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A single-step HSS method for non-Hermitian positive definite linear systems[☆]

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ABSTRACT

In this paper, based on the Hermitian and skew-Hermitian splitting (HSS) iteration method, a single-step HSS (SHSS) iteration method is introduced to solve the non-Hermitian positive definite linear systems. Theoretical analysis shows that, under a loose restriction on the iteration parameter, the SHSS method is convergent to the unique solution of the linear system. Furthermore, we derive an upper bound for the spectral radius of the SHSS iteration matrix, and the quasi-optimal parameter is obtained to minimize the above upper bound. Numerical experiments are reported to the efficiency of the SHSS method; numerical comparisons show that the proposed SHSS method is superior to the HSS method under certain conditions.

1. Introduction

Many problems in scientific computing result in a system of linear equations

$$Ax = b, \tag{1.1}$$

where A is a non-Hermitian and positive definite matrix (that is, the Hermitian part of A is positive definite), x is an unknown vector and b is a given vector. In order to more efficiently use the iteration methods for solving (1.1), usually, efficient matrix splittings of the coefficient matrix A are required. For example, splitting the matrix A into its diagonal and off-diagonal parts, the classical Jacobi and Gauss–Seidel iterations can be obtained [1–3]. To determine the asymptotic convergence rate of the iteration method, the value of the spectral radius of the corresponding iteration matrix has to be estimated.

Let $H = \frac{1}{2}(A + A^*)$ and $S = \frac{1}{2}(A - A^*)$. Then

$$A = H + S.$$

Obviously, the above matrix splitting is the Hermitian and skew-Hermitian splitting (HSS) of the coefficient matrix [4]. Based on this matrix splitting, the HSS iteration method is introduced in [4] to solve the large sparse non-Hermitian positive definite linear systems and described below.

The HSS method: Given an initial guess $x^{(0)}$, for $k = 0, 1, 2, \ldots$ until $\{x^{(k)}\}$ converges, compute

$$\begin{cases} (\alpha I + H)x^{(k+\frac{1}{2})} = (\alpha I - S)x^{(k)} + b, \\ (\alpha I + S)x^{(k+1)} = (\alpha I - H)x^{(k+\frac{1}{2})} + b, \end{cases} \tag{1.2}$$

where $H = \frac{1}{2}(A + A^*)$ and $S = \frac{1}{2}(A - A^*)$ are the Hermitian and skew-Hermitian parts of A, respectively, and α is a given positive constant.

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It is shown in [4] when H is positive definite, the HSS method converges unconditionally to the unique solution of the linear system. Meanwhile, in theory, the optimal iteration parameter $\alpha = \sqrt{\lambda_{\min}(H)\lambda_{\max}(H)}$, where $\lambda_{\min}(H)$ and $\lambda_{\max}(H)$ are the extreme eigenvalues of matrix H, is obtained to minimize an upper bound of the spectral radius of the iteration matrix associated with (1.2).

Due to its promising performance and elegant mathematical properties, the HSS method immediately attracts considerable attention and results in many papers devoted to various aspects of the new algorithms, such as the NSS method [5], the PSS iteration method [6], the GHSS iteration method [11,14], the MHSS iteration method [7], the PHSS iteration method [8], the AHSS iteration method [9], and the LHSS iteration method [12,13]. One can see [10] for a comprehensive survey on the HSS method.

Clearly, the HSS method is the need to solve two linear subsystems with $H + \alpha I$ and $S + \alpha I$. Since the coefficient matrix, $H + \alpha I$, of linear systems is Hermitian positive definite, there can employ CG method to gain its solution easily. Since the coefficient matrix, $S + \alpha I$, of linear systems is skew-Hermitian, in general, its solution is not easy to obtain. In some cases, its solution is as difficult as that of the original linear system [11,14].

In this paper, the SHSS method is introduced to solve the non-Hermitian positive definite linear systems to avoid solving a shifted skew-Hermitian linear subsystem with coefficient matrix $S + \alpha I$ and is described below.

$$(\alpha I + H)x^{(k+1)} = (\alpha I - S)x^{(k)} + b, \quad k = 0, 1, \ldots. \tag{1.3}$$

Theoretical analysis shows that the SHSS method is convergent to the unique solution of the linear system for a loose restriction on the iteration parameter α. The contraction factor of the SHSS iteration can be bounded by a function, which is dependent only on the choice of the iteration parameter α, the smallest eigenvalue of matrix H and the largest singular-value of matrix S. Numerical experiments are reported to the efficiency of the SHSS method; numerical comparisons show that the proposed SHSS method is superior to the HSS method under certain conditions.

