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Modified Hermitian and skew-Hermitian splitting methods for non-Hermitian positive-definite linear systems

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SUMMARY

To further study the Hermitian and non-Hermitian splitting methods for a non-Hermitian and positive-definite matrix, we introduce a so-called lopsided Hermitian and skew-Hermitian splitting and then establish a class of lopsided Hermitian/skew-Hermitian (LHSS) methods to solve the non-Hermitian and positive-definite systems of linear equations. These methods include a two-step LHSS iteration and its inexact version, the inexact Hermitian/skew-Hermitian (ILHSS) iteration, which employs some Krylov subspace methods as its inner process. We theoretically prove that the LHSS method converges to the unique solution of the linear system for a loose restriction on the parameter α. Moreover, the contraction factor of the LHSS iteration is derived. The presented numerical examples illustrate the effectiveness of both LHSS and ILHSS iterations.

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1. INTRODUCTION

Many problems in scientific computing require to solve the system of linear equations

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

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with $A \in \mathbb{C}^{n\times n}$ a large sparse non-Hermitian positive-definite matrix and $x, b \in \mathbb{C}^n$. To solve this problem iteratively, usually, efficient splittings of the coefficient matrix A are required. For example, the classic Jacobi and Gauss–Seidel iterations [1–3] split the matrix A into its diagonal and off-diagonal parts. Recently, a Hermitian/skew-Hermitian splitting [4–11] gains people's attention, which is

$$A = H + S$$

where

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

For non-Hermitian positive-definite systems, Bai *et al.* [4] presented the *HSS* iteration method: given an initial guess $x^{(0)}$, for $k = 0, 1, 2, \ldots$ until $\{x^{(k)}\}$ converges, compute

$$\begin{aligned}(\alpha I + H)x^{(k+1/2)} &= (\alpha I - S)x^{(k)} + b\\ (\alpha I + S)x^{(k+1)} &= (\alpha I - H)x^{(k+1/2)} + b\end{aligned} \tag{2}$$

where α is a given positive constant. They have also proved that for any positive α the HSS method converges unconditionally to the unique solution of the system of linear equations. The feasible IHSS iteration is discussed and can be adopted in actual implementations and has quite good performance.

Benzi and Golub [7] and Bai *et al*. [6] apply this method to the saddle point problem directly or as a preconditioner, which extends the application region of the HSS method to semidefinite linear systems. By further generalizing the concept of this method, Bai *et al*. [5] presented NSS method, where a normal/skew-Hermitian splitting ($A = N + S_0$, where $N \in \mathbb{C}^{n\times n}$ is a normal matrix and $S_0 \in \mathbb{C}^{n\times n}$ a skew-Hermitian matrix) is introduced and results in a two-stage iterative method: given an initial guess $x^{(0)}$, for $k = 0, 1, 2, \ldots$ until $\{x^{(k)}\}$ converges, compute

$$\begin{aligned}(\alpha I + N)x^{(k+1/2)} &= (\alpha I - S_0)x^{(k)} + b\\ (\alpha I + S_0)x^{(k+1)} &= (\alpha I - N)x^{(k+1/2)} + b\end{aligned}$$

where α is a given positive constant. Analogically to the HSS method, they also theoretically analyse the convergence properties of the NSS method and present a successive overrelaxation acceleration scheme for the NSS iteration.

Furthermore, Bai *et al*. [12] proposed PSS method, which essentially employs a positive-definite and skew-Hermitian splitting: $A = P + S$, $P \in \mathbb{C}^{n\times n}$ positive-definite and $S \in \mathbb{C}^{n\times n}$ skew-Hermitian and also produces a two-stage iteration. They specialize the PSS to block triangular and skew-Hermitian splitting and result in some feasible iteration [12], which can be applied to positive-definite systems of linear equations not only the non-Hermitian ones.

Moreover, based on the HS splitting, we can split A as

$$A = H + S = (\alpha I + S) - (\alpha I - H)$$

In this paper we present a different approach to solve Equations (1), called as the *Lopsided* Hermitian/skew-Hermitian splitting iteration, shortened as the *LHSS iteration*, and develop the HSS method in another direction. We describe it as follows.

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

$$\begin{aligned} Hx^{(k+1/2)} &= -Sx^{(k)} + b \\ (\alpha I + S)x^{(k+1)} &= (\alpha I - H)x^{(k+1/2)} + b \end{aligned} \tag{3}$$

where α is a given non-zero constant, and H is the Hermitian part of A, S the skew-Hermitian part. Since H is Hermitian positive definite and $\alpha I + S$ is also (positive of negative) definite, there is a good chance for LHSS iteration to converge to the unique solution of (1) fast.

Just like the HSS method (2), the LHSS iteration alternates between the Hermitian part H and the skew-Hermitian part S of the matrix A. Theoretical analysis shows that if the coefficient matrix A is positive definite the LHSS iteration (3) converges to the unique solution of the linear system (1) for a loose restriction on the choice of α. And the upper bound of the contraction factor of the LHSS iteration is dependent on the choice of α, the spectrum of the Hermitian part H and the maximum singular value of the skew-Hermitian part S, but is neither dependent on the rest singular values of S nor on the eigenvectors of the matrices H, S and A.

The two-half steps at each LHSS iterate require exact solutions with the matrices H and $\alpha I + S$. However, this is too costly to be practical in actual application. To overcome this disadvantage, the inexact lopsided Hermitian/skew-Hermitian splitting (ILHSS) iteration is employed. We solve the system of linear equations with coefficient matrix H by conjugate gradient (CG) method and $\alpha I + S$ by Krylov subspace method to some prescribed accuracies at each step of the LHSS iteration. Therefore, the ILHSS iteration can be regarded as a non-stationary iterative method for solving system (1).

This paper is organized as follows. In Section 2, we analyse the convergence properties of the LHSS iteration for non-Hermitian positive-definite linear systems. In Section 3, the ILHSS iteration is presented and its convergence property is studied. Numerical examples are presented in Section 4 to illustrate the effectiveness of our methods. Finally, in Section 5, we draw some conclusions.

2. CONVERGENCE ANALYSIS OF THE LHSS ITERATION

In this section, we study the choice of parameter α which results in convergent LHSS iteration and derive the upper bound of the contraction factor. The LHSS iteration method can be generalized to the two-step splitting iteration framework, we replicate the convergence criterion for a two-step splitting iteration from [4].

Lemma 2.1
Let $A \in \mathbb{C}^{n\times n}$, $A = M_i - N_i$ $(i=1, 2)$ be two splittings of A, and $x^{(0)} \in \mathbb{C}^n$ be a given initial vector. If $\{x^{(k)}\}$ is a two-step iteration sequence defined by

$$\begin{aligned} M_1 x^{(k+1/2)} &= N_1 x^{(k)} + b \\ M_2 x^{(k+1)} &= N_2 x^{(k+1/2)} + b \end{aligned} \qquad k = 0, 1, 2, \dots$$

then

$$x^{(k+1)} = M_2^{-1} N_2 M_1^{-1} N_1 x^{(k)} + M_2^{-1}(I + N_2 M_1^{-1})b, \quad k = 0, 1, 2, \dots$$

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Moreover, if the spectral radius $\rho(M_2^{-1}N_2M_1^{-1}N_1)<1$, then the iterative sequence $\{x^{(k)}\}$ converges to the unique solution $x^* \in \mathbb{C}^n$ of system (1) for all initial vectors $x^{(0)} \in \mathbb{C}^n$.

