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A single-step iteration method for non-Hermitian positive definite linear systems☆

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ABSTRACT

An efficient single-step iteration method is presented for solving the large sparse non-Hermitian positive definite linear systems. We theoretically prove that this method converges to the unique solution of the system of linear equations under suitable restrictions. Moreover, we derive an upper bound for the spectral radius of the new iteration matrix. Furthermore, we consider acceleration of the new iteration by Krylov subspace methods and some special properties of the new preconditioned matrix are proposed. Numerical experiments on a few model problems are presented to further examine the effectiveness of our new method.

1. Introduction

In this paper, we consider the following linear system

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

where $A \in C^{n\times n}$ is a non-Hermitian positive definite matrix (that is, the Hermitian part of A is positive definite), and $x \in C^n$ is an unknown vector and $b \in C^n$ is a given vector. Many problems in scientific computing result in a system of linear equations as (1). For example, molecular scattering, lattice quantum chromodynamics, quantum chemistry, diffuse optical tomography, FFT-based solution of certain time-dependent PDEs, eddy current problem and so on; see [1–15] and references therein.

Recently, many iteration methods have been presented for solving the non-Hermitian positive definite linear system (1). For example, the classic Jacobi and Gauss–Seidel methods [6,7,16], the generalized conjugate gradient (CG) method [17], the generalized Lanczos method [18] and Krylov subspace iterative methods [19–21]. Based on the Hermitian and skew-Hermitian parts of the coefficient matrix $A \in C^{n\times n}$: $A = H + S$ with

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

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Bai et al. proposed the HSS (Hermitian and skew-Hermitian splitting) iteration method [22] for solving non-Hermitian linear system as follows:

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

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

where α is a given positive constant. Then, many variant of this HSS iteration method such as preconditioned HSS (PHSS) method [23] and accelerated HSS (AHSS) [24] are proposed. In addition, the HSS-like iteration methods for system of linear equations have been extended to other equations and conditions in [25–34]. In [35], a shift-splitting iteration scheme and a shift-splitting preconditioner are presented for solving the large sparse system of linear equations of which the coefficient matrix is an ill-conditioned non-Hermitian positive definite matrix. In [36], Benzi proposed a generalization of the Hermitian and skew-Hermitian (HSS) splitting iteration and the new scheme can outperform the standard HSS method in some situations and can be used as an effective preconditioner for certain linear systems in saddle point form. Furthermore, in [11], a new Hermitian and skew-Hermitian splitting method is presented for solving non-Hermitian and normal positive definite linear systems with strong Hermitian parts. In [37], Wu studied several variants of the Hermitian and skew-Hermitian splitting iteration method. In [38], Zheng et al. proposed a block alternating splitting iteration method. Moreover, Li and Wu in [39] presented the following single-step HSS (SHSS) iteration method:

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

$$(\alpha I + H)x^{(k+1)} = (\alpha I - S)x^{(k)} + b, \tag{3}$$

where $\alpha > 0$ is a given constant. 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. Based on this SHSS method, Zeng and Ma in [40] proposed a parameterized SHSS iteration method for a class of complex symmetric system of linear equations.

In this paper, we propose a single-step iteration method for solving the large sparse non-Hermitian positive definite linear system (1). The convergence property of this new iteration method is studied. Furthermore, we derive an upper bound for the spectral radius of the iteration matrix of this new method. Acceleration of the new iteration by Krylov subspace methods and some special properties of the new preconditioned matrix are proposed and studied. Numerical examples are presented to illustrate the effectiveness of our new iteration method.

The remainder of this paper is organized as follows: in Section 2, the single-step iteration method is presented for the non-Hermitian positive definite linear system (1). The convergence of the new iteration method is studied in Section 3. Moreover, some spectral properties of the new preconditioned matrix are also given in this section. In Section 4, numerical experiments are provided to show the performance of the new iteration method and the new preconditioner. Finally, in Section 5, we end the paper with a few concluding remarks.

The following notations will be used throughout this paper. We denote the identity matrix with proper dimension by I. For a given vector v, we denote the l_2 norm of v by $\|v\|_2$. For a given matrix B, we denote the transpose and the inverse of B by B^T and B^{-1}, respectively. Moreover, $\Lambda(B)$ and $\rho(B)$ denote the spectrum and the spectral radius of B, respectively.

2. The new method

In this section, we first propose our new method for solving the non-Hermitian positive definite linear system (1) as follows:

New iteration method. Given an initial guess $x^{(0)}$, for $k = 0, 1, 2, \ldots$ until $\{x^{(k)}\}$ converges, compute the next iteration step according the following procedure:

$$(P + H)x^{(k+1)} = (P - S)x^{(k)} + b, \tag{4}$$

where P is a given Hermitian positive definite matrix.

With different choices of the matrix P, this new iteration method (4) covers several other methods. For example, if $P = \alpha I$, then the new iteration reduces to the SHSS iteration method (3). The matrix P can also be taken as $P = \alpha H$, $P = \Lambda$ (where $\Lambda = \mathrm{diag}(d_1, d_2, \ldots, d_n)$, $d_i > 0, i = 1, 2, \ldots, n$) or other different Hermitian matrices.

Since the coefficient matrix $H + P$ of the new method (4) is a Hermitian positive definite matrix, we can solve (4) by Cholesky method or conjugate gradient method. In fact, the coefficient matrix A of the linear system (1) can be rewritten as

$$A = (P + H) - (P - S).$$

Obviously, this is a splitting of the matrix A, because $P + H$ is nonsingular. It is easy to see that the iteration matrix of the new method is

$$\mathcal{T} = (P + H)^{-1}(P - S). \tag{5}$$

Moreover, the splitting preconditioner corresponding to the new iteration method (4) is given by

$$\mathcal{P}_{new} = P + H. \tag{6}$$

At each step of applying the new preconditioner $\mathcal{P}_{new}$ within a Krylov subspace method, it is necessary to solve sequences of generalized residual equations of the following form

$$\mathcal{P}_{new} z = (P + H)z = r, \tag{7}$$

where $r, z \in C^n$ are the current and the generalized residual vectors, respectively. Because $P + H$ is an Hermitian positive definite matrix, the above linear system (7) can be solved by Cholesky method or conjugate gradient method.