2. Convergence analysis

In this section, we will discuss the convergence properties of the SHSS method. To this end, the iterative scheme (1.3) can be transformed into the following form:

$$x^{(k+1)} = (\alpha I + H)^{-1}(\alpha I - S)x^{(k)} + (\alpha I + H)^{-1}b, \quad k = 0, 1, \ldots. \tag{2.1}$$

The SHSS iteration method given by (2.1) converges to the unique solution of (1.1) for an arbitrary initial guess if and only if the spectral radius of the iteration matrix,

$$T_\alpha = (\alpha I + H)^{-1}(\alpha I - S),$$

is less than one, i.e., $\rho(T_\alpha) < 1$.

Concerning the convergence property of the SHSS iteration method, we have the following theorem.

Theorem 2.1. *Let $A \in \mathbb{C}^{n\times n}$ be a positive definite matrix, let $H = \frac{1}{2}(A + A^*)$ and $S = \frac{1}{2}(A - A^*)$ be its Hermitian and skew-Hermitian parts, and let α be a positive constant. Then the spectral radius $\rho(T_\alpha)$ of the iteration matrix T_α of the SHSS iteration method is bounded by*

$$\delta_\alpha = \frac{\sqrt{\alpha^2 + \sigma_{\max}^2}}{\alpha + \lambda_{\min}}, \tag{2.2}$$

where $\lambda_{\min}$ is the smallest eigenvalue of matrix H and $\sigma_{\max}$ is the largest singular-value of matrix S. Moreover,

(i) *if $\lambda_{\min} \geq \sigma_{\max}$, then $\delta_\alpha < 1$ for any $\alpha > 0$, which means that the SHSS iteration method is unconditional convergent;*
(ii) *if $\lambda_{\min} < \sigma_{\max}$, then $\delta_\alpha < 1$ if and only if*

$$\alpha > \frac{\sigma_{\max}^2 - \lambda_{\min}^2}{2\lambda_{\min}}, \tag{2.3}$$

which means that the SHSS iteration method is convergent under the condition (2.3).

Proof. By direct computations, we have

$$\begin{aligned}
\rho(T_\alpha) &= \rho((\alpha I + H)^{-1}(\alpha I - S)) \\
&\leq \|(\alpha I + H)^{-1}(\alpha I - S)\|_2 \\
&\leq \|(\alpha I + H)^{-1}\|_2 \|\alpha I - S\|_2 \\
&= \max_{\lambda_i \in \lambda(H)} \frac{1}{\alpha + \lambda_i} \max_{\sigma_i \in \lambda(S)} \sqrt{\alpha^2 + \sigma_i^2} \\
&= \frac{\sqrt{\alpha^2 + \sigma_{\max}^2}}{\alpha + \lambda_{\min}}.
\end{aligned}$$

The upper bound of $\rho(T_\alpha)$ given in (2.2) is obtained.

By simple calculation, $\delta_\alpha < 1$ is equal to

$$\sigma_{\max}^2 - \lambda_{\min}^2 < 2\alpha\lambda_{\min}. \tag{2.4}$$

If $\lambda_{\min} \geq \sigma_{\max}$, then (2.4) holds true for any $\alpha > 0$, i.e., the SHSS iteration method converges to the unique solution of the system of linear equations (1.1); if $\lambda_{\min} < \sigma_{\max}$, then (2.4) or $\delta_\alpha < 1$ holds if and only if α satisfies (2.3). The proof is completed. □

Theorem 2.1 gives the convergence conditions of the SHSS iteration method for the system of linear equations (1.1) by analyzing the upper bound δ_α of the spectral radius $\rho(T_\alpha)$ of the iteration matrix T_α. Since the optimal parameter α minimizing the spectral radius $\rho(T_\alpha)$ is hardly obtained, we instead give the parameter α^*, which minimizes the upper bound δ_α of the spectral radius $\rho(T_\alpha)$, in the following corollary.

Corollary 2.1. *Let the conditions of Theorem 2.1 be satisfied. Then, the parameter α^* minimizing the upper bound δ_α of the spectral radius $\rho(T_\alpha)$ is*

$$\alpha^* = \arg\min_{\alpha}\left\{\frac{\sqrt{\alpha^2+\sigma_{\max}^2}}{\alpha+\lambda_{\min}}\right\} = \frac{\sigma_{\max}^2}{\lambda_{\min}}, \tag{2.5}$$

and

$$\delta_{\alpha^*} = \frac{\sigma_{\max}}{\sqrt{\lambda_{\min}^2+\sigma_{\max}^2}}. \tag{2.6}$$

Proof. Simple calculation gives

$$\delta_\alpha' = \frac{\alpha\lambda_{\min} - \sigma_{\max}^2}{(\alpha+\lambda_{\min})^2\sqrt{\alpha^2+\sigma_{\max}^2}}.$$

It is obviously that $\delta_\alpha' > 0$ for $\alpha > \frac{\sigma_{\max}^2}{\lambda_{\min}}$ and $\delta_\alpha' < 0$ for $\alpha < \frac{\sigma_{\max}^2}{\lambda_{\min}}$. Hence, the upper bound δ_α of the spectral radius $\rho(T_\alpha)$ achieves its minimum at $\alpha^* = \frac{\sigma_{\max}^2}{\lambda_{\min}}$, i.e., (2.5) holds true. Taking α^* into δ_α, the minimum value of δ_α given in (2.6) is obtained. □

Some remarks on Theorem 2.1 and Corollary 2.1 are given below.

