are forced to be zero. Denote the n_k nonzero entries of m_k by p_k and the n_k corresponding columns of A by A_k. The individual minimization problem (6) is thus reduced to a least squares problem of order $n \times n_k$

$$\min_{p_k} \|A_k p_k - e_k\|_2, \qquad k = 1, 2, \ldots, n. \tag{7}$$

Since A is sparse, its submatrix A_k may have many rows that are identically zero. The matrix A_k is usually a very small rectangular matrix. It has full rank if original matrix A is nonsingular, and can be solved very efficiently. The solves of these n problems yield an approximate inverse matrix M, which minimizes $\|AM - I\|_F$ for the given sparsity pattern.

The parallelism inherent in the technique is the computation of the columns p_k independently of each other. It can be implemented efficiently with a maximum degree of parallelism n on any modern parallel machine [12].

The remaining problem for constructing a sparse approximate inverse preconditioner is to decide how to choose a good sparsity pattern for M. There are a few heuristic strategies. Both static and dynamic sparsity pattern approaches have been proposed [6, 7, 8, 9, 10, 13, 15]. Each has a successful implementation, the ParaSails by Chow [9, 11] based on static sparsity pattern, and the SPAI by Barnard [1] based on dynamic sparsity pattern. A full performance comparison of these two strategies is reported at [17].

3 Theoretical Study of the Preconditoned System

Our study is based on the Frobenius norm minimization method introduced in the previous section. We assume that the original matrix A is a nonsingular matrix, and we assume that the diagonal pattern is always included in the selected sparsity pattern. From the introduction in Section 2, we know that the solution of each minimization problem is a vector p_k with length n_k, where $n_k \leq n$, and is equal to the number of nonzeros in the sparsity pattern.

The vector p_k can be computed by solving the normal equation

$$A_k^T A_k p_k = A_k^T e_k. \tag{8}$$

It is very difficult to study the properties of the SAI matrix M directly, since the columns of M are computed independently, and there is no direct relationship among them. However, we do know that a good SAI matrix M should make the preconditioned system AM close to an identity matrix I. We investigate the diagonal property of AM instead.

Theorem 3.1. *The diagonal elements of the AM matrix are nonnegative, and the value of each diagonal element is equal to the sum of the square values of all the elements in the same column.*

Proof: Let $AM = (d_{ij})_{i,j=1\ldots n}$. According to our previous discussion, the nonzero elements at each column of AM can be expressed as

$$A_k p_k, \quad k = 1, \ldots, n.$$

Here p_k stands for the solution of (8).

d_{kk}, the kth diagonal element of AM, corresponds to

$$d_{kk} = e_k^T A_k p_k = p_k^T A_k^T e_k.$$

According to (8), we get that

$$A_k^T e_k = A_k^T A_k p_k.$$

Multiplying this relation on the left by p_k^T gives

$$d_{kk} = p_k^T A_k^T e_k = (A_k p_k)^T A_k p_k = \sum_{j=1}^{n} d_{jk}^2.$$

□

Next, we show the relationship of AM and the identity matrix I.

Theorem 3.2. *The diagonal elements of the matrix $AM - I$ are nonpositive, and the value of each diagonal element is equal to the negative sum of the square values of all the elements in the same column.*

Proof: Let $AM - I = (c_{ij})_{i,j=1...n}$. The proof is straightforward. Considering $c_{jk} = d_{jk}$ when $j \neq k$, and $c_{jk} = d_{jk} - 1$, when $j = k$, where d_{jk} is the element of AM, we have

$$\begin{array}{ll} & c_{kk} = d_{kk} - 1 \\ \Rightarrow & c_{kk} = -(d_{kk} - 1)^2 - d_{kk} + d_{kk}^2 \\ \Rightarrow & c_{kk} = -c_{kk}^2 - \sum_{j=1}^{n} d_{jk}^2 + d_{kk}^2 \\ \Rightarrow & c_{kk} = -c_{kk}^2 - \sum_{j=1, j\neq k}^{n} d_{jk}^2 \\ \Rightarrow & c_{kk} = -\sum_{j=1}^{n} c_{jk}^2. \end{array}$$

□

Using the Frobenius norm, we can give following theorem..

Theorem 3.3. *The Frobenius norm $\|AM - I\|_F$ is the square root of the sum of the absolute values of the diagonal elements of $AM - I$.*

Proof: This can be proved by

$$\begin{array}{ll} & \|AM - I\|_F^2 \\ = & \sum_{k=1}^{n} \|A_k p_k - e_k\|_2 \\ = & \sum_{k=1}^{n} \sum_{j=1}^{n} c_{jk}^2. \end{array}$$

From Theorem 3.2, we get

$$\|AM - I\|_F^2 = -\sum_{k=1}^{n} c_{kk}.$$

Here c_{kk} is the diagonal element of $AM - I$.