3. Analysis for the new method

In this section, for the single-step iteration method (4), we first study its convergence property. Note that the iteration matrix of the new iteration method is $\mathcal{T}$ and coefficient matrix A is a nonsingular matrix, we can see that the iteration (4) is convergent if and only if $\rho(\mathcal{T}) < 1$.

Theorem 3.1. *Assume that $A \in C^{n\times n}$ is a non-Hermitian positive definite matrix. Let P be Hermitian positive definite and let $H = \frac{1}{2}(A + A^*)$ and $S = \frac{1}{2}(A - A^*)$ be its Hermitian and skew-Hermitian, respectively. Then the spectral radius $\rho(\mathcal{T})$ of the iteration matrix of the single-step iteration method (4) is bounded by*

$$\delta = \frac{\sqrt{1 + \mu_{\max}^2}}{1 + \lambda_{\min}}, \tag{8}$$

where $\lambda_{\min}$ is the smallest singular-value of matrix $\widetilde{H}$ and $\mu_{\max}$ is the largest singular-value of matrix $\widetilde{S}$. Here, $\widetilde{H} = P^{-\frac{1}{2}} H P^{-\frac{1}{2}}$ and $\widetilde{S} = P^{-\frac{1}{2}} S P^{-\frac{1}{2}}$.

Moreover, the new iteration method (4) is convergent if the following condition holds true:

$$\frac{\mu_{\max}^2 - \lambda_{\min}^2}{2\lambda_{\min}} < 1. \tag{9}$$

Proof. From (5), we see that the iteration matrix of the new iteration method is $\mathcal{T} = (P + H)^{-1}(P - S)$. Hence, we can obtain

$$\begin{aligned}
\mathcal{T} &= (I + P^{-1}H)^{-1}(I - P^{-1}S) \\
&= [P^{-\frac{1}{2}}(I + P^{-\frac{1}{2}} H P^{-\frac{1}{2}})P^{\frac{1}{2}}]^{-1}[P^{-\frac{1}{2}}(I - P^{-\frac{1}{2}} S P^{-\frac{1}{2}})P^{\frac{1}{2}}] \\
&= P^{-\frac{1}{2}}(I + P^{-\frac{1}{2}} H P^{-\frac{1}{2}})^{-1}(I - P^{-\frac{1}{2}} S P^{-\frac{1}{2}})P^{\frac{1}{2}}.
\end{aligned}$$

By the similarity invariance of the matrix spectrum, we have

$$\begin{aligned}
\rho(\mathcal{T}) &= \rho((I + P^{-\frac{1}{2}} H P^{-\frac{1}{2}})^{-1}(I - P^{-\frac{1}{2}} S P^{-\frac{1}{2}})) \\
&\le \|(I + P^{-\frac{1}{2}} H P^{-\frac{1}{2}})^{-1}(I - P^{-\frac{1}{2}} S P^{-\frac{1}{2}})\|_2 \\
&\le \|(I + P^{-\frac{1}{2}} H P^{-\frac{1}{2}})^{-1}\|_2 \|(I - P^{-\frac{1}{2}} S P^{-\frac{1}{2}})\|_2 \\
&= \max_{\lambda_i \in \Lambda(\widetilde{H})} \frac{1}{1 + \lambda_i} \max_{\mu_i \in \sigma(\widetilde{S})} \sqrt{1 + \mu_i^2} \\
&= \frac{\sqrt{1 + \mu_{\max}^2}}{1 + \lambda_{\min}} \\
&= \delta.
\end{aligned}$$

Here, $\sigma(\widetilde{S})$ is the singular-value set of $\widetilde{S}$. Because $\widetilde{H}$ is an Hermitian positive definite matrix, we can obtain $\Lambda(\widetilde{H}) = \sigma(\widetilde{H})$. So $\lambda_{\min}$ is also the smallest singular-value of the matrix $\widetilde{H}$.

If condition in (9) is satisfied, then we can obtain

$$\begin{aligned}
(9) &\Rightarrow \mu_{\max}^2 < \lambda_{\min}^2 + 2\lambda_{\min} \\
&\Rightarrow \mu_{\max}^2 + 1 < \lambda_{\min}^2 + 2\lambda_{\min} + 1 \\
&\Leftrightarrow \delta < 1.
\end{aligned}$$

So we have $\rho(\mathcal{T}) \le \delta < 1$. Hence, the single-step method (4) is convergent. The proof is completed. □

Corollary 3.1. *Assume that $A \in C^{n\times n}$ is a non-Hermitian positive definite matrix. Let P be Hermitian positive definite and let $H = \frac{1}{2}(A + A^*)$ and $S = \frac{1}{2}(A - A^*)$ be its Hermitian and skew-Hermitian, respectively. If $\lambda_{\min} > \mu_{\max}$ holds true, then the new iteration method (4) is convergent.*

Proof. From the result in Theorem 3.1, we can obtain the conclusion directly. □

Corollary 3.2. *Assume that $A \in C^{n\times n}$ is a non-Hermitian positive definite matrix. Let P be Hermitian positive definite and let $H = \frac{1}{2}(A + A^*)$ and $S = \frac{1}{2}(A - A^*)$ be its Hermitian and skew-Hermitian, respectively. From the result in Theorem 3.1, we can obtain that the contraction factor of the new iteration method can be bounded by a function, which is dependent only on the choice of the smallest singular-value of matrix $\widetilde{H}$ and the largest singular-value of matrix $\widetilde{S}$ but is independent of the spectrum of the skew-Hermitian part matrix $\widetilde{S}$ as well as the eigenvectors of the matrices H, S, and A.*