Applying this lemma to the LHSS iteration, we get convergence property in the following theorem.

Theorem 2.2
Let $A \in \mathbb{C}^{n\times n}$ be a positive-definite matrix, $H=\frac{1}{2}(A+A^*)$ and $S=\frac{1}{2}(A-A^*)$ be its Hermitian and skew-Hermitian parts, α be a non-zero constant. Then the iteration matrix $M(\alpha)$ of the LHSS method is

$$M(\alpha)=(\alpha I+S)^{-1}(\alpha I-H)H^{-1}(-S) \tag{4}$$

and its spectral radius $\rho(M(\alpha))$ is bounded by

$$\delta(\alpha)\equiv \frac{\sigma_{\max}}{\sqrt{\alpha^2+\sigma_{\max}^2}} \max_{\lambda_i \in \lambda(H)} \left|\frac{\alpha-\lambda_i}{\lambda_i}\right| \tag{5}$$

where $\lambda(H)$ is the spectral set of the matrix H and $\sigma_{\max}$ is the maximum singular value of the matrix S.

Assuming $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ we have

(i) If $\sigma_{\max} \leqslant \lambda_n$, when

$$\alpha>0 \quad \text{or} \quad \alpha<\frac{2\lambda_1\sigma_{\max}^2}{\sigma_{\max}^2-\lambda_1^2}$$

the bound $\delta(\alpha)<1$, i.e. the LHSS iteration converges;

(ii) if $\lambda_n<\sigma_{\max}<\lambda_1$, when

$$0<\alpha<\frac{2\lambda_n\sigma_{\max}^2}{\sigma_{\max}^2-\lambda_n^2} \quad \text{or} \quad \alpha<\frac{2\lambda_1\sigma_{\max}^2}{\sigma_{\max}^2-\lambda_1^2}$$

the bound $\delta(\alpha)<1$, i.e. the LHSS iteration converges;

(iii) if $\sigma_{\max} \geqslant \lambda_1$, when

$$0<\alpha<\frac{2\lambda_n\sigma_{\max}^2}{\sigma_{\max}^2-\lambda_n^2}$$

the bound $\delta(\alpha)<1$, i.e. the LHSS iteration converges.

Proof
Setting

$$M_1=H, \quad N_1=-S, \quad M_2=\alpha I+S \quad \text{and} \quad N_2=\alpha I-H$$

in Lemma 2.1, since H and $\alpha I+S$ are non-singular for any non-zero constant α, we get (4).

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By similarity transformation, we have

$$\begin{aligned}\rho(M(\alpha)) &= \rho((\alpha I + S)^{-1}(\alpha I - H)H^{-1}(-S)) \\ &\leqslant \|(\alpha I + S)^{-1}(\alpha I - H)H^{-1}(-S)\|_2 \\ &= \|(\alpha I - H)H^{-1}(-S)(\alpha I + S)^{-1}\|_2 \\ &\leqslant \|(\alpha I + S)^{-1}(-S)\|_2 \|H^{-1}(\alpha I - H)\|_2 \\ &= \max_{\sigma_i \in \sigma(S)} \frac{\sigma_i}{\sqrt{\alpha^2 + \sigma_i^2}} \max_{\lambda_i \in \lambda(H)} \left| \frac{\alpha - \lambda_i}{\lambda_i} \right|\end{aligned}$$

where $\sigma(S)$ is the singular-value set of matrix S. Apparently,

$$\max_{\sigma_i \in \sigma(S)} \frac{\sigma_i}{\sqrt{\alpha^2 + \sigma_i^2}} = \frac{\sigma_{\max}}{\sqrt{\alpha^2 + \sigma_{\max}^2}}$$

We have the bound for $\rho(M(\alpha))$ given by (5).

There exists a α^*, where $\alpha^* > 0$ such that

$$\max_{\lambda_i \in \lambda(H)} \left| \frac{\alpha - \lambda_i}{\lambda_i} \right| = \begin{cases} \dfrac{\alpha - \lambda_n}{\lambda_n} & \text{if } \alpha \geqslant \alpha^* \\[2ex] \dfrac{\lambda_1 - \alpha}{\lambda_1} & \text{if } \alpha \leqslant \alpha^* \end{cases}$$

We discuss $\delta(\alpha)$ as follows.

(1) If $\alpha \geqslant \alpha^*$, then

$$\delta(\alpha) = \frac{\sigma_{\max}(\alpha - \lambda_n)}{\lambda_n \left(\sqrt{\alpha^2 + \sigma_{\max}^2}\right)}$$

With $\delta(\alpha) < 1$ and $\alpha \geqslant \alpha^* > 0$, we get

$$\alpha < \frac{2\lambda_n \sigma_{\max}^2}{\sigma_{\max}^2 - \lambda_n^2} \quad \text{where } \sigma_{\max} > \lambda_n$$

$$\alpha > \frac{2\lambda_n \sigma_{\max}^2}{\sigma_{\max}^2 - \lambda_n^2} \quad \text{where } \sigma_{\max} < \lambda_n$$

(2) If $\alpha \leqslant \alpha^*$, then

$$\delta(\alpha) = \frac{\sigma_{\max}(\lambda_1 - \alpha)}{\lambda_1 \left(\sqrt{\alpha^2 + \sigma_{\max}^*}\right)}$$

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With $\delta(\alpha)<1$, by simple computing we get
if $\alpha>0$, then

$$\alpha < \frac{2\lambda_1\sigma_{\max}^2}{\sigma_{\max}^2-\lambda_1^2} \quad \text{where } \sigma_{\max}>\lambda_1$$

$$\alpha > \frac{2\lambda_1\sigma_{\max}^2}{\sigma_{\max}^2-\lambda_1^2} \quad \text{where } \sigma_{\max}<\lambda_1$$

if $\alpha<0$, then

$$\alpha<\frac{2\lambda_1\sigma_{\max}^2}{\sigma_{\max}^2-\lambda_1^2} \quad \text{where } \sigma_{\max}>\lambda_1$$

With similar analysis, we have,

$$\alpha>0 \quad \text{or} \quad \alpha<-\frac{2\lambda_1\lambda_n^2}{\lambda_1^2-\lambda_n^2} \quad \text{where } \sigma_{\max}=\lambda_n$$

$$0<\alpha<\alpha<\frac{2\lambda_1^2\lambda_n}{\lambda_1^2-\lambda_n^2} \quad \text{where } \sigma_{\max}=\lambda_1$$

Resorting these results by the relationship of $\sigma_{\max}$ and λ_1, λ_n we can complete the proof of this theorem. □

Theorem 2.2 shows the choice of α which results in convergent LHSS iteration and the convergence speed is bounded by $\delta(\alpha)$, which depends on the spectrum of the Hermitian part H and the skew-Hermitian part S, but does not depend on the spectrum of A, and neither on the eigenvalues of the matrices H, S, A. Moreover, it is observed that the restriction put on α is very loose and the available region for α is becoming large and the bound of $\rho(M(\alpha))$ is becoming small with the decrease of $\sigma_{\max}$.

