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ON CONVERGENCE PROPERTY OF THE LANCZOS METHOD FOR SOLVING A COMPLEX SHIFTED HERMITIAN LINEAR SYSTEM*

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Abstract

We discuss the convergence property of the Lanczos method for solving a complex shifted Hermitian linear system $(\alpha I + H)x = f$. By showing the colinear coefficient of two system's residuals, our convergence analysis reveals that under the condition $Re(\alpha) + \lambda_{min}(H) > 0$, the method converges faster than that for the real shifted Hermitian linear system $(Re(\alpha)I + H)x = f$. Numerical experiments verify such convergence property.

Mathematics subject classification: 65F10, 65Y20.
Key words: Hermitian matrix, Complex shifted linear system, Lanczos method.

1. Introduction

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

$$(\alpha I + H)x = f, \tag{1.1}$$

where $H \in C^{n\times n}$ is a Hermitian matrix, α is a complex number, called shift. Below, the linear system (1.1) will be termed the CSH linear system. Such shifted linear system arises in a variety of practical applications and has been discussed for many years; see [6-7,9,12,15]. The fundamental work of Faber and Manteuffel [8] ensured that the Arnoldi recurrence simplifies, yielding an optimal short-term recurrence. The issue was further explored and some theoretical results have been derived in [10-11,16-17].

Our motivation to discuss (1.1) comes from the HSS iteration method [5]; see also [1-2,4]. We know that in the HSS iteration method, two shifted linear sub-systems as inner iteration have to be solved per iteration step. In [14], a complex parameter α in the HSS iteration method is employed and the HSS iteration method with a suitable nonreal parameter has a smaller spectral radius of the iteration matrix than with a real parameter, even than with the experimental optimal real parameter; see also the numerical experiment 2 in this paper. Since a complex parameter α is employed in HSS, two linear sub-systems are the complex shifted linear systems, not the real shifted linear systems. In such case, an interesting discussion on the convergence rate of the shifted linear sub-system (*i.e.*, the linear system (1.1)) in the HSS iteration method is which is better, nonreal shift α, or real shift α.

In this paper, we discuss the convergence property of the Lanczos method for solving the CSH linear system (1.1). By showing the colinear coefficient of two system's residuals, our convergence analysis reveals that under the condition $Re(\alpha)+\lambda_{min}(H) > 0$, the method converges

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for the CSH linear system (1.1) faster than that for the real shifted Hermitian system

$$(Re(\alpha)I + H)x = f, \tag{1.2}$$

which indicates that the method benefits from the imaginary part of a complex shift α when solving the CSH linear system (1.1). It is known that for solving the system (1.2), the Lanczos method is equivalent to the CG method since the coefficient matrix $Re(\alpha)I + H$ is Hermitian positive definite under the condition $Re(\alpha)+\lambda_{min}(H) > 0$. This demonstrates that the Lanczos method for the CSH linear system (1.1) has a faster convergence than the CG method for the real shifted system (1.2). Numerical experiments verify such convergence property.

2. Lanczos Method and Its Convergence Property

In this section we briefly describe the direct version of the Lanczos method for solving the CSH linear system (1.1), and then give an analysis on the convergence property of the method.

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

For $j = 1, \cdots, m$, *Do*

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

EndDo

We refer to [18] for a detailed description about the Lanczos procedure. By setting $V_m = [v_1, \cdots, v_m]$ and a symmetric tridiagonal matrix $T_m = tridiag(\beta_i, \alpha_i, \beta_{i+1})$, where $\beta_i, \alpha_i, \beta_{i+1}$ are the entries in the ith row of the matrix T_m, we have the shifted factorization

$$(\alpha I + H)V_m = V_m(\alpha I + T_m) + \beta_{m+1}v_{m+1}e_m^T, \tag{2.1}$$

where V_m is an orthonormal basis of $K_m \equiv K_m(H, v_1)$. Note that the Krylov subspace keeps shift invariance $K_m(H, v_1) = K_m(\alpha I + H, v_1)$. An approximation to the solution of (1.1) in $\{x_0\} + K_m$ can be written as $x_m = x_0 + V_m y_m$ and its residual is

$$\begin{aligned}
r_m =& f - (\alpha I + H)x_m\\
=& r_0 - V_m(\alpha I + T_m)y_m - \beta_{m+1}v_{m+1}e_m^T y_m.
\end{aligned} \tag{2.2}$$

