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Convergence Properties of the Single-Step Preconditioned HSS Method for Non-Hermitian Positive Semidefinite Linear Systems

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Abstract. For the nonsingular, non-Hermitian and positive semidefinite linear systems, we derive the convergence results of the single-step preconditioned HSS (SPHSS) method under suitable constraints. Additionally, we consider the acceleration of the SPHSS method by Krylov subspace methods and some spectral properties of the preconditioned matrix are established. Numerical experiments are presented to further examine the effectiveness of the proposed method either as a solver or a preconditioner.

Mathematics Subject Classification. 65F10, 65F50.

Keywords. Nonsingular non-Hermitian, positive semidefinite linear systems, SPHSS method, convergence, spectral properties.

1. Introduction

In this paper, we consider the following systems of linear equations:

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

where $A \in \mathbb{C}^{n\times n}$ is a large, sparse and nonsingular matrix, $x \in \mathbb{C}^n$ is an unknown vector and $b \in \mathbb{C}^n$ is a given vector. Moreover, we assume $A \neq \pm A^*$, which implies that A is not Hermitian, while A is not skew-Hermitian, where A^* denotes the conjugate transpose of the matrix A. Linear systems of the form (1.1) come from many problems in scientific computing and engineering applications, such as molecular scattering, lattice quantum chromodynamics,

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quantum chemistry, diffuse optical tomography, FFT-based solution of certain time-dependent PDEs, eddy current problem and so on; see [1–18] and references therein.

Based on the Hermitian and skew-Hermitian (HS) splitting,

$$A = H + S, \quad \text{with} \quad H = \frac{1}{2}(A + A^*) \quad \text{and} \quad S = \frac{1}{2}(A - A^*).$$

Bai et al. [19–22] presented a class of the Hermitian and skew-Hermitian splitting (HSS) iteration method for solving non-Hermitian linear systems.

When the coefficient matrix A is positive definite, i.e., its Hermitian part H is Hermitian positive definite, Bai et al. [19] masterly designed a class of Hermitian and skew-Hermitian splitting (HSS) iteration method and described it as follows:

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

where α is a given positive constant and I is identity matrix with proper dimension. To accelerate the convergence of the HSS method, Bai et al. [20] further proposed a preconditioned HSS (PHSS) iteration method and described below:

$$\begin{cases} (\alpha P + H)x^{(k+\frac{1}{2})} = (\alpha P - S)x^{(k)} + b, \\ (\alpha P + S)x^{(k+1)} = (\alpha P - H)x^{(k+\frac{1}{2})} + b, \end{cases} \tag{1.3}$$

where P is a prescribed Hermitian positive definite matrix. Additionally, Li et al. [27] presented a single-step HSS (SHSS) iteration method, which can be described as follows:

$$(\alpha I + H)x^{(k+1)} = (\alpha I - S)x^{(k)} + b. \tag{1.4}$$

Furthermore, Wu et al. [28] proposed a non-alternating preconditioned HSS (NPHSS) iteration method as follows:

$$(\alpha P + H)x^{(k+1)} = (\alpha P - S)x^{(k)} + b. \tag{1.5}$$

Due to the performance and elegant mathematical properties of the HSS method, a number of considerable attentions and results have been presented; see [23–26, 29, 31] and references therein.

When the coefficient matrix A is positive semidefinite, but nonsingular, Bai et al. [21] proved that the HSS method is convergent if and only if the coefficient matrix A does not have a (reducing) eigenvalue of the form $i\varsigma$ with $\varsigma \in \mathbb{R}$ and i the imaginary unit, or, equivalently, the null space of Hermitian part H of coefficient matrix does not contain an eigenvector of skew-Hermitian part S of coefficient matrix.

In this paper, we use the SHSS and SPHSS methods for a class of nonsingular, non-Hermitian and positive semidefinite linear system (1.1).

The remainder of this paper is organized as follows. In Sect. 2, the convergence conditions of the proposed method and the spectral properties of the preconditioned matrices are derived under suitable constraints. In Sect. 3, numerical experiments are presented to show the correctness of theoretical analyses and the effectiveness of the proposed method either as a solver or a preconditioner. Finally, some conclusions are given in Sect. 4.