Now, our task is to give a determination for parameter α minimizing the bound $\delta(\alpha)$ on $\rho(M(\alpha))$, that is determining the *optimal* α. We have the following corollary.

Corollary 2.3
Let A, H and S be defined as those in Theorem 2.2, and $\lambda_{\max}$, $\lambda_{\min}$ be the maximum and minimum eigenvalues of the matrix H, $\sigma_{\max}$ be the maximum singular value of the matrix S. Then the optimal parameter α is

$$\alpha^*=\frac{2\lambda_{\max}\lambda_{\min}}{\lambda_{\max}+\lambda_{\min}}$$

and the bound for $\rho(M(\alpha))$ is

$$\delta(\alpha^*)=\frac{(\lambda_{\max}-\lambda_{\min})\sigma_{\max}}{\sqrt{4\lambda_{\max}^2\lambda_{\min}^2+\sigma_{\max}^2(\lambda_{\max}-\lambda_{\min})^2}}<1$$

Proof
Now that

$$\delta(\alpha) \equiv \frac{\sigma_{\max}}{\sqrt{\alpha^2+\sigma_{\max}^2}} \max_{\lambda_i \in \lambda(H)} \left| \frac{\alpha-\lambda_i}{\lambda_i} \right|$$

$$= \max \left\{ \frac{\sigma_{\max}}{\sqrt{\alpha^2+\sigma_{\max}^2}} \left| \frac{\alpha-\lambda_{\max}}{\lambda_{\max}} \right|, \frac{\sigma_{\max}}{\sqrt{\alpha^2+\sigma_{\max}^2}} \left| \frac{\alpha-\lambda_{\min}}{\lambda_{\min}} \right| \right\}$$

To minimize the upper bound $\delta(\alpha)$ of $\rho(M(\alpha))$, the following equality must hold:

$$\frac{\sigma_{\max}}{\sqrt{\alpha^2+\sigma_{\max}^2}} \left| \frac{\alpha-\lambda_{\max}}{\lambda_{\max}} \right| = \frac{\sigma_{\max}}{\sqrt{\alpha^2+\sigma_{\max}^2}} \left| \frac{\alpha-\lambda_{\min}}{\lambda_{\min}} \right|$$

therefore

$$\alpha^* = \frac{2\lambda_{\max}\lambda_{\min}}{\lambda_{\max}+\lambda_{\min}}$$

and the results follow. $\square$

It should be noted that the optimal parameters α^* in Corollary 2.3 minimize the bound $\delta(\alpha)$ of the iteration matrix, not the spectral radius of the iteration matrix.

We shall compare the LHSS and HSS method and give a criterion for choosing between these two methods. We first introduce a lemma briefly reviewing the convergence analysis of the HSS method established in [4].

Lemma 2.4
Let A, H and S be defined as those in Theorem 2.2 and α be a non-zero constant. Then the spectral radius $\rho(M(\alpha))$ of the iteration matrix of the HSS method (2) is bounded by

$$\gamma(\alpha) = \max_{\lambda_i \in \lambda(H)} \left| \frac{\alpha-\lambda_i}{\lambda_i+\alpha} \right|$$

where $\lambda(H)$ is the spectral set of the matrix H. Thus, it holds that

$$\rho(M(\alpha)) \leqslant \gamma(\alpha) < 1 \quad \forall \alpha > 0$$

Moreover, if $\lambda_{\min}$ and $\lambda_{\max}$ are the lower and upper bounds of the eigenvalues of the matrix H, then

$$\overline{\alpha} = \arg\min_{\alpha} \left\{ \max_{\lambda_{\min} \leqslant \lambda \leqslant \lambda_{\max}} \left| \frac{\alpha-\lambda}{\lambda+\alpha} \right| \right\} = \sqrt{\lambda_{\min}\lambda_{\max}}$$

and

$$\gamma(\overline{\alpha}) = \frac{\sqrt{\lambda_{\max}}-\sqrt{\lambda_{\min}}}{\sqrt{\lambda_{\max}}+\sqrt{\lambda_{\min}}}$$

With this lemma and Corollary 2.3, we give the following theorem that can be used for choosing between the two methods.

Theorem 2.5
Let $\lambda_{\min}$, $\lambda_{\max}$, $\sigma_{\max}$, α^* and $\delta(\alpha^*)$ be defined as those in Corollary 2.3 and $\bar{\alpha}$ and $\gamma(\bar{\alpha})$ be those in Lemma 2.4, then, if

$$\sigma_{\max}^2 \leqslant \frac{\lambda_{\min}^2 \lambda_{\max}^2}{(\lambda_{\max} - \lambda_{\min})^2 \sqrt{\lambda_{\min}\lambda_{\max}}} \tag{6}$$

then the following inequality holds:

$$\delta(\alpha^*) \leqslant \gamma(\bar{\alpha})$$

Proof
Suppose that $\delta(\alpha^*) \leqslant \gamma(\bar{\alpha})$, then

$$\frac{(\lambda_{\max} - \lambda_{\min})\sigma_{\max}}{\sqrt{4\lambda_{\max}^2\lambda_{\min}^2 + \sigma_{\max}^2(\lambda_{\max} - \lambda_{\min})^2}} \leqslant \frac{\sqrt{\lambda_{\max}} - \sqrt{\lambda_{\min}}}{\sqrt{\lambda_{\max}} + \sqrt{\lambda_{\min}}}$$

This implies

$$(\lambda_{\max} - \lambda_{\min})^2 \sigma_{\max} \leqslant \sqrt{4\lambda_{\max}^2\lambda_{\min}^2 + \sigma_{\max}^2(\lambda_{\max} - \lambda_{\min})^2} \left(\lambda_{\max} + \lambda_{\min} - 2\sqrt{\lambda_{\max}\lambda_{\min}}\right)^2$$

then, applying squaring operation on both sides and combining the coefficients of $\sigma_{\max}$, we have

$$\begin{aligned}&\left((\lambda_{\max}-\lambda_{\min})^2 - \left(\lambda_{\max} + \lambda_{\min} - 2\sqrt{\lambda_{\max}\lambda_{\min}}\right)^2\right)(\lambda_{\max}-\lambda_{\min})^2\sigma_{\max}^2 \\ &\leqslant 4\lambda_{\max}^2\lambda_{\min}^2\left(\sqrt{\lambda_{\max}} - \sqrt{\lambda_{\min}}\right)^2\end{aligned}$$