2.1. Lanczos method

By imposing the Galerkin condition $r_m \perp K_m$, we have

$$(\alpha I + T_m)y_m = V_m^H r_0 = \beta e_1, \tag{2.3}$$

where $\beta = \|r_0\|$. Thus the Lanczos solution of the CSH linear system (1.1) has the form $x_m = x_0 + V_m(\alpha I + T_m)^{-1}(\beta e_1)$. Note that the shifted matrix $\alpha I + T_m$ is nonsingular under the condition $Re(\alpha) + \lambda_{min}(H) > 0$ in the Theorem 2.2. Let $y_m = (\eta_1, \cdots, \eta_m)^T$. By (2.2), we have the following result [18]; see also [13].

Property 2.1 *The residual r_m of the Lanczos solution has the expression*

$$r_m = -\beta_{m+1} e_m^T y_m v_{m+1} = -\beta_{m+1}\eta_m v_{m+1}. \tag{2.4}$$

This expression is important for our convergence analysis in the next subsection.

In practical computation, we can solve y_m in (2.3) by $L_m U_m y_m = \beta e_1$, where $\alpha I + T_m = L_m U_m$ is the LU factorization of $\alpha I + T_m$. The factorization is of the form

$$\alpha I + T_m \quad = \begin{pmatrix} 1 & & & & \\ l_2 & 1 & & & \\ & l_3 & 1 & & \\ & & \ddots & \ddots & \\ & & & l_m & 1 \end{pmatrix} \begin{pmatrix} d_1 & \beta_2 & & & \\ & d_2 & \beta_3 & & \\ & & d_3 & \beta_4 & \\ & & & \ddots & \ddots \\ & & & & d_m \end{pmatrix}.$$

The formulas of the elements are

$$\begin{cases} d_1 = \alpha + \alpha_1, & l_2 = \beta_2/d_1, \\ d_k = \alpha + \alpha_k - \beta_k l_k, & l_k = \beta_k/d_{k-1}, \qquad k = 2, \cdots, m. \end{cases} \tag{2.5}$$

We omit derivation of the following direct version of the Lanczos method (D-Lanczos); see [11,18].

Algorithm 2.1. D-Lanczos method for solving the CSH linear system (1.1).

1. Choose x_0, and let $r_0 = f - (\alpha I + H)x_0,\ \zeta_1 = \beta = \|r_0\|,\ v_1 = r_0/\beta$.
2. Setting $l_1 = \beta_1 = 0,\ p_0 = 0$.
3. For $m = 1, 2, \cdots,$ until Convergence, Do

$$w_m = Hv_m - \beta_m v_{m-1},$$
$$\alpha_m = (w_m, v_m),$$

If $m > 1$,

$$l_m = \beta_m/d_{m-1}, \quad \zeta_m = -l_m \zeta_{m-1} \tag{2.6}$$

endIf

$$d_m = \alpha + \alpha_m - \beta_m l_m,$$
$$\eta_m = \zeta_m/d_m, \tag{2.7}$$
$$p_m = \frac{1}{d_m}(v_m - \beta_m p_{m-1}),$$
$$x_m = x_{m-1} + \zeta_m p_m,$$
$$w_m = w_m - \alpha_m v_m,$$
$$\beta_{m+1} = \|w_m\|,$$

If $|\beta_{m+1}||\eta_m| < \epsilon$, Stop.

$$v_{m+1} = w_m/\beta_{m+1}.$$

EndDo

2.2. Convergence property

In this subsection, we give an analysis on the convergence property of the Lanczos method for the CSH linear system (1.1). By letting the shift $\alpha = a + ib$, the CSH linear system (1.1) can be written as

$$(ibI + \hat{H})x = f, \tag{2.8}$$

where $\hat{H} = aI + H$. Let $\lambda_{min}(H)$ be the smallest eigenvalue of the Hermitian matrix H. We now assume $a + \lambda_{min}(H) > 0$. 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 the symmetric tridiagonal matrix T_m by the Lanczos procedure with $\hat{H}$ and $v_1 = r_0/\|r_0\|$. Then we have

$$\begin{aligned} \hat{H}V_m &= V_m T_m + \beta_{m+1} v_{m+1} e_m^T, \\ (ibI + \hat{H})V_m &= V_m(ibI + T_m) + \beta_{m+1} v_{m+1} e_m^T. \end{aligned} \tag{2.9}$$