2. Convergence and Preconditioning Properties

In this section, we discuss the convergence properties of the SHSS and SPHSS methods, and study the spectral properties of the preconditioned matrices with respect to the SHSS and SPHSS preconditioner for a class of nonsingular non-Hermitian positive semidefinite linear systems (1.1). Without loss of generality, we take the SHSS method as an example.

It is easy to see that (1.4) can be rewritten as

$$x^{(k+1)} = \mathcal{T}_\alpha x^{(k)} + M_\alpha^{-1} b, \quad k = 0, 1, 2, \ldots, \tag{2.1}$$

where

$$\mathcal{T}_\alpha = (\alpha I + H)^{-1}(\alpha I - S), \quad M_\alpha = (\alpha I + H). \tag{2.2}$$

Here, $\mathcal{T}_\alpha$ is the iteration matrix of the SHSS method. In fact, the scheme (2.1) can also be obtained from the splitting $A = M_\alpha - N_\alpha$ of the coefficient matrix with $N_\alpha = (\alpha I - S)$. Evidently, the SHSS method can naturally induce a preconditioner M_α to the matrix A, which is called the SHSS preconditioner. Then, in every step of the SHSS iteration scheme (2.1) or applying the preconditioner M_α to accelerate a Krylov subspace methods, we need to solve generalized residual equations of the form $M_\alpha z = r$, where $r, z \in \mathbb{C}^n$ are the current and generalized residual vectors, respectively. Notice $\alpha I + H$ is Hermitian positive definite matrix for any $\alpha > 0$ and Hermitian positive semidefinite matrix H ; hence the linear systems can be exactly solved by the Cholesky factorization or inexactly by the CG algorithm.

Now, we turn to study the convergence properties of the SHSS method. It is well known that the iteration method (2.1) is convergent for every initial guess $x^{(0)}$ if and only if $\rho(\mathcal{T}_\alpha) < 1$, where $\rho(\mathcal{T}_\alpha)$ denotes the spectral radius of $\mathcal{T}_\alpha$.

To obtain the convergence of the SHSS method, we first assume that $\lambda \neq 0$ and give a lemma.

Lemma 2.1. *Assume that $A \in \mathbb{C}^{n\times n}$ is a nonsingular positive semidefinite matrix. If λ is an eigenvalue of iteration matrix $\mathcal{T}_\alpha$ defined by (2.2), then $\lambda \neq 1$.*

Proof. If $\lambda = 1$ and x are the corresponding eigenvector, then it follows that $Ax = 0$. Since the matrix A is nonsingular, we have $x = 0$, which contradicts the assumption that x is an eigenvector of the iteration matrix $\mathcal{T}_\alpha$. Hence, $\lambda \neq 1$. □

The following theorem gives sufficient and necessary conditions for convergence of the SHSS method.

Theorem 2.1. *Assume that $A \in \mathbb{C}^{n\times n}$ is a nonsingular positive semidefinite matrix with $A \neq \pm A^*$, and let α be a positive constant. If x is an eigenvector* *of the iteration matrix $\mathcal{T}_\alpha$ corresponding to the eigenvalue λ, then*

$$\lambda = \frac{\alpha - \tilde{b}}{\alpha + \tilde{a}},$$

where

$$\tilde{a} = \frac{x^* H x}{x^* x}, \quad \tilde{b} = \frac{x^* S x}{x^* x}. \tag{2.3}$$

Moreover, the SHSS method is convergent if and only if parameter α satisfies

$$\alpha > \max\left\{0, \ \frac{\tilde{b}^2 - \tilde{a}^2}{2\tilde{a}}\right\}, \tag{2.4}$$

with $\tilde{a} > 0$.

