

On Convergence Property of MINRES Method for Solving a Complex Shifted Hermitian Linear System

Guiding Gu and Guo Liu

Abstract—We discuss the convergence property of the minimum residual (MINRES) method for the solution of complex shifted Hermitian system $(\alpha I + H)x = f$. Our convergence analysis shows that the method has a faster convergence than that for real shifted Hermitian system $(Re(\alpha)I + H)x = f$ under the condition $Re(\alpha) + \lambda_{min}(H) > 0$, and a larger imaginary part of the shift α has a better convergence property. Numerical experiments show such convergence properties.

Keywords—complex shifted linear system, Hermitian matrix, MINRES method.

I. INTRODUCTION

WE are interested in the iterative solution of the following complex shifted Hermitian system

$$(\alpha I + H)x = f, \quad (1)$$

where $H \in C^{n \times n}$ is a Hermitian matrix, α is a complex number, called shift. Such the shifted systems arise in a variety of practical applications such as the complex Helmholtz equation, lattice gauge computations in QCD and structural dynamics, see [4], [6], [9], [10], [12].

We know that the Krylov subspace keeps shift invariance, *i.e.* for any α ,

$$K_m \equiv K_m(H, v) = K_m(\alpha I + H, v),$$

where $K_m(H, v) = \text{span}(v, Hv, H^2v, \dots, H^{m-1}v)$. Thus we can seek the approximation solution of the system (1) in $K_m(H, v)$. It is important that the basis of K_m can be produced by the Hermitian matrix H (therefore using short vector recurrences) rather than by the shifted matrix $\alpha I + H$, which is not Hermitian matrix. We know that such shifted system has been discussed for many years. The fundamental work of Faber and Manteuffel [5] ensured that the Arnoldi recurrence simplifies, yielding an optimal short-term recurrence. The issue was further explored and some theoretical results has been derived by [7], [8], [14], [15].

However, our motivation to discuss (1) comes from the HSS method [3]. We know that in the HSS method, two shifted sub-systems as inner iteration have to be solved per iteration step. In [10], a complex parameter α in the HSS method is employed and the HSS method with a suitable complex

parameter has a smaller spectral radius of the iteration matrix than with a real parameter, even than with the experimental 'optimal' real parameter; also see the numerical experiment 3 in this paper. Since a complex parameter α is employed in HSS, two sub-system become the complex shifted system, not the real shifted system. In such case, an interesting discussion on the convergence rate of the shifted sub-system (*i.e.* the system (1)) in the HSS method is which is better, complex shift α , or real shift α . In [11], we have shown that the Lanczos method has a better convergence property for solving the system (1) than that for solving the real shifted Hermitian system

$$(Re(\alpha)I + H)x = f. \quad (2)$$

In this paper, we discuss the convergence property of the MINRES method for solving the system (1). Similar to the Lanczos method, our convergence analysis also shows that under the condition $Re(\alpha) + \lambda_{min}(H) > 0$, the method have faster convergence than that for the system (2), and the method has the better convergence property if the shift has a larger imaginary part $Im(\alpha)$. Numerical experiments show such convergence properties.

II. CONVERGENCE PROPERTY OF MINRES METHOD

In this section we first briefly describe the MINRES method, and then give an analysis on its convergence property for the system (1).

The main ingredient of the MINRES method is the following Lanczos procedure [13] applied to the Hermitian matrix H with $v_1 = r_0 / \|r_0\|_2$ as a starting vector:

For $j = 1, 2, \dots, m$, Do

$$\begin{aligned} w_j &= Hv_j - \beta_j v_{j-1}, & (\text{if } j = 1, \text{ let } \beta_1 v_0 = 0) \\ \alpha_j &= (w_j, v_j), \\ w_j &= w_j - \alpha_j v_j, \\ \beta_{j+1} &= \|w_j\|, & (\text{if } \beta_{j+1} = 0, \text{ stop.}) \\ v_{j+1} &= w_j / \beta_{j+1}. \end{aligned}$$