Since

$$\begin{aligned}&(\lambda_{\max} - \lambda_{\min})^2 - \left(\lambda_{\max} + \lambda_{\min} - 2\sqrt{\lambda_{\max}\lambda_{\min}}\right)^2 \\ &= \left(\lambda_{\max} - \lambda_{\min} + \left(\lambda_{\max} + \lambda_{\min} - 2\sqrt{\lambda_{\max}\lambda_{\min}}\right)\right) \\ &\quad \times \left(\lambda_{\max} - \lambda_{\min} - \left(\lambda_{\max} + \lambda_{\min} - 2\sqrt{\lambda_{\max}\lambda_{\min}}\right)\right) \\ &= \left(2\lambda_{\max} - 2\sqrt{\lambda_{\max}\lambda_{\min}}\right)\left(2\sqrt{\lambda_{\max}\lambda_{\min}} - 2\lambda_{\min}\right) \\ &= 4\left(\sqrt{\lambda_{\max}} - \sqrt{\lambda_{\min}}\right)^2 \sqrt{\lambda_{\max}\lambda_{\min}}\end{aligned}$$

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Then by some simple symbolic computations, we get

$$\sigma_{\max}^2 \leqslant \frac{\lambda_{\min}^2 \lambda_{\max}^2}{(\lambda_{\max} - \lambda_{\min})^2 \sqrt{\lambda_{\min}\lambda_{\max}}}$$

and complete the proof. □

It should be noted that Theorem 2.5 compares the bounds on the spectral radius of the iteration matrices of the HSS method and the LHSS method when optimal parameter α is employed. When inequality (6) holds, it is not indicated that the LHSS method will converge faster than the HSS method, however, we can learn from this theorem that if the skew-Hermitian part of the coefficient matrix is less dominant then the LHSS method would be a good choice and if the skew-Hermitian part becomes more dominant we need to improve the LHSS method, but the improvement is not covered in this paper.

3. THE ILHSS ITERATION

In the process of LHSS iteration, we need to solve two systems of linear equations whose coefficient matrices are H and $\alpha I + S$. This is a tough task which is costly and even impractical in actual implementations. To improve computing efficiency of the LHSS iteration, we employ ILHSS iteration, that is to solve the two subproblems iteratively. Since H is Hermitian positive definite, we can solve this system of linear equations by employing CG method, and some Krylov subspace method [1, 2, 9, 13] to solve the system of linear equations with coefficient matrix $\alpha I + S$. We write the ILHSS iteration schemes in the following algorithm.

Algorithm 1
ILHSS: (if $A \in \mathbb{C}^{n\times n}$ is a non-Hermitian positive-definite matrix, $b \in \mathbb{C}^n$ and $x^{(0)} \in \mathbb{C}^n$ is the initial guess, then this algorithm leads to the solution of the system (1))
$k = 0$;
while (not convergent)
  $r^{(k)} = b - Ax^{(k)}$;
  approximately solve $Hz^{(k)} = r^{(k)}$ by employing CG method, such that the residual $p^{(k)} = r^{(k)} - Hz^{(k)}$ of the iteration satisfies $\|p^{(k)}\| \leqslant \eta_k \|r^{(k)}\|$;
  $x^{(k+1/2)} = x^{(k)} + z^{(k)}$;
  $r^{(k+1/2)} = b - Ax^{(k+1/2)}$;
  approximately solve $(\alpha I + S)z^{(k+1/2)} = r^{(k+1/2)}$ by employing some Krylov sub-space method, such that the residual $q^{(k)} = r^{(k+1/2)} - (\alpha I + S)z^{(k+1/2)}$ of the iteration satisfies $\|q^{(k)}\| \leqslant \tau_k \|r^{(k+1/2)}\|$;
  $x^{(k+1)} = x^{(k+1/2)} + z^{(k+1/2)}$;
  $k = k + 1$;
end

We remark that the convergent criterion for outer iteration is chosen at will. If the inner systems is solved exactly, the tolerances $\{\eta_k\}$ and $\{\tau_k\}$ are all zeros, then the ILHSS iteration essentially becomes the LHSS iteration. In fact, to obtain convergent ILHSS iteration, the sequences $\{\eta_k\}$ and $\{\tau_k\}$ are not required to go to zero as k increases. Bai *et al*. [4] had carefully studied the

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convergence properties for the two-step iteration, which is represented in the following lemma. We introduce a vector norm $|||x|||_M = \|Mx\|_2$ $(\forall x \in \mathbb{C}^n)$.

Lemma 3.1
Let $A \in \mathbb{C}^{n\times n}$ and $A = M_i - N_i$ $(i = 1, 2)$ be two splittings of the matrix A. If $\{x^{(k)}\}$ is an iteration sequence defined as follows:

$$x^{(k+1/2)} = x^{(k)} + z^{(k)} \quad \text{with } M_1 z^{(k)} = r^{(k)} + p^{(k)}$$

satisfying $\|p^{(k)}\| \leqslant \eta_k \|r^{(k)}\|$, where $r^{(k)} = b - Ax^{(k)}$; and

$$x^{(k+1)} = x^{(k+1/2)} + z^{(k+1/2)} \quad \text{with } M_2 z^{(k+1/2)} = r^{(k+1/2)} + q^{(k)}$$

satisfying $\|q^{(k)}\| \leqslant \tau_k \|r^{(k+1/2)}\|$, where $r^{(k+1/2)} = b - Ax^{(k+1/2)}$, then $\{x^{(k)}\}$ is of the form

$$\begin{aligned} x^{(k+1)} = {} & M_2^{-1} N_2 M_1^{-1} N_1 x^{(k)} + M_2^{-1}(I + N_2 M_1^{-1}) b \\ & + M_2^{-1}(N_2 M_1^{-1} p^{(k)} + q^{k+1/2}) \end{aligned} \tag{7}$$

Moreover, if $x^* \in \mathbb{C}^n$ is the exact solution of the system of linear equation (1), then we have

$$|||x^{(k+1)} - x^*|||_{M_2} \leqslant (\zeta + \mu\theta\eta_k + \theta(\rho + \theta v \eta_k)\tau_k) |||x^{(k)} - x^*|||_{M_2}, \quad k = 0, 1, \ldots \tag{8}$$

where

$$\zeta = \|N_2 M_1^{-1} N_1 M_2^{-1}\|, \quad \rho = \|M_2 M_1^{-1} N_1 M_2^{-1}\|, \quad \mu = \|N_2 M_1^{-1}\|$$
$$\theta = \|A M_2^{-1}\|, \quad v = \|M_2 M_1^{-1}\|$$

In particular, if

$$\zeta + \mu\theta\eta_{\max} + \theta(\rho + \theta v \eta_{\max})\tau_{\max} < 1$$

then the iteration sequence $\{x^{(k)}\}$ converges to $x^* \in \mathbb{C}^n$, where $\eta_{\max} = \max_k \{\eta_k\}$ and $\tau_{\max} = \max_k \{\tau_k\}$.

According to this lemma, we derive convergence properties for ILHSS iteration.