Lemma 3.1. *Assume that $K \in C^{n\times n}$ is a non-Hermitian positive definite matrix. Then K is positive stable, i.e., the eigenvalues of K have positive real parts: $Re(\xi) > 0$ for all $\xi \in \Lambda(K)$.*

Proof. Let (ξ, θ) be an eigenpair of K, with $\|\theta\|_2 = 1$. Then

$$\xi = \theta^* K\theta \quad \text{and} \quad \overline{\xi} = (\theta^* K\theta)^* = \theta^* K^*\theta.$$

Therefore, we have

$$\begin{aligned}\mathfrak{Re}(\xi) &= \frac{\xi + \overline{\xi}}{2} = \frac{1}{2}\theta^*(K + K^*)\theta \\ &= \frac{1}{2}[(\mathfrak{Re}(\theta)^T - \mathrm{i}\mathfrak{Im}(\theta)^T)(K + K^*)(\mathfrak{Re}(\theta) + \mathrm{i}\mathfrak{Im}(\theta))] \\ &= \frac{1}{2}[\mathfrak{Re}(\theta)^T(K + K^*)\mathfrak{Re}(\theta) + \mathfrak{Im}(\theta)^T(K + K^*)\mathfrak{Im}(\theta)],\end{aligned}$$

where $\mathrm{i} = \sqrt{-1}$.

Since $\frac{1}{2}(K + K^*)$ is the Hermitian part of the matrix K, it must be an Hermitian positive definite matrix. So we have $\mathfrak{Re}(\xi) > 0$. This implies that the matrix K is positive stable. The proof is completed. □

Theorem 3.2. *Assume that $A \in C^{n\times n}$ is a non-Hermitian positive definite matrix. Let P be Hermitian positive definite and let $H = \frac{1}{2}(A + A^*)$ and $S = \frac{1}{2}(A - A^*)$ be its Hermitian and skew-Hermitian, respectively. Then the preconditioned matrix $\mathcal{P}_{new}^{-1}A$ is positive stable. That is, the eigenvalues of the preconditioned matrix $\mathcal{P}_{new}^{-1}A$ have positive real parts: $Re(\eta) > 0$ for all $\eta \in \Lambda(\mathcal{P}_{new}^{-1}A)$.*

Proof. Let $\widehat{P} = \mathcal{P}_{new}$, then we have

$$\mathcal{P}_{new}^{-1}A = \widehat{P}^{-1}A = \widehat{P}^{-\frac{1}{2}}\widehat{P}^{-\frac{1}{2}}A\widehat{P}^{-\frac{1}{2}}\widehat{P}^{\frac{1}{2}}.$$

So $\mathcal{P}_{new}^{-1}A$ is similar to $\widehat{P}^{-\frac{1}{2}}A\widehat{P}^{-\frac{1}{2}}$.

Note

$$\widehat{P}^{-\frac{1}{2}}A\widehat{P}^{-\frac{1}{2}} = \widehat{P}^{-\frac{1}{2}}(H + S)\widehat{P}^{-\frac{1}{2}} = \widehat{P}^{-\frac{1}{2}}H\widehat{P}^{-\frac{1}{2}} + \widehat{P}^{-\frac{1}{2}}S\widehat{P}^{-\frac{1}{2}} = \widehat{H} + \widehat{S}.$$

Here, $\widehat{H} = \widehat{P}^{-\frac{1}{2}}H\widehat{P}^{-\frac{1}{2}}$ and $\widehat{S} = \widehat{P}^{-\frac{1}{2}}S\widehat{P}^{-\frac{1}{2}}$. Since

$$\widehat{H}^* = \widehat{P}^{-\frac{1}{2}}H^*\widehat{P}^{-\frac{1}{2}} = \widehat{P}^{-\frac{1}{2}}H\widehat{P}^{-\frac{1}{2}} = \widehat{H}$$

and

$$\widehat{S}^* = \widehat{P}^{-\frac{1}{2}}S^*\widehat{P}^{-\frac{1}{2}} = -\widehat{P}^{-\frac{1}{2}}S\widehat{P}^{-\frac{1}{2}} = -\widehat{S},$$

we can obtain that $\widehat{H}$ and $\widehat{S}$ are the Hermitian part and skew-Hermitian part of $\widehat{P}^{-\frac{1}{2}}A\widehat{P}^{-\frac{1}{2}}$, respectively. Because $\widehat{H}$ is an Hermitian positive definite matrix, we can obtain $\widehat{P}^{-\frac{1}{2}}A\widehat{P}^{-\frac{1}{2}}$ is a positive definite matrix. Then we have $\mathcal{P}_{new}^{-1}A$ is positive stable by making use of the result in Lemma 3.1. The proof is completed. □

In particular, when $P = \alpha H$ with α being a positive constant, the new iteration method is given by

$$(\alpha + 1)Hx^{(k+1)} = (\alpha H - S)x^{(k)} + b, \tag{10}$$

and the iteration matrix of the new method becomes

$$\mathcal{T}_\alpha = \frac{1}{\alpha + 1}H^{-1}(\alpha H - S). \tag{11}$$

In addition, the splitting preconditioner of the new iteration method (10) is

$$\mathcal{P}_{new}^{\alpha} = (\alpha + 1)H. \tag{12}$$

Let $\widetilde{S}_H = H^{-\frac{1}{2}}SH^{-\frac{1}{2}}$, then from the proof of Theorem 3.1, it is easy to obtain the following results by the fact that $\widetilde{H} = \frac{1}{\alpha}I$ and $\widetilde{S} = \frac{1}{\alpha}\widetilde{S}_H$.