EndDo

We refer to [16] for a detailed discussion of the Lanczos procedure. By setting $V_m = [v_1, \dots, v_m]$, an orthonormal basis of $K_m \equiv K_m(H, v_1)$, and a symmetric tridiagonal matrix $T_m = \text{tridiag}(\beta_i, \alpha_i, \beta_{i+1})$, we have the shifted factorization,

$$(\alpha I + H)V_m = V_m(\alpha I + T_m) + \beta_{m+1} v_{m+1} e_m^T.$$

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An approximation to the solution of the system (1) in $\{x_0\} + K_m$ can be written as $x_m = x_0 + V_m y_m$ and its residual is

$$\begin{aligned} r_m &= f - (\alpha I + H)x_m \\ &= r_0 - (\alpha I + H)V_m y_m \\ &= V_{m+1}(\beta e_1 - (\alpha I + \tilde{T}_m))y_m, \end{aligned}$$

where

$$\tilde{T}_m = \begin{pmatrix} T_m & \\ & \beta_{m+1} e_m^T \end{pmatrix}.$$

A. MINRES method

We solve y_m such that the residual r_m has the minimum norm,

$$\begin{aligned} \|r_m\| &= \min_{y \in C^m} \|V_{m+1}(\beta e_1 - (\alpha I + \tilde{T}_m))y\| \\ &= \min_{y \in C^m} \|\beta e_1 - (\alpha I + \tilde{T}_m)y\|. \end{aligned} \quad (3)$$

The following is the MINRES method for the system (1); see [8], [16].

Algorithm (MINRES method for the solution of the system (1)).

- 1) Choose x_0 , and let $r_0 = f - (\alpha I + H)x_0$, $\beta = \|r_0\|$, $v_1 = r_0/\beta$.
- 2) Run m steps of the Lanczos procedure to generate V_m and \tilde{T}_m .
- 3) Solve the solution: $y_m = \arg \min_{y \in C^m} \|\beta e_1 - (\alpha I + \tilde{T}_m)y\|$.
- 4) $x_m = x_0 + V_m y_m$.

In practical computation we can use the Givens complex rotation to solve the linear least-square problem (3), by which the direct version of the MINRES method (denoted by the D-MINRES method) can be derived. We omit the description and refer to [8], [16] for a detailed derivation. Our numerical experiments in the section 3 is based on the D-MINRES method.

B. Convergence Property

In this subsection, we give an analysis on the convergence property of the MINRES method for the system (1). By letting the shift $\alpha = a + ib$, the system (1) can be written as

$$(ibI + \hat{H})x = f, \quad (4)$$

where $\hat{H} = aI + H$. Let $\lambda_{max}(H)$, $\lambda_{min}(H)$ be the largest and smallest eigenvalue of the Hermitian matrix H . We now assume that $a + \lambda_{min}(H) > 0$. Thus the matrix \hat{H} is Hermitian positive definite (HPD). We produce the orthonormal basis V_m of $K_m(\hat{H}, r_0)$ and T_m by the Lanczos procedure with \hat{H} and $v_1 = r_0/\beta$, $\beta = \|r_0\|$, and then we have

$$\hat{H}V_m = V_m T_m + \beta_{m+1} v_{m+1} e_m^T$$

and

$$(ibI + \hat{H})V_m = V_m(ibI + T_m) + \beta_{m+1} v_{m+1} e_m^T.$$

It is clear that the convergence property of the method for solving the system (1) is equivalent to that for solving the system (4).

Note that the residual of any approximation solution x_m of (4) in $\{x_0\} + K_m(\hat{H}, r_0) = \{x_0\} + K_m(biI + \hat{H}, r_0)$ can be expressed by

$$\begin{aligned} r_m &= f - (biI + \hat{H})x_m \\ &= r_0 - (biI + \hat{H})q_{m-1}(biI + \hat{H})r_0 \\ &= p_m(biI + \hat{H})r_0, \end{aligned}$$

where $p_m(x)$ is a polynomial with $p_m(0) = 1$. By the minimum property, the residual r_m of the MINRES method, denoted by r_m^{min} , for the system (4) satisfies with