Proof. Let (λ, x) be the eigenpair of the iteration matrix $\mathcal{T}_\alpha$; we have

$$(\alpha I - S)x = \lambda(\alpha I + H)x.$$

Multiplying both sides from the left by x^*, yield

$$\alpha x^* x - x^* S x = \lambda(\alpha x^* x + x^* H x).$$

Thus, it follows from the denote (2.3) that

$$\lambda = \frac{\alpha - \tilde{b}}{\alpha + \tilde{a}}.$$

Next, we first prove $\tilde{a} > 0$. Since H is a Hermitian positive semidefinite, we only need to prove $\tilde{a} \neq 0$. In fact, if $\tilde{a} = 0$, i.e., $Hx = 0$, we have $Sx \neq 0$, i.e., $\tilde{b} \neq 0$. Thus, we conclude that $|\lambda| \geqslant 1$, so it must have $\tilde{a} > 0$ so that the SHSS method is convergent. After simple algebraic manipulations, we get the SHSS iteration method to be convergent if and only if parameter α satisfies (2.4) with $\tilde{a} > 0$. Thus, we complete the proof of Theorem 2.1. □

Denote

$$\tilde{\eta}_{\max} = \max_{\eta_j \in sp(H)} \{\eta_j\}, \ \tilde{\eta}_{\min} = \min_{\eta_j \in sp(H)} \{\eta_j \backslash \{0\}\}, \ \tilde{\mu}_{\max} = \max_{\mu_j \in sp(S)} \{|\mu_j|\}. \tag{2.5}$$

Accordingly, combining Theorem 2.1 and the denote (2.5), we derive the following sufficient convergence conditions of the SHSS method.

Lemma 2.2. *Under the assumption of Theorem 2.1, the spectral radius $\rho(\mathcal{T}_\alpha)$ of the iteration matrix $\mathcal{T}_\alpha$ satisfies $\rho(\mathcal{T}_\alpha) \leqslant \delta_\alpha$, with*

$$\delta_\alpha = \frac{\sqrt{\alpha^2 + \tilde{\mu}_{\max}^2}}{\alpha + \tilde{\eta}_{\min}},$$

where $\tilde{\mu}_{\max}$ and $\tilde{\eta}_{\min}$ are denoted in (2.5). Moreover, the SHSS method is convergent if $\delta_\alpha < 1$ or equivalently parameter α satisfies

$$\alpha > \max\left\{0, \ \frac{\tilde{\mu}_{\max}^2 - \tilde{\eta}_{\min}^2}{2\tilde{\eta}_{\min}}\right\}. \tag{2.6}$$

Proof. By Theorem 2.1 and using the Courant–Fisher minmax theorem [30], we have

$$\rho(\mathcal{T}_\alpha) = \max\{|\lambda|\} = \max\left\{\frac{\sqrt{\alpha^2+\tilde{b}^2}}{\alpha+\tilde{a}}\right\} \leqslant \frac{\sqrt{\alpha^2+\tilde{\mu}_{\max}^2}}{\alpha+\tilde{\eta}_{\min}} = \delta_\alpha.$$

Thus, after the same algebraic manipulations of Theorem 2.1, the SHSS method is convergent if $\delta_\alpha < 1$ or equivalently parameter α satisfies (2.6). Therefore, we complete the proof of Lemma 2.2. □

On the other hand, as we know, the clustered spectrum of the preconditioned matrix often leads to rapid convergence [14,30] of the preconditioning Krylov subspace iteration methods such as restarted GMRES, so possessing the clustering properties of the eigenvalues of the preconditioned matrix and playing an important role in estimating the convergence rate of the preconditioned Krylov subspace iteration methods. In the following lemmas, we describe the spectral properties of the eigenvalues of the preconditioned matrix $M_\alpha^{-1}A$ with respect to the SHSS preconditioner.

Lemma 2.3. *Under the assumption of Theorem 2.1, the eigenvalues ξ of the preconditioned matrix $M_\alpha^{-1}A$ are*

$$\xi = \frac{\tilde{a}+\tilde{b}}{\alpha+\tilde{a}},$$

where $\tilde{a}$ and $\tilde{b}$ denote in (2.3). Moreover, it holds that

$$\frac{\tilde{\eta}_{\min}}{\alpha+\tilde{\eta}_{\min}} \leqslant \Re(\xi) \leqslant \frac{\tilde{\eta}_{\max}}{\alpha+\tilde{\eta}_{\max}} \quad \text{and} \quad \left|\Im(\xi)\right| \leqslant \frac{\tilde{\mu}_{\max}}{\alpha+\tilde{\eta}_{\min}}, \tag{2.7}$$

where $\tilde{\mu}_{\max}, \tilde{\eta}_{\min}$ and $\tilde{\eta}_{\max}$ denote in (2.5).