Theorem 3.3. *Assume that $A \in C^{n\times n}$ is a non-Hermitian positive definite matrix. Let $H = \frac{1}{2}(A + A^*)$ and $S = \frac{1}{2}(A - A^*)$ be its Hermitian and skew-Hermitian, respectively. Then the spectral radius $\rho(\mathcal{T}_\alpha)$ of the iteration matrix of the single-step iteration method (10) is bounded by*

$$\delta(\alpha) = \frac{\sqrt{1 + \frac{1}{\alpha^2}(\mu_{\max}^H)^2}}{1 + \frac{1}{\alpha}} = \frac{\sqrt{\alpha^2 + (\mu_{\max}^H)^2}}{\alpha + 1}, \tag{13}$$

where $\mu_{\max}^H$ is the largest singular-value of matrix $\widetilde{S}_H$. Moreover,
(i) if $\mu_{\max}^H \le 1$, then $\delta(\alpha) < 1$ i.e. the iteration converges for any $\alpha > 0$;
(ii) if $\mu_{\max}^H > 1$, then $\delta(\alpha) < 1$ if and only if

$$\alpha > \frac{(\mu_{\max}^H)^2 - 1}{2}. \tag{14}$$

Corollary 3.3. *Under the conditions of Theorem 3.3, the optimal parameter α_* which minimizes the upper bound $\delta(\alpha)$ of the spectral radius $\rho(\mathcal{T}_\alpha)$ is given by*

$$\alpha_* = \arg\min_\alpha \left\{ \frac{\sqrt{\alpha^2 + (\mu_{\max}^H)^2}}{\alpha + 1} \right\} = (\mu_{\max}^H)^2, \tag{15}$$

and

$$\delta(\alpha_*) = \frac{\mu_{\max}^H}{\sqrt{1 + (\mu_{\max}^H)^2}}. \tag{16}$$

Proof. By simple calculations, we obtain

$$\delta(\alpha)' = \frac{\alpha - (\mu_{\max}^H)^2}{(\alpha + 1)^2\sqrt{\alpha^2 + (\mu_{\max}^H)^2}}.$$

Thus, it is clear that the upper bound $\delta(\alpha)$ of the spectral radius $\rho(\mathcal{T}_\alpha)$ achieves its minimum at $\alpha_* = (\mu_{\max}^H)^2$, i.e., (15) holds true. Taking α_* into $\delta(\alpha)$, we get the minimum value of $\delta(\alpha)$ given by (16). □

Note that according to (16), if $\mu_{\max}^H \le 1$, then by taking the optimal parameter α_*, we have $\rho(\mathcal{T}_{\alpha_*}) \le \delta(\alpha_*) \le \frac{1}{\sqrt{2}}$.

Remark 3.1. When $P = \alpha I$, the new iteration method (4) is reduced to the SHSS iteration [39], and the minimal upper bound δ_α of the spectral radius $\rho(T_\alpha)$ for the SHSS iteration is given by

$$\delta_{\alpha^*} = \frac{\sigma_{max}}{\sqrt{\nu_{min}^2 + \sigma_{max}^2}} = \frac{\frac{\sigma_{max}}{\nu_{min}}}{\sqrt{1 + (\frac{\sigma_{max}}{\nu_{min}})^2}}, \tag{17}$$

where $\nu_{\min}$ is the smallest eigenvalue of matrix H and σ_{max} is the largest singular-value of matrix S. While from (16) and (17), using the fact that

$$\mu_{\max}^H = \|\widetilde{S}_H\|_2 = \|H^{1/2}(H^{-1}S)H^{-1/2}\|_2 = \|H^{-1}S\|_2 \le \|H^{-1}\|_2\|S\|_2 = \frac{\sigma_{max}}{\nu_{min}},$$

we obtain

$$\delta(\alpha_*) \le \delta_{\alpha^*},$$

since $f(x) \equiv \frac{x}{\sqrt{1+x^2}}$ is a strictly monotonic increasing function. Therefore, the new iteration (10) may be more efficient than the SHSS iteration when the optimal parameters are used. Here, we should note that the new iteration method is not always better than the SHSS iteration when the optimal parameters α_* are used. This is because that the upper bound of the radius is smaller cannot guarantee the corresponding spectral radius itself is always smaller.

4. Numerical experiments

In this section, we present two numerical experiments to illustrate the theoretical results and the effectiveness of our single-step iteration method for solving the large sparse non-Hermitian positive definite linear system (1) in terms of both iteration count (denoted as IT) and computing time (in seconds, denoted as CPU), and the norm of the residual (denoted as "RES") defined by

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

In actual computations, the iteration schemes are started from the zero vector and terminated if the current iterations satisfy ERR$\leq 10^{-6}$ or the number of the prescribed iteration steps $k = 400$ are exceeded, where

$$\text{ERR} = \frac{\|b - Ax^{(k)}\|_2}{\|b\|_2}.$$

All experiments are performed in MATLAB (R2010b) with machine precision 10^{-16}, and all experiments are implemented on a personal computer with 2.00G memory.

The new iteration method is compared with the PMHSS method [37], the HSS method (2), the MHSS method [41] and the SHSS method (3). Moreover, the new preconditioner induced by the new iteration method is compared with the GMRES(10) method [42] without preconditioning, the GMRES(10) method with the PMHSS preconditioner and the GMRES(10) method with the SHSS preconditioner. The iteration parameter α used in PMHSS preconditioner is 1 (which is the best parameter; see [37]). The parameter matrix P of the new method in our tests is taken as αH. Moreover, the iteration parameters α in our experiments for the new method are chosen by trial and error in interval [0,1.25]. More precisely, we test five values, i.e., 0.25, 0.50, 0.75, 1.00, 1.25 to get the numerical optimal values of iteration parameter α in our new method.

Example 1. In this text, we consider the following Stokes equation:

$$-\nu\triangle \boldsymbol{u} + \nabla \boldsymbol{f} = f, \text{ in } \Omega \tag{18}$$

$$\nabla \cdot \boldsymbol{u} = 0, \text{ in } \Omega \tag{19}$$

$$\boldsymbol{u} = 0, \text{ on } \partial\Omega \tag{20}$$

$$\int_{\Omega} p(x)dx = 0. \tag{21}$$

Here $\Omega = [0, 1] \times [0, 1] \subset R^2$, $\partial\Omega$ is the boundary of Ω, ν is the viscous coefficient of fluid, $\triangle$ denote the Laplace operator, $\boldsymbol{u}$ and p represent the velocity and pressure of fluid, respectively.