$$\|r_m^{min}\| = \min_{p_m(0)=1} \|p_m(biI + \hat{H})r_0\|.$$

Since the matrix \hat{H} is Hermitian, there exists a unitary matrix U , such that $\hat{H} = U\hat{\Lambda}U^H$, where $\hat{\Lambda} = \text{diag}(\hat{\lambda}_1, \dots, \hat{\lambda}_n)$ and $\hat{\lambda}_i$ is eigenvalue of \hat{H} , which is real. Then,

$$ibI + \hat{H} = U\tilde{\Lambda}U^H, \quad p_m(ibI + \hat{H}) = Up_m(\tilde{\Lambda})U^H,$$

where $\tilde{\Lambda} = \text{diag}(ib + \hat{\lambda}_1, \dots, ib + \hat{\lambda}_n)$. Thus,

$$\begin{aligned} \|r_m^{min}\| &= \min_{p_m(0)=1} \|Up_m(\tilde{\Lambda})U^H r_0\| \\ &\leq \min_{p_m(0)=1} \|p_m(\tilde{\Lambda})\| \|r_0\| \\ &= \min_{p_m(0)=1} \max_{\hat{\lambda}_j \in \Lambda(\hat{H})} |p_m(ib + \hat{\lambda}_j)| \|r_0\|. \end{aligned}$$

The eigenvalues $ib + \hat{\lambda}_j$ of the matrix $ibI + \hat{H} = \alpha I + H$ are all located on the line $L: \lambda + ib$, $\lambda \in [\hat{\lambda}_{min}, \hat{\lambda}_{max}]$, where $\hat{\lambda}_{min} = a + \lambda_{min}(H)$, $\hat{\lambda}_{max} = a + \lambda_{max}(H)$. Thus

$$\|r_m^{min}\| \leq \min_{p_m(0)=1} \max_{z \in L} |p_m(z)| \|r_0\|.$$

Consider the complex Chebyshev polynomial

$$T_m(z) = \frac{(z + \sqrt{z^2 - 1})^m + (z - \sqrt{z^2 - 1})^m}{2}.$$

It also can be expressed by

$$T_m(z) = \frac{\omega^m + \omega^{-m}}{2},$$

where z has the relation with ω as the following,

$$z = \frac{\omega + \omega^{-1}}{2}.$$

Let $c_0 = \frac{1}{2}(\hat{\lambda}_{max} + \hat{\lambda}_{min})$ and $e_0 = \frac{1}{2}(\hat{\lambda}_{max} - \hat{\lambda}_{min})$. We now define a mapping between the z -plane and the ω -plane:

$$\frac{z - c_0 - bi}{e_0} = \frac{\omega + \omega^{-1}}{2}.$$

This mapping transforms an unit circle $\omega = e^{i\theta}$ in the ω -plane onto the line L in the z -plane. Therefore, it holds that

$$T_m\left(\frac{z - c_0 - bi}{e_0}\right) = \frac{\omega^m + \omega^{-m}}{2}.$$

Let

$$\hat{T}_m(z) = \frac{T_m\left(\frac{z - c_0 - bi}{e_0}\right)}{T_m\left(\frac{-c_0 - bi}{e_0}\right)},$$

then $\hat{T}_m(0) = 1$. Thus we have

$$\|r_m^{min}\| \leq \max_{z \in L} \left| \frac{T_m\left(\frac{z-c_0-bi}{e_0}\right)}{T_m\left(\frac{-c_0-bi}{e_0}\right)} \right| \|r_0\|.$$