Proof. Let ξ be the eigenvalues of the preconditioned matrix $M_\alpha^{-1}A$. By Theorem 2.1, we have

$$\xi = 1-\lambda = \frac{\tilde{a}+\tilde{b}}{\alpha+\tilde{a}}.$$

Since H and S are Hermitian and skew-Hermitian matrices, respectively,

$$\Re(\xi) = \frac{\tilde{a}}{\alpha+\tilde{a}} \quad \text{and} \quad \Im(\xi) = \frac{\tilde{b}}{\alpha+\tilde{a}}.$$

By making use of the Courant–Fisher minmax theorem [30], after simple algebraic manipulations, we obtain that the conclusion of (2.7) holds. Thus, we complete the proof. □

From the view of Lemma 2.3, we obtain the asymptotic behavior of the eigenvalue ξ of the preconditioned matrix $M_\alpha^{-1}A$ under some conditions.

Lemma 2.4. *Under the assumption of Theorem 2.1, the Hermitian part of matrix A is dominantly stronger than the skew-Hermitian part. Then the eigenvalue ξ of the preconditioned matrix $M_\alpha^{-1}A$ are clustered at 1_- as α tends to 0_+.*

Proof. According to Lemma 2.3 and since the Hermitian part of the coefficient matrix is dominantly stronger than the skew-Hermitian part, we obtain $\Re(\xi) \to 1_-$ and $\Im(\xi) \to 0_+$ as α tends to 0_+. Thus, we have $\xi \to 1_-$ as α tends to 0_+. Hence, we complete the proof. □

Based on the algebraic estimation technique [34], we may expect that M_α is close to A as much as possible and $N_\alpha \approx 0$. If the expectation comes true, more precisely, the SHSS method will have fast convergence rates and the preconditioned matrix will have clustered eigenvalue distribution when we minimize the function $\phi(\alpha) = \|N_\alpha\|_F^2$ with respect to α. By direct computations, we have

$$\begin{aligned}\phi(\alpha) &= \|N_\alpha\|_F^2 = tr(N_\alpha N_\alpha^*)\\ &= \alpha^2 tr(I_n) + tr(S^* S).\end{aligned}$$

By taking the first-order derivative of $\phi(\alpha)$ and making use of the necessary condition for the extreme value of a function, we conclude that $\phi(\alpha)$ has a minimum if $\alpha \to 0_+$ (since $\alpha > 0$).

Similar to the SHSS method, the iteration matrix of the SPHSS method is

$$\mathcal{T}_{\alpha,P} = (\alpha P + H)^{-1}(\alpha P - S),$$

which is similar to

$$\tilde{\mathcal{T}}_{\alpha,P} = (\alpha I + \tilde{H})^{-1}(\alpha I - \tilde{S}),$$

where $\tilde{H} = P^{-\frac{1}{2}} H P^{-\frac{1}{2}}$ and $\tilde{S} = P^{-\frac{1}{2}} S P^{-\frac{1}{2}}$. Then, similar to the analysis method, in the SHSS method, we can obtain the convergence of the SPHSS method and the spectral properties of the preconditioned matrix $M_{\alpha,P}^{-1}A$; since it is similar to the above results, it is omitted here. Moreover, we have $\alpha \to 0_+$ and matrix P dominant matrix S by minimizing the function $\alpha^2 tr(I_n) + tr\big((P^{-1}S)^*(P^{-1}S)\big)$.