Theorem 3.2
Let $A \in \mathbb{C}^{n\times n}$ be a positive-definite matrix, H and S be its Hermitian and skew-Hermitian parts, and α be a non-zero constant. If $\{x^{(k)}\}$ is an iterative sequence generated by the ILHSS iteration method (Algorithm 1) and if $x^* \in \mathbb{C}^n$ is the exact solution of the system of linear equation (1), then it holds that

$$\begin{aligned} & |||x^{(k+1)} - x^*||| \leqslant \left(\delta(\alpha) + \theta\rho\tau_k \frac{\sigma_{\max}}{\sqrt{\alpha^2 + \sigma_{\max}^2}}\right)\left(1 + \theta\eta_k \frac{\sqrt{\alpha^2 + \sigma_{\max}^2}}{\sigma_{\max}}\right) |||x^{(k)} - x^*||| \\ & \quad k = 0, 1, \ldots \end{aligned} \tag{9}$$

where $|||x|||$ represents $|||x|||_{(\alpha I + S)}$, and

$$\rho = \|(\alpha I + S)(H)^{-1}\|_2, \quad \theta = \|A(\alpha I + S)^{-1}\|_2$$

Particularly, when

$$\left(\delta(\alpha)+\theta\rho\tau_{\max}\frac{\sigma_{\max}}{\sqrt{\alpha^2+\sigma_{\max}^2}}\right)\left(1+\theta\eta_{\max}\frac{\sqrt{\alpha^2+\sigma_{\max}^2}}{\sigma_{\max}}\right)<1$$

the iterative sequence $\{x^{(k)}\}$ converges to x^*, where $\tau_{\max}=\max_k\{\tau_k\}$ and $\eta_{\max}=\max_k\{\eta_k\}$.

Proof
Replacing M_i, N_i $(i=1,2)$ in Lemma 3.1 with

$$M_1=H, \quad N_1=-S$$
$$M_2=\alpha I+S, \quad N_2=\alpha I-H$$

and noting that $\sigma_{\max}/\sqrt{\alpha^2+\sigma_i^2}\geqslant 1$, then we have

$$\begin{aligned}|||x^{(k+1)}-x^*||| &\leqslant \left(\delta(\alpha)+\theta\eta_k\max_{\lambda_i\in\lambda(H)}\left|\frac{\alpha-\lambda_i}{\lambda_i}\right|+\theta\tau_k\left(\rho\frac{\sigma_{\max}}{\sqrt{\alpha^2+\sigma_{\max}^2}}+\eta_k\rho\theta\right)\right)|||x^{(k)}-x^*|||\\
&\leqslant \left(\delta(\alpha)+\theta\eta_k\delta(\alpha)\frac{\sqrt{\alpha^2+\sigma_{\max}^2}}{\sigma_{\max}}+\theta\rho\tau_k\frac{\sigma_{\max}}{\sqrt{\alpha^2+\sigma_{\max}^2}}\right.\\
&\quad\times\left.\left(1+\theta\eta_k\frac{\sqrt{\alpha^2+\sigma_{\max}^2}}{\sigma_{\max}}\right)\right)|||x^{(k)}-x^*|||\\
&=\left(\delta(\alpha)+\theta\rho\tau_k\frac{\sigma_{\max}}{\sqrt{\alpha^2+\sigma_{\max}^2}}\right)\left(1+\theta\eta_k\frac{\sqrt{\alpha^2+\sigma_{\max}^2}}{\sigma_{\max}}\right)|||x^{(k)}-x^*|||\end{aligned}$$

Then inequality (9) holds, and the results follow straightforwardly. □

Theorem 3.2 tells us the choice of the tolerances $\{\eta_k\}$ and $\{\tau_k\}$ for convergence. Apparently, we find that there is a trade-off between inner and outer iteration with the choice of $\{\eta_k\}$ and $\{\tau_k\}$, which we can attest in the numerical examples. However, the optimal tolerances $\{\eta_k\}$ and $\{\tau_k\}$ are hard to analyse.

4. NUMERICAL EXAMPLES

In this section, we give some numerical examples to illustrate the effectiveness of both LHSS and ILHSS iterations. For the convenience of comparison, we consider the three-dimensional convection–diffusion equation

$$-(u_{xx}+u_{yy}+u_{zz})+q(u_x+u_y+u_z)=f(x,y,z) \tag{10}$$

on the unit cube $\Omega=[0,1]\times[0,1]\times[0,1]$, with constant coefficient q and subject to Dirichlet-type boundary conditions. Greif and Varah [14, 15] have carefully studied this kind of problems,

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and Cheung and Ng [10] proposed other efficient methods, however, we used this problem as an example to illustrate the efficiency of our methods.

Discretizing this equation with seven-point finite difference and assuming the numbers (n) of grid points in all three directions are the same, we obtain a positive-definite system with linear equations A ($n^3 \times n^3$), and for details, we recommend you turn to [4, 14, 15]. Different q and n result in different matrix A. If we define $h=1/(n+1)$ as the step size, $r=qh/2$ is the mesh Reynolds number, according to the analysis in [4, 14, 15] we know for the centred difference scheme that

$$\min_{1\leqslant i\leqslant n^3} \lambda_i(H)=6(1-\cos\pi h), \qquad \max_{1\leqslant i\leqslant n^3} \lambda_i(H)=6(1+\cos\pi h)$$

$$\max_{1\leqslant i\leqslant n^3} \sigma_i(S)=6r\cos\pi h$$

and for the upwind difference scheme that

$$\min_{1\leqslant i\leqslant n^3} \lambda_i(H)=6(1+r)(1-\cos\pi h), \qquad \max_{1\leqslant i\leqslant n^3} \lambda_i(H)=6(1+r)(1+\cos\pi h)$$

$$\max_{1\leqslant i\leqslant n^3} \sigma_i(S)=6r\cos\pi h$$

Therefore, the *optimal* parameters (α^* and $\overline{\alpha}$ in Corollary 2.3 and Lemma 2.4) for both the HSS and LHSS method can be easily calculated out.

4.1. Spectral radius

In this subsection, we test the spectral radius of the iteration matrix M_α (4) with different q and different difference schemes. All the matrices tested are 512×512 unless otherwise mentioned, that is $n=8$. In Figures 1 and 2, we show the spectral radius $\rho(M(\alpha))$ of the iteration matrices of both LHSS method and HSS method with different α, and also the bound $\delta(\alpha)$ (5). From these two figures we find that when q is small (the Hermitian part is dominant), the spectral radius of the iteration matrix LHSS method is much smaller than that of HSS method, but as q becomes large (the skew-Hermitian part is dominant) the HSS method seems to perform better. When α is small, the bound $\delta(\alpha)$ is tight for $\rho(M(\alpha))$.

In Table I it is shown that α^* generated by Corollary 2.3 can result in fast convergence (when q is not large), however, α^* is a little far away from the optimal parameter α, which we present as α^{t} where t means *tested* and also *optimal*. We also see that $\rho(M(\alpha^*))$ is always less than one, which confirms the corollary.

Figure 3 shows the spectral radius of the iteration matrix of LHSS method for different q, where α^* represents $\rho(M(\alpha^*))$, α^{t} $\rho(M(\alpha^{\mathrm{t}}))$. We see that with the increasing of q (the matrix becomes dominant) the spectral radius becomes large, especially when $q>100$.

In Figures 4 and 5, we depict the distributions of the eigenvalues of the iteration matrices, where the parameter α^* which minimize the bound $\delta(\alpha)$ is applied.