Assume that the point ω_0 in the ω - plane corresponds the point $z_0 = \frac{-c_0-bi}{e_0}$ in the z - plane, which satisfies with

$$\frac{-c_0 - bi}{e_0} = \frac{\omega_0 + \omega_0^{-1}}{2},$$

i.e., ω_0 satisfies with the following equation,

$$\omega_0^2 + 2q\omega_0 + 1 = 0,$$

where $q = \frac{c_0+bi}{e_0}$. We choose a larger root in the modulus as ω_0 ,

$$\omega_0 = -q - \sqrt{q^2 - 1}. \quad (5)$$

Then there is the following estimate by setting $\omega_0 = \rho_0 e^{i\phi}$,

$$\begin{aligned} \|r_m^{min}\| &\leq \max_{\omega=e^{i\theta}} \left| \frac{\omega^m + \omega^{-m}}{\omega_0^m + \omega_0^{-m}} \right| \|r_0\| \\ &\leq \frac{2}{|\omega_0^m + \omega_0^{-m}|} \|r_0\| \\ &= \frac{2}{\rho_0^m |1 + e^{-2i\phi} \rho_0^{-2m}|} \|r_0\|. \end{aligned}$$

Note that $Re(q) = \frac{c_0}{e_0} = \frac{\kappa+1}{\kappa-1} > 1$, where $\kappa = \frac{\lambda_{max}}{\lambda_{min}}$ is the condition number of the Hermitian positive matrix H . Since the complex number q is either in the first quadrant (if $b > 0$) or the fourth quadrant (if $b < 0$) of the complex plane, q and $\sqrt{q^2 - 1}$ are both in the same quadrant as $|q| > 1$. Thus by (5), it holds that

$$\rho_0 = |\omega_0| = |q + \sqrt{q^2 - 1}| > |q| > 1.$$

Then we have that $\frac{2}{|\omega_0^m + \omega_0^{-m}|} \rightarrow 0$, $m \rightarrow \infty$, i.e., the MINRES converges.

Remark Note that

$$|q|^2 = \frac{c_0^2 + b^2}{e_0^2} = \frac{b^2}{e_0^2} + \left(\frac{\kappa+1}{\kappa-1}\right)^2.$$

This demonstrates that the larger the imaginary b of the shift α is, the larger $|q|$ is, and therefore the larger $|\omega_0| = \rho_0$. In this case, the MINRES has a faster convergence rate.

We conclude these as the following convergence property of the MINRES method for solving the system (1).

Theorem Suppose that the matrix H be Hermitian, and the complex shift α be satisfied with $Re(\alpha) + \lambda_{min}(H) > 0$. Then the MINRES method for the system $(\alpha I + H)x = f$ converges and has a faster convergence than that for the Hermitian positive system $(Re(\alpha)I + H)x = f$.

III. NUMERICAL EXPERIMENTS

In this section, we give three numerical experiments to show the convergence property of the MINRES method revealed by the theorem for the complex shifted Hermite system $(\alpha I + H)x = f$ and the real shifted Hermitian system $(Re(\alpha)I + H)x = f$.

We report the results of our numerical experiments with a Fortran 77 implementation of the method based on the D-MINRES method. The right-hand side of the linear system is formed by $f = (\alpha I + H)x$, or $f = (Re(\alpha)I + H)x$, where $x = (1 - i, 1 - i, \dots, 1 - i)^T$. The initial value is set by $x^{(0)} = 0$, and the stopping criterion is based on the residual of system $\|r^{(k)}\| < 10^{-6}$.

Experiment 1 We form a Hermitian matrix $H = \frac{1}{2}(A + A^H)$, where

$$A = (-\omega^2 M + K) + i(\omega C_V + C_H)$$

is a complex matrix with the inertia and a modified stiffness matrices M , K , the viscous and the hysteretic damping matrices C_V , C_H , and the driving circular frequency ω (see [1], [2]). In our test, we also take (see [2]) $C_H = \mu K$ with μ a damping coefficient, $M = I$, $C_V = 10I$, and K the five-point centered difference matrix approximating the operator $L = -\Delta + \gamma(\partial_x + \partial_y)$, $\gamma \in R$ with homogeneous Dirichlet boundary conditions on a uniform mesh in the unit square $[0, 1] \times [0, 1]$ with the mesh-size $h = \frac{1}{m+1}$. In addition, we set $\omega = \pi$, $\mu = 0.02$, and normalize coefficient matrix and right-hand side by multiplying both by h^2 . The mesh-size $m = 128$ and the parameter $\gamma = 8$ is tested. The Hermitian matrix H is positive definite. Thus for all shift α with $Re(\alpha) \geq 0$, the MINRES method converges according to the theorem.