3. Numerical Experiments

In this section, we perform two examples to illustrate the effectiveness of the proposed method and the corresponding preconditioner for solving linear systems (1.1). In actual computations, we use left preconditioning with restarted GMRES(10) [33] as the Krylov subspace method. We compare the SPHSS method with the HSS [19] method and compare the corresponding preconditioner for the GMRES(10) method from the point of view of the number of iterations (denoted by "IT", including the outside iteration numbers and the inner iteration numbers), elapsed CPU time in seconds (denoted by "CPU") and relative residual error (denoted by "RES") defined by

$$\text{RES} := \frac{\|b - Ax^{(k)}\|_2}{\|b\|_2},$$

where $x^{(k)}$ are the current approximate solutions. Moreover, we choose the null vectors as an initial guess and the stopping criterion $RES < 10^{-6}$ or the maximum prescribed number of iteration $k_{\max} = 600$. All the computation results are run in MATLAB [version 7.10.0.499 (R2010a)] in double precision and performed on a personal computer with 3.20 GHz central processing unit (Intel(R) Core(TM) i5-6500) and 16.00G memory. In our experiments, the linear subsystems involved in each step of the HSS and SPHSS methods can be solved effectively using the sparse Cholesky factorization [32].

Example 1. Consider the complex Helmholtz equation:

$$-\Delta u + \sigma_1 u + i\sigma_2 u = b, \tag{3.1}$$

where σ_1 and σ_2 are real coefficient functions, u satisfies Dirichlet boundary conditions in $D = [0,1] \times [0,1]$ and $i = \sqrt{-1}$. We discretize the problem with finite differences on a $m \times m$ grid with mesh size $h = 1/(m+1)$. Then it leads to the following linear equations:

$$\big[(K + \sigma_1 I) + i\sigma_2 I\big] = b,$$

where $K = I \otimes V_m + V_m \otimes I$ is the discretization of $-\Delta$ by means of centered differences, wherein $V_m = h^{-2} tridiag(-1, 2, -1) \in \mathbb{R}^{m\times m}$. The right-hand side vector b is taken as $b = (1+i)A\mathbf{1}$, with $\mathbf{1}$ being the vector of all entries equal to 1. Moreover, we also normalize the coefficient matrix and in right-hand side of (3.1) by multiplying both by h^2. For the numerical tests we take $\sigma_1 = \sigma_2 = 100$.

Example 2 [22,32]. Consider the nonsingular linear system of equations (1.1) with

$$W = 10(I \otimes V_c + V_c \otimes I) + 9(e_1 e_m^T + e_m^T e_1) \otimes I \quad \text{and} \quad T = I \otimes V + V \ \otimes \ I,$$

where $V_c = V - e_1 e_m^T - e_m e_1^T \in \mathbb{R}^{m\times m}$, $V = tridiag(-1, 2, -1) \in \mathbb{R}^{m\times m}$, and e_1 and e_m are the first and last unit vectors in $\mathbb{R}^m$, respectively. Hence, we take the right-hand side vector b to be of the form $b = (1+i)Ae$, with e being the vector of all entries equal to 1 and $A = W + iT$. Here, T and K correspond to the five-point centred difference matrices approximating the negative Laplacian operator with homogeneous Dirichlet boundary conditions and periodic boundary conditions, respectively, on a uniform mesh in the unit square $[0,1] \times [0,1]$ with the mesh size $h = 1/(m+1)$.

Table 1. Numerical results of different splitting iteration methods for Example 1

Grid	Method	α_*	IT	CPU	RES
16×16	HSS	1.45	25	0.0456	5.95e−08
	SPHSS	0.79	30	0.0398	6.20e−08
32×32	HSS	1.49	86	2.6899	1.49e−08
	SPHSS	0.62	29	0.8559	1.31e−08
48×48	HSS	1.22	149	32.5328	8.40e−09
	SPHSS	0.75	28	6.2937	6.05e−09
64×64	HSS	1.01	208	68.1580	5.53e−08
	SPHSS	0.89	27	19.5856	4.85e−08

Table 2. Numerical results of different preconditioned GMRES methods for Example 1

Grid	Preconditioner	α_*	IT	CPU	RES
16×16	HSS-GMRES(10)	1.45	2(3)	0.0387	3.60e−07
	SPHSS-GMRES(10)	0.79	2(1)	0.0259	6.27e−07
32×32	HSS-GMRES(10)	1.49	4(1)	1.1569	9.75e−07
	SPHSS-GMRES(10)	0.62	2(2)	0.5917	3.95e−07
48×48	HSS-GMRES(10)	1.22	5(7)	16.6351	8.36e−07
	SPHSS-GMRES(10)	0.75	2(2)	4.1917	5.79e−07
64×64	HSS-GMRES(10)	1.01	7(1)	46.6169	9.44e−07
	SPHSS-GMRES(10)	0.89	2(2)	9.3528	6.86e−07