4.2. Results for LHSS and ILHSS iteration

We study the LHSS and ILHSS iterations in this subsection. We try to solve the systems of linear equations $Ax=b$, where A is the matrix discretized from (10), and $f(x, y, z)$ is adjusted such that

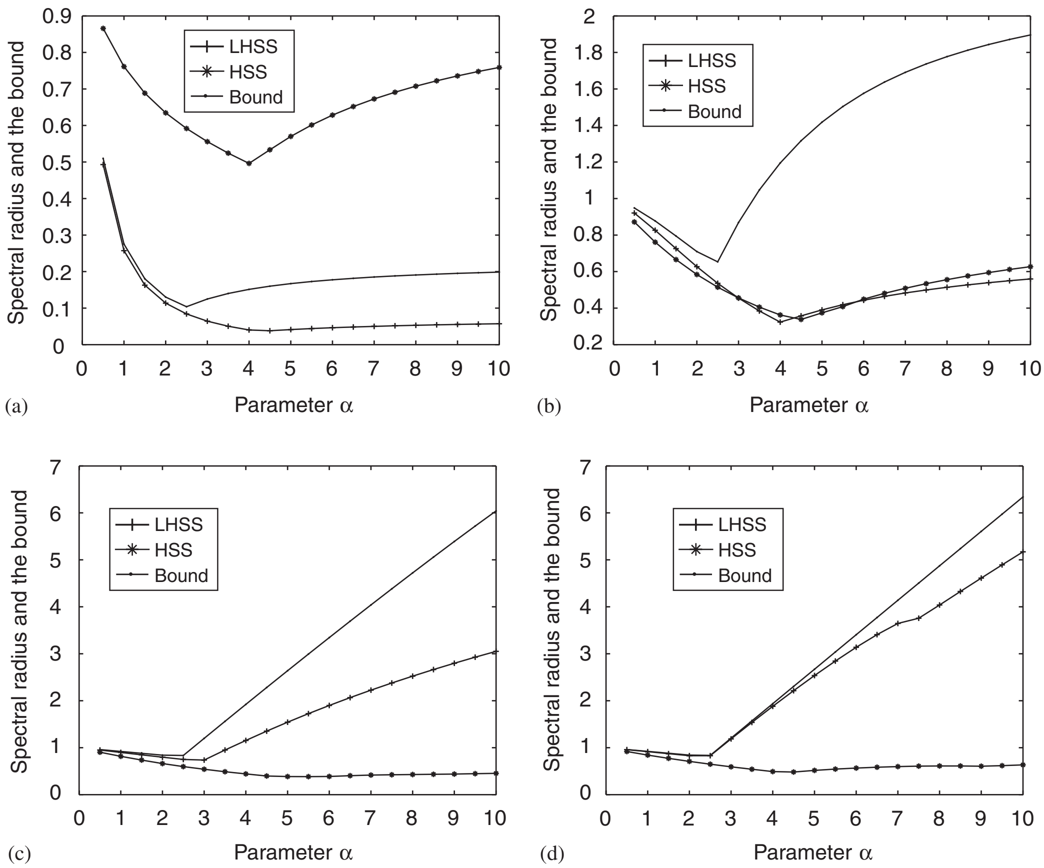

Figure 1. Centred difference scheme. The spectral radius $\rho(M(\alpha))$ of the iteration matrices of LHSS method and HSS method, and the bound $\delta(\alpha)$ with different α: (a) $q = 1$; (b) $q = 10$; (c) $q = 100$; and (d) $q = 1000$.

$b = Ae$ (e is $(1, 1, \ldots, 1)^{\mathrm{T}} \in \mathbb{C}^m$). All tests are started from the zero vector, performed in MATLAB with machine precision 10^{-16}, and terminated when the current iterate satisfies $\|r^{(k)}\|_2 < 10^{-6}$, where $r^{(k)}$ is the residual of the kth LHSS iteration. In Table II, we show the iteration numbers (it.s) of the LHSS method and the associate parameter α with different differential scheme and different q. When n increases the matrix the scale of A ($n^3 \times n^3$) increases very fast, therefore, it is hard to compute the spectral radius of A, and the α_{t} is hard to obtain, however, according to the experience and the test above, we can give a good estimation of it. We find that when n is large, the optimal parameter α is nearly the same with that when n is small, and the needed iterations are even less. And it is shown that the LHSS performs very good for a wide range of the parameter α, when q is not very large.

In the two-half steps of LHSS iteration, it is required to solve two systems of linear equations with matrices H and $\alpha I + S$, which is very costly. We employ ILHSS method in the actual implementation, that is solving the systems with coefficient matrix H iteratively by the CG method

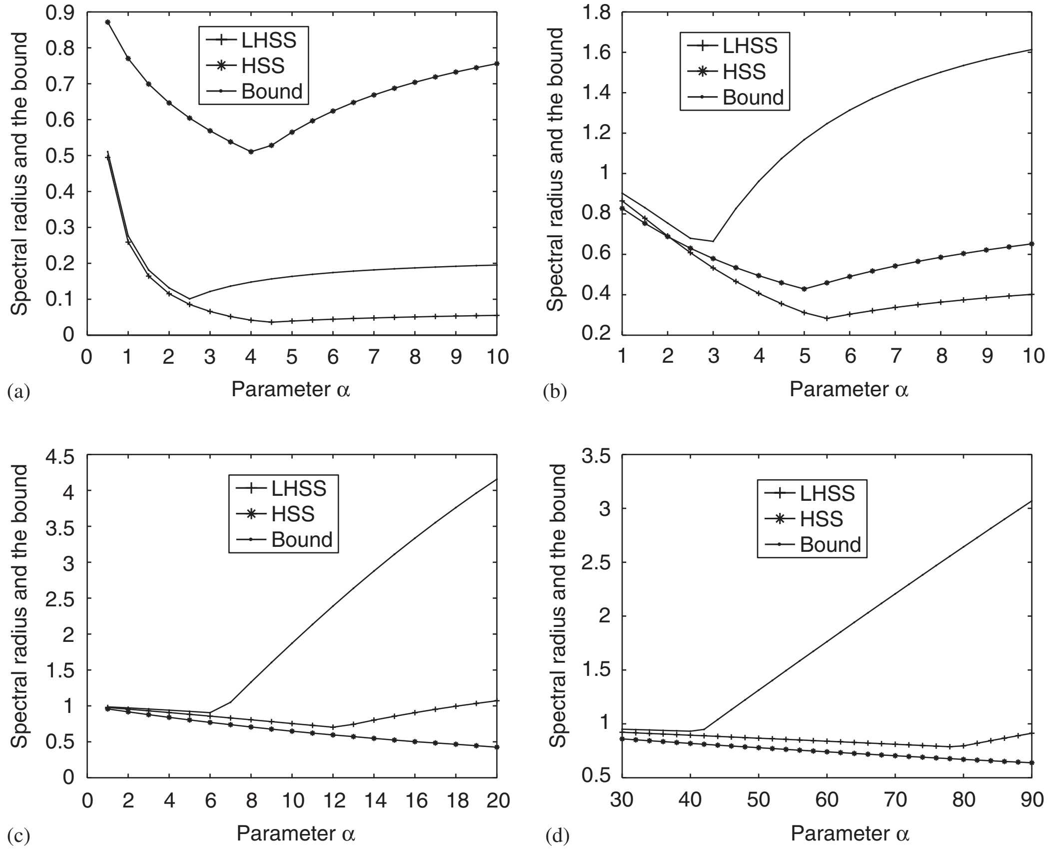

Figure 2. Upwind difference scheme. The spectral radius $\rho(M(\alpha))$ of the iteration matrices of LHSS method and HSS method, and the bound $\delta(\alpha)$ with different α: (a) $q=1$; (b) $q=10$; (c) $q=100$; and (d) $q=1000$.