We reveal the convergence property of the MINRES method for the shifted system with zero imaginary part of the shift α (i.e. for the system (2)) and nonzero imaginary part of α (i.e. for the system (1)) by showing convergence curves for norm of residuals. We test two groups of values for the shift α : one is with $Re(\alpha) = 0$ (see the left of Fig. 1) and another is with $Re(\alpha) = 0.2$ (see the right of Fig. 1).

The curves in the Fig. 1 show the following facts:

1. the MINRES method for the linear system (1) converges faster than that for the linear system (2); e.g., the method converges respectively after 42 iteration (IT) steps for the linear system (1) with the shift $\alpha = 0.2 + 0.5i$; however it converges after IT=56 for the linear system (2) with the real shift $Re(\alpha) = 0.2$;

2. for the complex shifted linear system, a larger the imaginary part $Im(\alpha)$ has a better convergence property; e.g., IT=77 with $\alpha = 0 + 0.2i$ and IT=50 with $\alpha = 0 + 0.5i$;

3. the convergence property is irrelevant to the sign of the imaginary of the shift.

Experiment 2 We form a Hermitian matrix $H = \frac{1}{2}(A + A^H)$, where

$$A = W + iZ$$

is a complex matrix with $W = K + w_1 I$, $Z = K + w_2 I$, $w_1 = \frac{3-\sqrt{3}}{h}$, $w_2 = \frac{3+\sqrt{3}}{h}$ (see [2], [10]) and the matrix K the five-point centered difference matrix approximating the operator $L = -\Delta + \gamma(\partial_x + \partial_y)$, $\gamma \in R$ with homogeneous Dirichlet boundary conditions on a uniform mesh in the unit square $[0, 1] \times [0, 1]$ with the mesh-size $h = \frac{1}{m+1}$. We also normalize coefficient matrix and right-hand side by multiplying both by h^2 . The mesh-size $m = 128$ and the parameter $\gamma = 8$ are

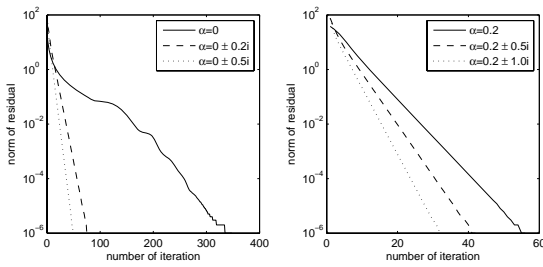


Fig. 1. Norm of residuals for Ex. 1. Left: the first group with $Re(\alpha) = 0$. Right: the second group with $Re(\alpha) = 0.2$.

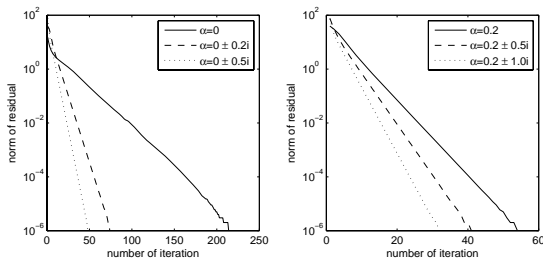


Fig. 2. Norm of residuals for Ex. 2. Left: the first group with $Re(\alpha) = 0$. Right: the second group with $Re(\alpha) = 0.2$.

tested, and in this case, the Hermitian matrix H is positive definite. Thus for all shift α with $Re(\alpha) \geq 0$, $Re(\alpha)I + H$ is Hermitian positive definite matrix, and the MINRES method converges according to the theorem.

We also test two groups of values for the shift α : one is with $Re(\alpha) = 0$ (see the left of Fig. 2) and another is with $Re(\alpha) = 0.2$ (see the right of Fig. 2).

The curves in the Fig. 2 show again the above three issues for the experiment 1. These numerical results illustrate that the method benefits from the imaginary part of a complex shift α when solving the linear system (1).