Firstly, discrete Laplace operator with center difference scheme, and also discrete the pressure and continuity parts with the first-order forward difference scheme. Then we can obtain the linear system like the form (which is a saddle point problem; see [43,44] for more detail)

$$\begin{pmatrix} A & B \\ -B^{\top} & C \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} p \\ -q \end{pmatrix}, \tag{22}$$

with nonsingular coefficient matrix of the following matrix blocks

$$A = \begin{pmatrix} I \otimes T + T \otimes I & 0 \\ 0 & I \otimes T + T \otimes I \end{pmatrix} \in R^{2l^2 \times 2l^2}$$

and

$$B = \begin{pmatrix} I \otimes F \\ F \otimes I \end{pmatrix} \in R^{2l^2 \times l^2},$$

with

$$T = \frac{\nu}{h^2} \cdot \text{tridiag}(-1, 2, -1) \in R^{l\times l} \text{ and } F = \frac{1}{h} \cdot \text{tridiag}(-1, 1, 0) \in R^{l\times l}$$

being tridiagonal matrices. Here, the (2,2) block sub-matrix of the coefficient matrix of (22) is $C = 0$. Moreover, $\otimes$ denotes the Kronecker product and $h = \frac{1}{l+1}$ is the size of the mesh. If we let the (2,2) block sub-matrix be $C = 5 * I$, then we can see that linear system (22) is a non-Hermitian positive definite linear system. This kind of example can also be seen in [24].

For Example 1, the numerical results about IT, CPU and RES of the HSS, SHSS methods and the new method are proposed in Table 1. From Table 1, we can see that our new method outperforms the HSS and SHSS iteration methods, because our new method needs much less time. Moreover, the numerical results about IT, CPU and RES of GMRES(10), the GMRES(10) method with the SHSS preconditioner and the GMRES(10) method with the new preconditioner are presented in Table 2. Obviously, from Table 2, we can see the new preconditioner outperforms other two methods.

Example 2 (*See [38,41]*)**.** In this test, we consider the following non-Hermitian positive definite linear equation:

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

where $V = tridiag(-1, 2, -1) \in R^{l\times l}$, $V_c = V - e_1 e_l^{\top} - e_l e_1^{\top} \in R^{l\times l}$, e_1 and e_l are the first and the last unit vectors in R^l, respectively. We take the right-hand side vector b to be $b = (1 + \mathrm{i})A\mathbf{1}$, with $\mathbf{1}$ being the vector of all entries equal to 1. Here T and W correspond to the five-point centered 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 $h = \frac{1}{m+1}$.

Table 1
Numerical results of different iterative methods.

Method	$l \times l$	8×8	16×16	32×32	64×64	128×128
HSS	α	56.06	107.06	208.47	410.01	807.21
	IT	60	107	194	360	682
	CPU	0.0563	0.3207	2.8591	27.4145	318.0620
	RES	8.51e−7	9.70e−7	9.72e−7	9.60e−7	9.99e−7
SHSS	α	18.09	19.50	20.30	21.01	19.05
	IT	43	43	41	38	332
	CPU	0.0251	0.0132	0.0671	0.4387	2.5804
	RES	9.28e−7	9.49e−7	9.19e−7	9.53e−7	8.68e−7
NEW	α	0.25	0.25	0.25	0.25	0.25
	IT	13	13	13	13	13
	CPU	0.0038	0.0133	0.0325	0.1951	1.3437
	RES	5.47e−7	5.68e−7	5.80e−7	5.90e−7	5.97e−7

Table 2
Numerical results of different preconditioners.

Method	$l \times l$	8×8	16×16	32×32	64×64	128×128
GMRES(10)	IT	6(7)	24(2)	–	–	–
	CPU	0.0457	0.0381	–	–	–
	RES	7.42e−7	9.90e−7	–	–	–
SHSS–GMRES(10)	IT	1(7)	1(7)	1(7)	1(7)	1(6)
	CPU	0.0198	0.0086	0.0445	0.2378	1.6202
	RES	7.57e−7	7.66e−8	4.55e−7	2.16e−7	4.30e−7
NEW–GMRES(10)	IT	1(6)	1(6)	1(6)	1(5)	1(4)
	CPU	0.0015	0.0039	0.0230	0.1776	0.8687
	RES	3.76e−7	6.31e−7	2.86e−7	8.25e−7	7.52e−7

Table 3
Numerical results of different iterative methods.

Method	$l \times l$	8×8	16×16	32×32	64×64	128×128
PMHSS	α	1.00	1.00	1.00	1.00	1.00
	IT	31	31	31	31	31
	CPU	0.0136	0.0151	0.3365	0.4721	3.8987
	RES	3.41e−5	4.82e−5	6.74e−5	9.43e−5	1.32e−4
HSS	α	3.45	4.41	2.71	1.61	0.93
	IT	107	83	136	222	389
	CPU	0.1566	0.3819	2.4116	17.0392	97.2819
	RES	5.03e−5	6.75e−5	9.57e−5	1.41e−4	2.03e−4
MHSS	α	1.86	1.79	1.05	0.55	0.27
	IT	50	51	75	128	241
	CPU	0.0902	0.2057	0.7529	5.3268	60.5282
	RES	4.10e−5	5.93e−5	1.01e−5	1.39e−4	2.05e−4
SHSS	α	0.45	0.43	0.15	0.16	0.28
	IT	14	22	28	43	229
	CPU	0.0119	0.0133	0.0590	0.5756	19.5000
	RES	2.73e−5	4.59e−5	1.03e−4	1.23e−4	2.05e−4
NEW	α	0.25	0.50	1.25	1.25	1.25
	IT	13	20	46	169	330
	CPU	0.0022	0.0087	0.0514	2.0001	20.8701
	RES	2.17e−5	7.00e−5	9.69e−5	2.40e−4	3.34e−4

The numerical results about IT, CPU and RES of the PMHSS, HSS, SHSS methods and the new method are proposed in Table 3. From Table 3, we can see that our new method outperforms the other four iteration methods for $l = 8, 16, 32$. For the large l ($l = 64,128$), our new method is better than the HSS method and MHSS method but is not effective than the PMHSS method and SHSS method. Thus, we accelerate the new method by GMRES(10); see [42] (Also, we compare this new preconditioner with the shift-splitting (SS) preconditioner [45], because the test of Example 2 can also be rewritten as a block two-by-two linear system).