□

The above theorems illustrate some interesting properties of the preconditioned matrix AM. In the following discussion, we show that these results can be used in discovering the condition to guarantee the nonsingularity of SAI preconditioners.

4 Nonsingularity Study of SAI Preconditioning

Utilizing the theorems given in the previous section, we investigate the nonsingularity of the SAI preconditioning. First, we study the SAI preconditioning for general matrices, and give a practical method to check its nonsingularity. Then, we study the SAI preconditioning for a type of special structured matrix — the M-matrix, and prove that the nonnegativeness is the key to its nonsingularity.

4.1 Nonsingularity of SAI Preconditioning for General Matrices

The nonsingularity justification of a matrix is an NP-Completeness problem. However, using the theorems in the previous section, we can easily give a practical method to check the nonsingularity of the computed SAI matrix M for any general sparse matrix A.

Theorem 4.1. *If the sum of the absolute values of the diagonal elements of $AM - I$ is less than 1 then M is nonsingular.*

Proof: Let $AM - I = (c_{ij})_{i,j=1...n}$. Theorem 3.3 shows the Frobenius norm of $AM - I$ can be written as

$$\|AM - I\|_F^2 = \sum_{k=1}^{n} |c_{kk}|.$$

So $\sum_{k=1}^{n} |c_{kk}| < 1$ implies

$$\|AM - I\|_F < 1.$$

It is well known that when

$$\|AM - I\|_F = \|I - AM\|_F < 1,$$

then $I - (I - AM) = AM$ is a nonsingular matrix [14], so M is nonsingular.

□

From above theorem, we can see that, to verify the nonsingularity of an approximate inverse matrix, we only need to calculate the sum of the diagonal elements of $AM - I$. This is particularly useful for the multistep successive preconditioning strategies proposed in [16], where multiple matrices, $M_1, ..., M_s$, are computed to approximate the inverse of A. We need to guarantee the nonsingularity of all computed M_i. Because at each step i, the product of $A * M_1 * ... * M_{i-1}$ will be calculated, and then a SAI preconditioner M_i is constructed to approximate the inverse of the product of $A * M_1 * ... * M_{i-1}$, the justification based on Theorem 4.1 will be straightforward and incur no additional computational cost.

4.2 Nonsingularity Study of SAI Preconditioning for M-matrix

In this section, we study the nonsingularity of SAI preconditioning For M-matrix. First, we give some known properties of M-matrix [5], which will be used in the following discussion. If a matrix A is an M-matrix, then [5]:

- The diagonal elements of A are nonnegative (≥ 0), and the off-diagonal elements of A are nonpositive (≤ 0).
- The primary submatrices of A are M-matrix.
- The inverse of A is nonnegative.
- There exists a positive diagonal matrix D which makes AD a strictly column diagonally dominant M-matrix.

For the convenience of discussion, we reorder the rectangular matrix A_k by a permutation so that A_k can be written in the block form

$$\begin{pmatrix} B_k \\ E_k \end{pmatrix}. \tag{9}$$

Here B_k is a primary submatrix of A with rank n_k, and E_k is a rectangular matrix formed by the remaining elements. We can easily see that all elements in E_k are from the off-diagonal elements of A. Particularly, we point out that the permutation makes kth diagonal element of A be permuted to some places in the diagonal of B_k. Not losing generality, we assume it is permuted to be the first diagonal element of B_k.

After permutation, the minimization problems (7) will be rewritten as

$$\min_{p_k} \|A_k p_k - e_1\|_2, \quad k = 1, \ldots, n \tag{10}$$

Here, e_1 is the corresponding permutation of e_k with the first element equals to 1, and all other elements equals to 0.

Using the block form of A_k in 9, the normal equation to solve the minimization problems will be

$$\begin{aligned} & A_k^T A_k p_k = A_k^T e_1 \\ \Rightarrow \quad & (B_k^T B_k + E_k^T E_k) p_k = A_k^T e_1. \end{aligned} \tag{11}$$

Note that $A_k^T e_1$ is the first row of A_k, which is also the first row of B_k, we have

$$(B_k^T B_k + E_k^T E_k) p_k = B_k^T \tilde{e}_1. \tag{12}$$

Here $\tilde{e}_1$ is different from e_1 in its length. When the original matrix A is an M-matrix, we get following Theorem.