Experiment 3 As a source of the shifted Hermitian linear system and also as our motivation to discuss the linear system (1), in this experiment we use the HSS iteration method with a complex parameter α (see [10]) to solve the linear system

$$Ax = b, \quad (6)$$

with respect to the positive definite complex matrix A of (6). The mesh size $m = 32$ and the parameter $\gamma = 2$ are tested. In the HSS iteration method, two shifted linear sub-systems with respect to $\alpha I + H$ and $(-\alpha i)I + (-iS)$ have to be solved per iteration step, where $H = \frac{1}{2}(A + A^H)$, $S = \frac{1}{2}(A - A^H)$. Both sub-systems are the linear system (1) and we use the D-MINRES method to solve these sub-systems in the HSS iteration method. In [10], a suitable nonreal parameter $\alpha_{est} = 0.3520 + 1.0835i$ could be estimated according to the extremal eigenvalues of H and S . We test this estimated parameter α_{est} in the HSS iteration method to solve the linear system (6). As a comparison, we also test an experimental optimal real parameter $\alpha = a_{exp} = 0.6819$ in the HSS iteration method,

TABLE I
 $\rho(T(\alpha))$, IT AND CPU TIME FOR CONVERGENCE OF HSS FOR EXPERIMENT 3, AND IT FOR CONVERGENCE OF MINRES FOR SUB-SYSTEMS

$\alpha = a + bi$	$\rho(T(\alpha))$	IT	CPU	IT(H)	IT(S)
$\alpha_{est} = 0.3520 + 1.0835i$	0.7368	55	1.48	32	16
$a_{exp} = 0.6819$	0.8433	100	3.59	33	42

which is given by

$$a_{exp} = \arg \min_{\alpha_j} \rho(T(\alpha_j)),$$

where $\rho(T(\alpha))$ is the spectral radius of the HSS iterative matrix $T(\alpha)$, and real number α_j ($j = 1, \dots, 401$) is the equally-spaced points in $[0, \lambda_{max}(H)]$; see [10]. In our test, the eigenvalues of a matrix are solved by the function *eig* in *Matlab(7.4 ed)*.

In Table I, we show the spectral radius $\rho(T(\alpha))$, IT and CPU time (sec.) for convergence of the HSS iteration method with the nonreal parameter $\alpha = \alpha_{est}$ and the real parameter $\alpha = a_{exp}$, respectively. The stopping criterion is based on the system (6) residual $\|r^{(k)}\| < 10^{-6}$. Also, we show IT for convergence of the inner iteration using the D-MINRES method for solving two shifted linear sub-systems with these shift parameters, denoted by IT(H) for $(\alpha I + H)u = g$, and IT(S) for $((-\alpha i)I + (-iS))u = (-ig)$. The stopping criterion is based on the sub-system residual $\|r_{in}^{(l)}\| < 10^{-7}$. The numbers shown in the last two columns of Table I are stable iteration numbers for convergence of the inner iteration after nearly 3 outer iteration steps k .

The numerical results in Table I show the following facts:

1) the HSS iteration method with the nonreal parameter α_{est} has a smaller spectral radius and a considerable faster convergence rate than that with the experimental optimal real parameter a_{exp} ;

2) in the inner iteration, the D-MINRES method converges for the two shifted linear sub-systems with the nonreal shift α_{est} faster than that with the real shift a_{exp} . In particular, for the shifted linear sub-system $((-\alpha i)I + (-iS))u = (-ig)$, although the shift $a_{exp} = 0.6819 > Re(\alpha_{est}) = 0.3520$, but α_{est} has its imaginary part $Im(\alpha_{est}) = 1.0835$, which illustrates again that the method benefits from the imaginary part of a complex shift when solving the linear system (1).

3. as above issue 1 and 2, it is possible that the HSS iteration method with a suitable nonreal parameter α_{est} take less CPU time to solve the linear system (6) than with an experimental optimal real parameter a_{exp} , in particular, for the 'dominant' imaginary part of the matrix; see [10].

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