The numerical results about IT, CPU and RES of GMRES(10), the GMRES(10) method with the PMHSS preconditioner, the GMRES(10) method with the SHSS preconditioner and the GMRES(10) method with the new preconditioner are presented in Table 4. As we can see from Table 4 that new preconditioner considerably outperforms other three preconditioners, because it needs less iteration counts and CPU time to reach the stopping criterion.

Table 4
Numerical results of different preconditioners.

Method	$l \times l$	8×8	16×16	32×32	64×64	128×128
GMRES(10)	IT	8(8)	23(3)	–	–	–
	CPU	0.0082	0.0355	–	–	–
	RES	8.77e−7	9.85e−7	–	–	–
PMHSS–GMRES(10)	IT	1(8)	1(8)	1(10)	2(2)	2(3)
	CPU	0.0080	0.0449	0.1809	1.1968	6.5108
	RES	2.63e−8	6.60e−7	3.45e−7	4.57e−7	9.12e−7
SHSS–GMRES(10)	IT	1(8)	1(9)	2(2)	3(4)	6(1)
	CPU	0.0025	0.0093	0.0693	0.5450	5.3421
	RES	3.18e−7	6.51e−8	1.18e−7	4.48e−7	8.85e−7
SS–GMRES(10)	IT	1(7)	1(9)	1(10)	1(11)	2(8)
	CPU	0.0046	0.0103	0.0763	0.5780	5.4928
	RES	4.79e−7	5.97e−8	4.47e−7	4.59e−7	2.63e−7
NEW–GMRES(10)	IT	1(6)	1(8)	1(9)	1(11)	2(6)
	CPU	0.0019	0.0075	0.0415	0.2276	1.5024
	RES	4.25e−7	5.37e−8	4.88e−7	7.11e−7	9.08e−7

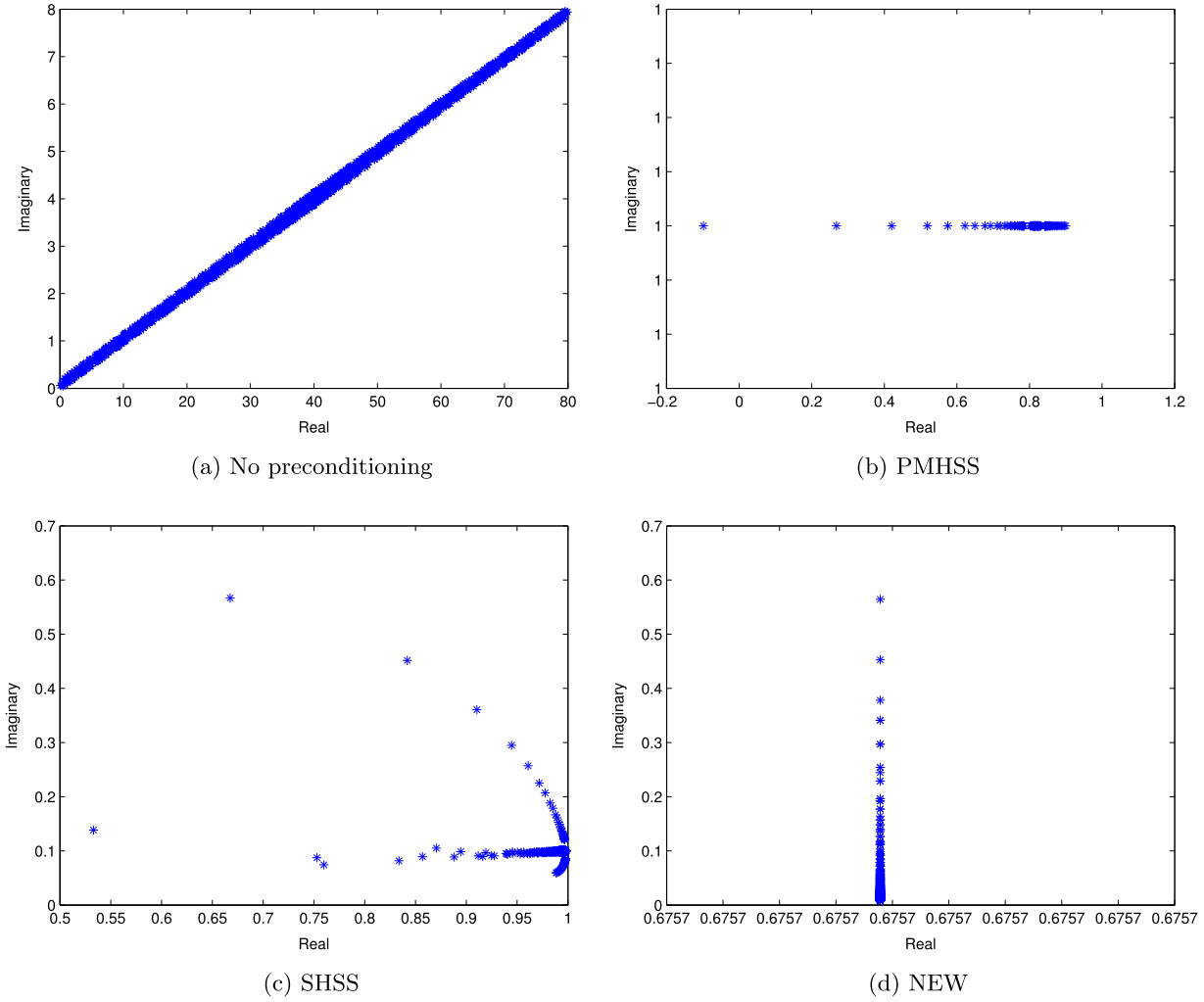


Fig. 1. The eigenvalue distributions of the matrix A and different preconditioned matrices when $l = 32$.