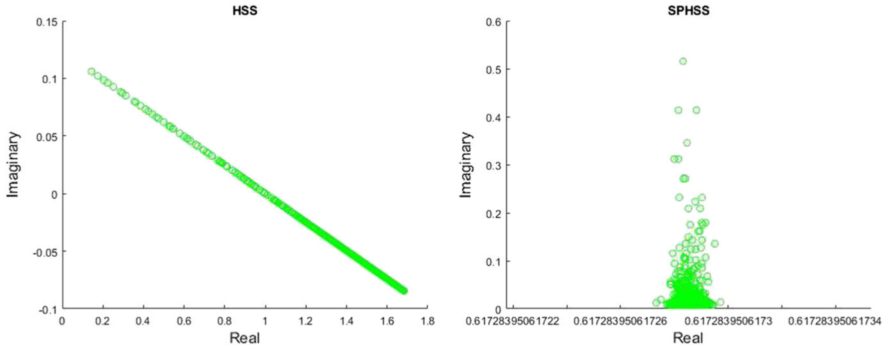

Figure 1. Eigenvalue distribution of different preconditioned matrices for Example 1 with $m = 32$

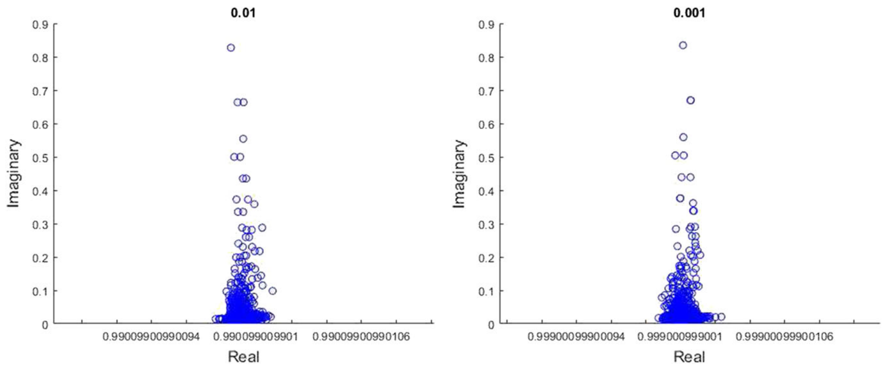

Figure 2. Eigenvalue distribution of the preconditioned matrix $M_{\alpha,P}^{-1}A$ for Example 1 with $m = 32$

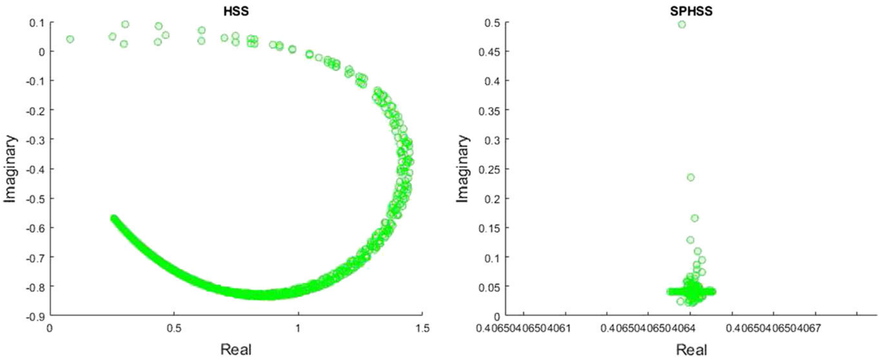

Figure 3. Eigenvalue distribution of different preconditioned matrices for Example 2 with $m = 32$