Table I. Spectral radius of the iteration matrix of the LHSS method.

Difference scheme	q	α^*	$\rho(\alpha^*)$	α^{t}	$\rho(\alpha^{\mathrm{t}})$
Centred	1	2.5	0.0839	4.5	0.0380
Centred	10	2.5	0.5359	4	0.3232
Centred	100	2.5	0.7500	3	0.7361
Centred	1000	2.5	0.8290	2.5	0.8290
Upwind	1	2.5	0.0856	4.5	0.0362
Upwind	10	3	0.5326	5.5	0.2832
Upwind	100	6	0.8573	12	0.7033
Upwind	1000	40	0.8945	79	0.7853

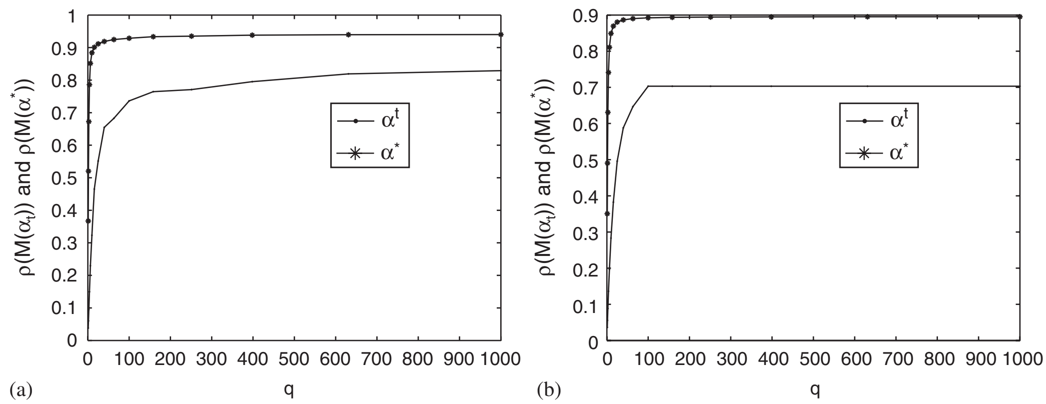

Figure 3. The spectral radius of the iteration matrices for different q; using α^* and α_t: (a) centred difference scheme; and (b) upwind difference scheme.

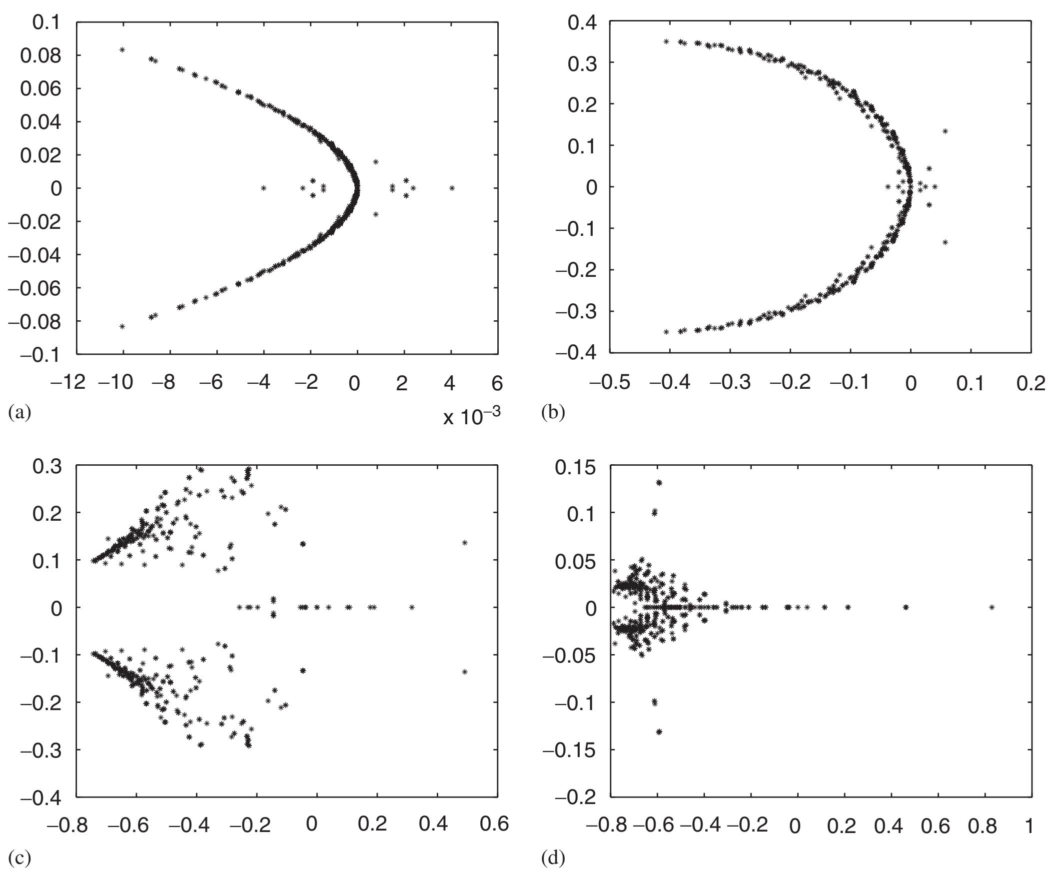

Figure 4. Centred difference scheme: (a) $q = 1$; (b) $q = 10$; (c) $q = 100$; and (d) $q = 1000$.