In Fig. 1, we depict the eigenvalue distributions of the coefficient matrix A, the PMHSS preconditioned matrix, the SHSS preconditioned matrix and the new preconditioned matrix when $l = 32$. From Fig. 1, we can see that all the eigenvalues of

Table 5
Numerical results of different iterative methods.

Method	$l \times l$	8×8	16×16	32×32	64×64	128×128
PMHSS	α	1.00	1.00	1.00	1.00	1.00
	IT	23	30	35	38	39
	CPU	0.0027	0.0088	0.0352	0.2438	1.6019
	RES	2.31e−7	4.65e−8	1.55e−8	4.50e−9	1.57e−9
HSS	α	1.46	1.45	1.49	1.01	0.82
	IT	27	24	85	207	–
	CPU	0.0513	0.1038	0.3494	2.3189	–
	RES	2.30e−7	5.95e−8	1.49e−8	5.53e−9	–
SHSS	α	0.63	0.46	0.15	0.36	0.10
	IT	32	31	41	158	157
	CPU	0.0047	0.0092	0.0390	0.7971	5.3040
	RES	2.43e−7	5.65e−8	1.59e−8	5.36e−9	1.89e−9
NEW	α	0.75	0.75	0.75	0.75	0.75
	IT	30	29	28	27	24
	CPU	0.0041	0.0065	0.0232	0.1609	1.1045
	RES	2.59e−7	5.97e−8	1.27e−8	4.04e−9	1.25e−9

Table 6
Numerical results of different preconditioners.

Method	$l \times l$	8×8	16×16	32×32	64×64	128×128
GMRES(10)	IT	3(2)	5(8)	12(8)	25(4)	–
	CPU	0.0203	0.0483	0.1358	0.8953	–
	RES	8.29e−7	9.16e−7	9.42e−7	9.98e−7	–
PMHSS–GMRES(10)	IT	1(10)	2(3)	2(4)	2(6)	2(6)
	CPU	0.0166	0.0406	0.1263	0.8683	5.2362
	RES	3.17e−7	8.18e−7	8.96e−7	3.41e−7	6.12e−7
SHSS–GMRES(10)	IT	1(10)	2(2)	2(4)	4(7)	5(1)
	CPU	0.0042	0.0112	0.0471	0.5647	3.5090
	RES	3.18e−7	6.51e−8	1.18e−7	4.48e−7	8.85e−7
NEW–GMRES(10)	IT	1(10)	2(1)	2(2)	2(2)	2(3)
	CPU	0.0040	0.054	0.0281	0.1920	1.0023
	RES	1.18e−7	6.40e−7	3.65e−7	7.40e−7	2.50e−7

the new preconditioned matrix are more clustered than others. Moreover, from Fig. 1 we can also see that all real part of the eigenvalues of the preconditioned matrix $\mathcal{P}_{new}^{-1}A$ are positive, which is in accordance with the results in Theorem 3.2.

Example 3 (*See [38]*)**.** In the second test, we consider the complex Helmholtz equation

$$-\Delta u + \sigma_1 u + i\sigma_2 u = f, \tag{23}$$

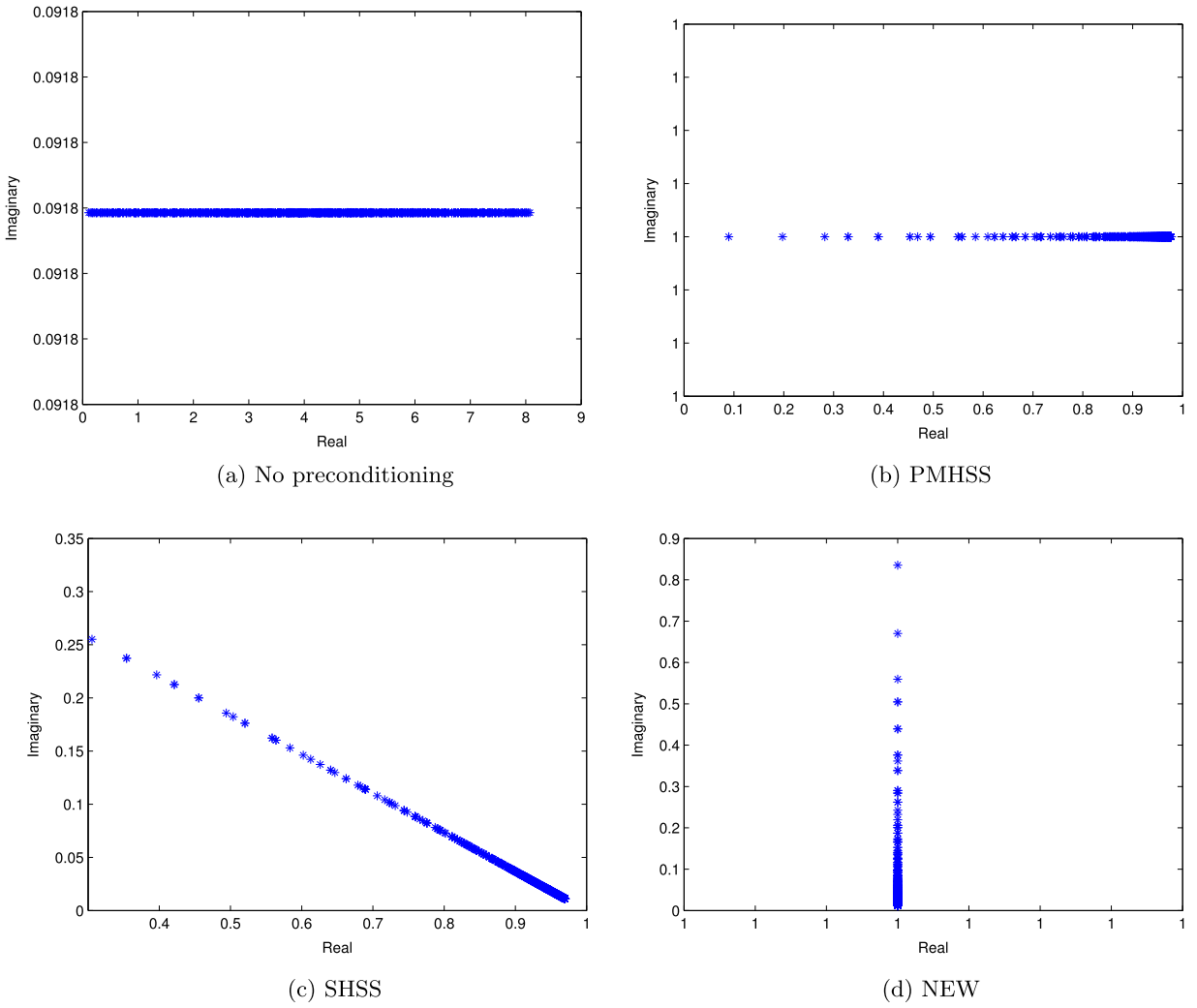
where σ_1 and σ_2 are real coefficient functions, u satisfies Dirichlet boundary conditions in $D = [0, 1] \times [0, 1]$ and $i = \sqrt{-1}$. We discretize the problem with finite differences on a $l \times l$ grid with mesh size $h = 1/(l+1)$. This leads to a system of linear equations