Theorem 4.2. *If the SAI matrix M of an M-matrix A is nonnegative, then AM is a matrix with nonnegative diagonal elements and nonpositive off-diagonal elements, and $AM - I$ is a nonpositive matrix.*

Proof: From Theorem 3.1 and Theorem 3.2, we know that the diagonal elements of AM and $AM - I$ are nonnegative and nonpositive respectively. Next we only need to prove the off-diagonal elements of $AM - I$, which are also the off-diagonal elements of AM, are nonpositive.

Each column of $AM - I$ can be expressed by a permutation of

$$\begin{pmatrix} B_k p_k - \tilde{e}_1 \\ E_k p_k \end{pmatrix}. \tag{13}$$

We only need to prove that, when $p_k \geq 0$, $B_k p_k - \tilde{e}_1$ and $E_k p_k$ are nonpositive.

Obviously, when A is a nonsingular M-matrix, B_k is a nonsingular M-matrix because it is a primary submatrix of A; and the matrix E_k is a nonpositive matrix as it is formed by the off-diagonal elements of A.

$E_k p_k \leq 0$ is clear because $E_k \leq 0$ and $p_k \geq 0$. Next we prove $B_k p_k - \tilde{e}_1 \leq 0$.

From (12), we get

$$\begin{array}{rl} & B_k^T B_k p_k + E_k^T E_k p_k - B_k^T \tilde{e}_1 = 0 \\ \Rightarrow & B_k^T B_k p_k - B_k^T \tilde{e}_1 = E_k^T E_k p_k \\ \Rightarrow & B_k p_k - \tilde{e}_1 = -B_k^{-T} E_k^T E_k p_k. \end{array}$$

B_k is a nonsingular M-matrix, so B_k^{-1} is a nonnegative matrix. Therefore,

$$-B_k^{-T} E_k^T E_k p_k$$

is a nonpositive vector, so $B_k p_k - \tilde{e}_1$ is nonpositive.

Therefore, the Theorem is obvious.

□

From the properties of M-matrix, we know that any M-matrix can be transformed to a strictly column diagonally dominant M-matrix, multiplied by a diagonal matrix D. The following discussion considers the original matrix A is a diagonally dominant M-matrix.

Theorem 4.3. *Suppose A is a column diagonally dominant M-matrix. If the computed sparse approximate inverse preconditioner M is a nonnegative matrix, then AM is a diagonally dominant matrix. Particularly, if A is strictly column diagonally dominant, then M is nonsingular, and AM is also an M-matrix.*

Proof: Let d_k be one column in AM. According to Theorem 4.2, when M is a nonnegative matrix,

$$d_{kk} \geq 0,$$

and

$$d_{ik} \leq 0, \quad i \neq k.$$

Since $d_{ik} = \sum_{j=1}^{n} a_{ij} m_{jk}$,

$$\begin{array}{rl} & \sum_{i=1}^{n} d_{ik} \\ = & \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} m_j \\ = & \sum_{j=1}^{n} \sum_{i=1}^{n} a_{ij} m_j \\ = & \sum_{j=1}^{n} m_j \sum_{i=1}^{n} a_{ij}. \end{array}$$

A is a diagonally dominant M-matrix, so we have

$$\sum_{i=1}^{n} a_{ij} \geq 0.$$

Therefore, we get

$$\sum_{i=1}^{n} d_{ik} = \sum_{j=1}^{n} m_j \sum_{i=1}^{n} a_{ij} \geq 0.$$

That means AM is a diagonally dominant matrix. Obviously, when A is strictly diagonally dominant, AM is also a strictly diagonally dominant M-matrix, which implies M is nonsingular.

□

From Theorem 4.3, we can see that for a strictly column diagonally dominant M-matrix, the nonsingularity of its approximate inverse matrix can be guaranteed by nonnegativeness. Since every M-matrix can be transformed to a diagonally dominant matrix by a diagonal matrix D, this theorem can be extended to general M-matrix by first transforming the M-matrix A into a diagonally dominant matrix A_1; then making A_1 diagonally dominant by adding a small value, say, 0.001 to the diagonal elements of A_1; finally, computing the nonnegative sparse approximate inverse preconditioner M for $\tilde{A}$. M and D will be the preconditioner of the M-matrix. Here we point out that improving the matrix property by an offset of the diagonal elements is a strategy used in many preconditioning techniques [14].

5 Conclusions

The theoretical study of preconditioning technique is important. In this paper, We conduct research on nonsingular sparse approximate inverse preconditioning. By studying the preconditioned system, we find that for general sparse matrices, as long as the diagonal elements of their preconditioned system are close enough to 1, their SAI preconditioner will be nonsingular; for M-matrices, a nonnegative SAI preconditioner can guarantee the computed SAI preconditioner nonsingular. These theoretical results can advise us for designing robust SAI preconditioner. That is our next step research plan.

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