- For case (ii) of Theorem 2.1, i.e., $\lambda_{\min} < \sigma_{\max}$, one sees that α^* given in Corollary 2.1 satisfies the condition (2.3) since
$$\frac{\sigma_{\max}^2}{\lambda_{\min}} > \frac{\sigma_{\max}^2 - \lambda_{\min}^2}{2\lambda_{\min}}.$$
- From Theorem 2.1 and Corollary 2.1, one can see that the convergence rate of the SHSS iteration method is bounded by δ_α, which only depends on the smallest eigenvalue $\lambda_{\min}$ of matrix H and the largest singular value $\sigma_{\max}$ of matrix S.
- Using Hermitian positive definite matrix V instead of the identity matrix I in (1.3) yields the preconditioned SHSS (PSHSS) iteration method. It is not difficult to find that the convergence properties of the PSHSS iteration method are similar to the SHSS iteration method.
- It should be noted that the parameter α^* in Corollary 2.1 minimizes only the upper bound δ_α of the spectral radius $\rho(T_\alpha)$ of the iteration matrix T_α, but not $\rho(T_\alpha)$ itself. In fact, the practical usefulness estimates of α for the SHSS method are questionable in actual implementations. By observing Corollary 2.1, it is easy to find that the estimated value of α depends on the smallest eigenvalue of matrix H and the largest singular value of matrix S, which may be not easy to obtain, as well as for the LHSS method [12,13]. Whereas, experience suggests that in most applications and for an appropriate scaling of the problem, a "small" value of α (usually between 0.01 and 0.5) gives good results [14]. In this case, the SHSS method is more efficient than the HSS method (to see the next section).

3. Numerical experiments

In this section, we give some numerical experiments to demonstrate the performance of the SHSS method for solving the linear system (1.1). Numerical comparisons with the SHSS and HSS methods are also presented to show the advantage of the SHSS method under certain conditions.

Example 1 (*[7]*). Consider the following non-Hermitian positive definite linear systems:

$$Ax \equiv (W + iT)x = b,$$

with $T = I \otimes V + V \otimes I$ and $W = 10(I \otimes V_c + V_c \otimes I) + 9(e_1 e_m^T + e_m e_1^T) \otimes I$, where $V = \text{tridag}(-1, 2, -1) \in \mathbb{R}^{m\times m}$, $V_c = V - e_1 e_m^T - e_m e_1^T \in \mathbb{R}^{m\times m}$, e_1 and e_m are the first and the last unit vectors in $\mathbb{R}^m$, respectively. We take the right-hand side vector b to be $b = (1+i)A\mathbf{1}$, with $\mathbf{1}$ being the vector of all entries equal to 1.

Table 1
CPU(s) and IT for SHSS and HSS with $m = 16$.

	α	0.01	0.05	0.1	0.5	1
SHSS	CPU(s)	0.0165	0.0156	0.0123	0.0123	0.0175
	IT	13	11	10	10	16
HSS	CPU(s)	35.5313	7.4063	3.5469	0.75	0.375
	IT	14323	2865	1433	287	143

Table 2
CPU(s) and IT for SHSS and HSS with $m = 32$.

	α	0.01	0.05	0.1	0.5	1
SHSS	CPU(s)	2.25	0.25	0.938	0.938	0.1563
	IT	500	58	19	20	37
HSS	CPU(s)	156.7656	32.0469	3.5469	3.2344	1.6719
	IT	13557	2712	1356	271	135

In our implementations, the initial guess is chosen to be $x^{(0)} = 0$ and the stopping criteria for the SHSS and HSS methods are $\frac{\|b-Ax^{(k)}\|_2}{\|b\|_2} \leq 10^{-6}$. We compare two methods from the point of view of the number of iterations (denoted as IT) and CPU times (denoted as CPU).

In Tables 1 and 2, we list the iteration numbers and CPU times for the SHSS and HSS methods. From Tables 1 and 2, we see that the presented results show that in all cases SHSS is superior to HSS method in terms of the iteration numbers and CPU times. That is to say, compared with the HSS method, the SHSS method may be given priority under certain conditions.

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