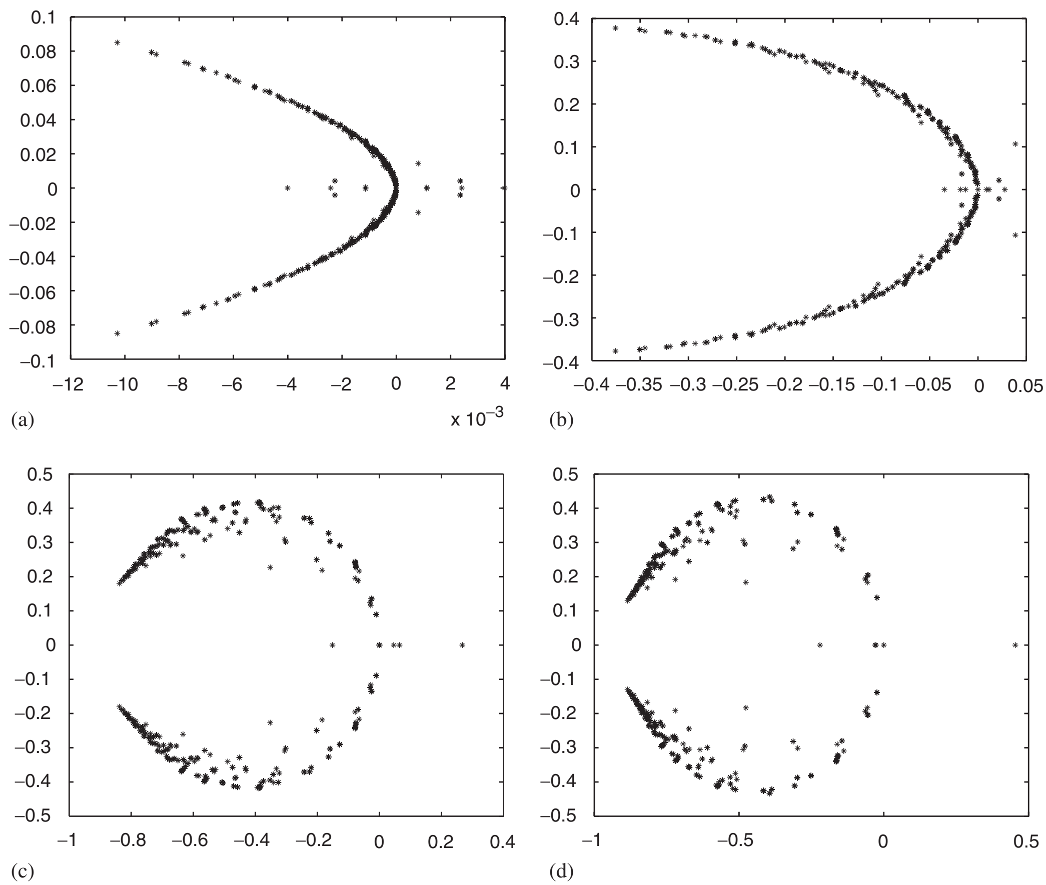

Figure 5. Upwind difference scheme: (a) $q = 1$; (b) $q = 10$; (c) $q = 100$; and (d) $q = 1000$.

Table II. Iterations of the LHSS method and the corresponding α.

		Centred difference scheme				Upwind difference scheme			
q	n	α^*	it.s	α^{t}	it.s	α^*	it.s	α^{t}	it.s
1	8	2.5	5	3	5	2.5	5	4.5	5
	16	1.2	6	3	4	1	6	$\geqslant 3.5$	$\leqslant 5$
	32	1.2	5	3	4	$\geqslant 1$	$\leqslant 5$	$\geqslant 3$	$\leqslant 4$
10	8	2.5	18	3.4	11	3	17	5.5	13
	16	1.5	16	3.6	8	3	9	5	8
	32	1.5	10	3.6	6	3	7	5	7

Table III. Centred difference scheme and $q=1$, the number of ILHSS iteration and inner iterations.

	$\tau=0.9$			$\tau=0.8$			$\tau=0.7$		
n	it.s	CG	GMRES	it.s	CG	GMRES	it.s	CG	GMRES
8	6	4.5	1	6	5	1	6	5.1	1
16	7	4	1	7	4.7	1.3	6	5.1	1.3
32	7	3.9	1	7	4.9	1	6	5.7	1.2

Table IV. Centred difference scheme and $q=10$, the number of ILHSS iteration and inner iterations.

	$\tau=0.9$			$\tau=0.8$			$\tau=0.7$		
n	it.s	CG	GMRES	it.s	CG	GMRES	it.s	CG	GMRES
8	13	4	3.7	13	5.3	4.3	12	6.6	5.2
16	10	4.2	2.6	9	6.1	2.8	9	6.9	3.2
32	8	4.4	1.8	8	5.5	2	8	6.1	2.4

Table V. Upwind difference scheme and $q=1$, the number of ILHSS iteration and inner iterations.

	$\tau=0.9$			$\tau=0.8$			$\tau=0.7$		
n	it.s	CG	GMRES	it.s	CG	GMRES	it.s	CG	GMRES
8	6	4.2	1	6	4.5	1.5	6	5.2	1.7
16	6	4.8	1	6	5.3	1.3	5	5.8	1
32	6	5	1	6	5.3	1	6	6.2	1

and solving the systems with coefficient matrix $\alpha I+S$ iteratively by the GMRES method (or other Krylov subspace methods, like BiCGSTAB and CGNE) in each outer iteration.

In our computations, the inner CG and GMRES iterates are terminated if the current residual of the inner iterations satisfy

$$\frac{\|p^{(j)}\|_2}{\|r^{(k)}\|_2}\leqslant 0.1\tau^k \quad \text{and} \quad \frac{\|q^{(j)}\|_2}{\|r^{(k)}\|_2}\leqslant 0.1\tau^k$$

(cf. Algorithm 1) where $p^{(j)}$ and $q^{(j)}$ are, respectively, the residuals of the jth inner CG and GMRES, $r^{(k)}$ is the kth outer ILHSS iteration, τ is a tolerance. In Tables III–VI, we list numerical results for the centred difference and upwind difference schemes when $q=1,10$.

We report the numbers of outer ILHSS iterations (it.s) and the average numbers of inner CG and GMRES iterations. According to these tables, the number of ILHSS iterations generally increases when τ increases and the inner iterations generally decrease. For the convenience of comparison, in our numerical tests we do not employ preconditioning technic in the inner iterations, even though, we find that our ILHSS method is very effective for not very large q.

Table VI. Upwind difference scheme and $q=10$, the number of ILHSS iteration and inner iterations.

	$\tau=0.9$			$\tau=0.8$			$\tau=0.7$		
n	it.s	PCG	GMRES	it.s	PCG	GMRES	it.s	PCG	GMRES
8	11	5.6	3	11	6.6	3.7	11	7.9	4
16	10	5.7	1.9	10	7	2	10	8.3	2.4
32	8	5.5	1.5	8	6.5	1.8	7	7.3	1.9

5. CONCLUSIONS

In this paper, we have introduced a modified HSS method called LHSS method for solving non-Hermitian positive-definite systems of linear equations. Theoretical analysis shows that for any initial guess the LHSS method converges to the unique solution of the system for a wide range of the parameter α. We also derive a bound for the spectral radius of the iteration matrix and give the α^* which minimizes the bound. To make the LHSS feasible, we present its inexact version ILHSS method, that is solving the linear systems at each iteration inexactly. In this manner, the ILHSS method can also converge to the unique solution, and save much CPU time.

Numerical tests show that when the Hermitian part of the coefficient matrix is dominant the LHSS method performs very well, however as the skew-Hermitian part becomes dominant the performance of the LHSS method becomes not so good as the HSS method. This fact is also indicated in Theorem 2.5. Therefore, we need to improve our method, such as introduce another parameter β in the first equation in (3), which we will study in the future.

Since the SSOR method is successfully used as preconditioner for the CG method [1, 2, 16], and recently, the HSS method preconditioned Keylov methods are considered for solving saddle point problems [6, 7, 9], it seems that a good splitting usually results in a good preconditioner. Thus, the LHSS method is promising for solving the non-Hermitian positive-definite systems, especially for those whose skew-Hermitian part are not so dominant.

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