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

where $K = I \otimes V_l + V_l \otimes I$ is the discretization of $-\Delta$ by means of centered differences, wherein $V_l = h^{-2}\text{tridiag}(-1, 2, -1) \in R^{l\times l}$. 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. Furthermore, before solving the system we normalize the coefficient matrix and the right-hand side vector by multiplying both by h^2. For the numerical tests we set $\sigma_1 = \sigma_2 = 100$.

For this test, the numerical results about IT, CPU and RES of the PMHSS, HSS, SHSS methods and the new method are proposed in Table 5. From Table 5, we can see that our new method outperforms the other three iteration methods, because our new method needs much less time than the PMHSS method, the HSS method and the SHSS method. Moreover, the numerical results about IT, CPU and RES of GMRES(10), the GMRES(10) method with the PMHSS preconditioner, the GMRES(10) method with the SHSS preconditioner and the GMRES(10) method with the new preconditioner are presented in Table 6. As we can see from Table 6 that new preconditioner also considerably outperforms other three methods, because it needs less iteration counts and CPU time to reach the stopping criterion than those of the other three preconditioners.

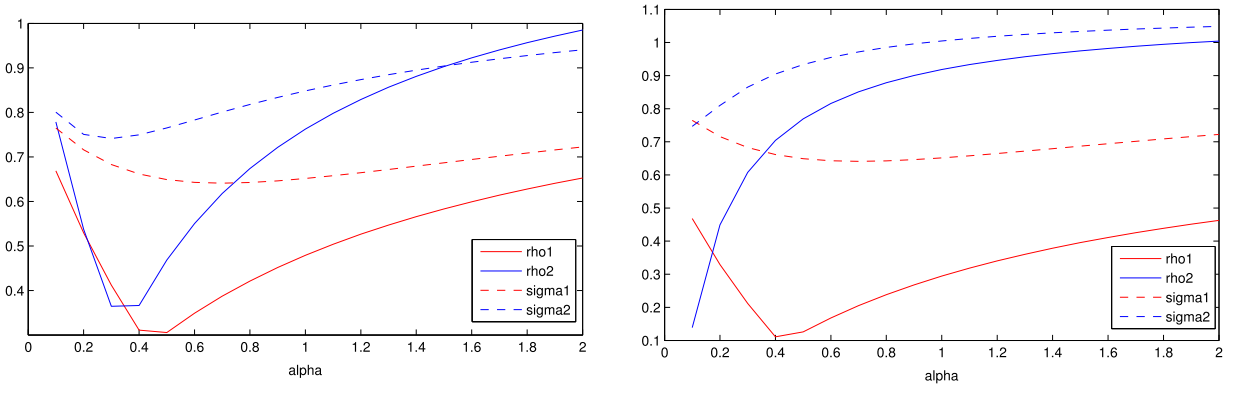
In Fig. 2, we depict the eigenvalue distributions of the matrix A, the PMHSS preconditioned matrix, the SHSS preconditioned matrix and the new preconditioned matrix for Example 3. We can see from Fig. 2 that all the eigenvalues of the new preconditioned matrix are more clustered than others. Furthermore, from Fig. 2 we can also see the results in Theorem 3.2



(a) No preconditioning (b) PMHSS

(c) SHSS (d) NEW

Fig. 2. The eigenvalue distributions of the matrix A and different preconditioned matrices when $l = 32$.



(a) $l = 16$ (b) $l = 32$

Fig. 3. The spectral radius: rho1 (NEW) and rho2 (SHSS); the upper bound of spectral radius: sigma1 (NEW) and sigma2 (SHSS).

hold true. Fig. 3 shows the curves of the spectral radius and their corresponding upper bound of the SHSS iteration method and our new iteration algorithm. As we can see from this figure that the spectral radius of our new method is smaller than the SHSS method and the upper bound of the new method is smaller than the SHSS iteration which is in accordance with the result of Remark 3.1.

5. Conclusions

In this paper, a single-step iteration method is presented for solving the large sparse non-Hermitian positive linear systems. The convergence property of the new iteration method for the linear system is given. Moreover, the optimal iteration parameter and some spectral properties of the new preconditioned matrices are analyzed. Numerical examples show the effectiveness of the new iteration method and new preconditioner for solving large sparse linear system (1).

For further reading

[46]

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