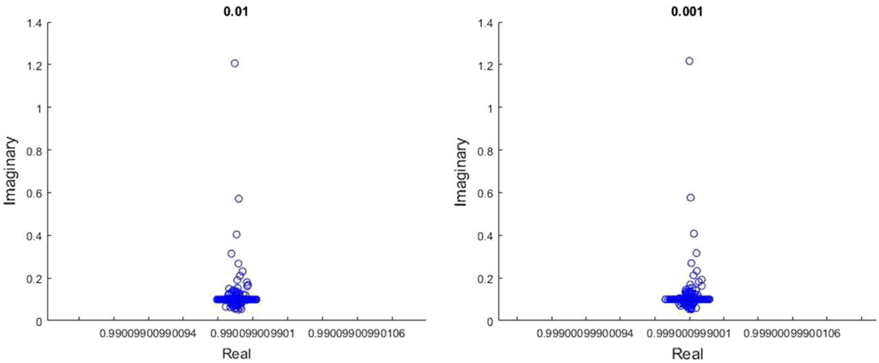

Figure 4. Eigenvalue distribution of preconditioned matrix $M_{\alpha,P}^{-1}A$ for Example 2 with $m = 32$

Table 3. Numerical results of different splitting iteration methods for Example 2

Grid	Method	α_*	IT	CPU	RES
16×16	HSS	4.41	84	0.2489	9.26e−07
	SPHSS	0.35	22	0.0256	5.81e−07
32×32	HSS	2.71	137	8.2371	9.28e−07
	SPHSS	1.46	47	0.6591	7.93e−07
48×48	HSS	2.12	185	43.1284	9.70e−09
	SPHSS	3.34	85	5.1283	9.98e−07
64×64	HSS	1.61	223	128.1285	9.72e−07
	SPHSS	5.38	138	21.2117	9.52e−07

Table 4. Numerical results of different preconditioned GMRES methods for Example 2

Grid	Preconditioner	α_*	IT	CPU	RES
16×16	HSS-GMRES(10)	4.41	4(8)	0.1387	8.72e−07
	SPHSS-GMRES(10)	0.35	1(9)	0.0642	6.58e−07
32×32	HSS-GMRES(10)	2.71	9(6)	6.2149	8.84e−07
	SPHSS-GMRES(10)	1.46	3(9)	0.3482	9.95e−07
48×48	HSS-GMRES(10)	1.22	13(9)	23.1284	9.99e−07
	SPHSS-GMRES(10)	0.75	7(10)	2.9124	9.14e−07
64×64	HSS-GMRES(10)	1.61	16(5)	85.5417	9.80e−07
	SPHSS-GMRES(10)	5.38	12(7)	8.1286	9.75e−07

In Table 1, we list the numerical results of various iteration methods with respect to different problem sizes for Example 1. The parameter α^* for HSS and SPHSS iteration methods is obtained by minimizing the numbers of iterations with respect to each test example and each spatial mesh size. Moreover, we take $P = H$ for Example 1. Additionally, the numerical results of IT, CPU and RES of the tested methods with respect to different problem sizes for Example 1 by using GMRES(10) in conjunction with the corresponding preconditioners are listed in Table 2. The eigenvalue distribution of the corresponding preconditioned matrices with $m = 32$ is given in Fig. 1. Furthermore, the eigenvalue distribution of the preconditioned matrix $M_{\alpha,P}^{-1}A$ is listed in Fig. 2 with $\alpha = 0.01$ and $\alpha = 0.001$, respectively. For Example 2, we have the same strategy as Example 1, see Tables 3, 4 and Figs. 3, 4

The numerical results clearly show that the SPHSS method and the corresponding preconditioner use less iteration steps and CPU times to achieve the stopping criterion. We also see that the distribution eigenvalues of the preconditioned matrices $M_{\alpha,P}^{-1}A$ are quite clustered in accordance with theoretical analysis. In other words, the numerical results show the feasibility of the SPHSS method for solving nonsingular linear system (1.1).

4. Conclusions

In this paper, we present the SPHSS method for solving a class of nonsingular non-Hermitian positive semidefinite linear system (1.1). Meanwhile, the convergence properties of the SPHSS method and the spectral properties of the preconditioned matrix are also derived. Numerical results show the effectiveness of the SPHSS method in terms of the number of iteration steps ("IT") and CPU times ("CPU"). However, its efficiency depends on the preconditioned matrix P. With regard to this case, we will need to study further.

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