It is clear that the convergence property of the method for solving the CSH linear system (1.1) is equivalent to that for solving the linear system (2.8). We consider its seed system

$$\hat{H}x = f, \tag{2.10}$$

i.e., the linear system (1.2). It is known that the Lanczos method converges for this linear system since $\hat{H}$ is a HPD matrix and the D-Lanczos method is equivalent to the CG method. Below we use the superscript 0 to express all of the linear system (2.10), *e.g.*, r_m^0 denotes the Lanczos residual of the linear system (2.10). By (2.4), the Lanczos residual r_m of the linear system (2.8) is colinear to r_m^0, *i.e.*,

$$r_m = c_m r_m^0. \tag{2.11}$$

Further, since

$$r_m^0 = -\beta_{m+1} e_m^T y_m^0 v_{m+1},$$

and β_m and v_{m+1} are irrelevant to the shift ib, we have

$$c_m = e_m^T y_m / e_m^T y_m^0 = \eta_m / \eta_m^0,$$

and $\eta_m = \zeta_m / d_m$ (see (2.7)). By (2.6) and (2.5), we can derive

$$\begin{aligned} \zeta_m &= -l_m \zeta_{m-1} = \cdots = (-1)^{m-1} l_m l_{m-1} \cdots l_2 \beta \\ &= (-1)^{m-1} \frac{\beta_m \cdots \beta_2}{d_{m-1} \cdots d_1} \beta. \end{aligned}$$

We now show $|c_m| \le |c| < 1$, with c a constant, which means that the Lanczos method for solving the CSH linear system (1.1) converges (since $r_m^0 \to 0$) faster than that for solving the real shifted linear system (1.2). Note that β_k is irrelevant to the shift ib. So

$$|c_m| = \frac{|\eta_m|}{|\eta_m^0|} = \frac{|d_m^0 \cdots d_1^0|}{|d_m \cdots d_1|}.$$

We next show $|d_k^0| < |d_k|, \quad \forall k$. Thus we have

$$|c_m| \le \frac{|d_1^0|}{|d_1|} = \frac{\alpha_1^2}{\alpha_1^2 + b^2} \equiv c < 1.$$

By (2.5) we have

$$\begin{cases} d_1 = \alpha + \alpha_1, \\ d_k = \alpha + \alpha_k - \beta_k^2 / d_{k-1}, & k = 2, 3, \cdots, \\ d_1^0 = \alpha_1, \\ d_k^0 = \alpha_k - \beta_k^2 / d_{k-1}^0, & k = 2, 3, \cdots, \end{cases} \tag{2.12}$$

where $\alpha = ib$ is a pure imaginary shift of the linear system (2.8). Note that by (2.9), the matrix $T_m = V_m^H \hat{H} V_m = L_m D_m L_m^T$ is HPD, as the matrix $\hat{H}$ is HPD, so the diagonal elements of

D_m, $d_k^0 > 0$, $k = 1, \cdots, m$. Also the coefficients of the Lanczos procedure $\alpha_k = (w_k, v_k) = (\hat{H}v_k, v_k) > 0$.

Lemma 2.1. *For the sequences of* (2.12)*, suppose that real number* $\alpha_k > 0$, $d_k^0 > 0$, β_k *is a real number and* $\alpha = ib$, $b \neq 0$. *Then, for any* k,

$$|d_k| > d_k^0, \quad \forall k.$$

Proof. Note that $|d_1|^2 = |\alpha + \alpha_1|^2 = |ib + \alpha_1|^2 = \alpha_1^2 + b^2 > \alpha_1^2 = (d_1^0)^2$. Next it only needs to show that $Re(d_k) > d_k^0$, $k > 1$, since $|d_k| \geq Re(d_k)$. For $k = 2$,

$$d_2 = \alpha + \alpha_2 - \beta_2^2/d_1 = ib + \alpha_2 - \frac{\beta_2^2(\alpha_1 - ib)}{b^2 + \alpha_1^2}.$$

Consequently,

$$Re(d_2) = \alpha_2 - \frac{\beta_2^2 \alpha_1}{b^2 + \alpha_1^2} > \alpha_2 - \frac{\beta_2^2}{\alpha_1} = d_2^0.$$

Assume $Re(d_{k-1}) > d_{k-1}^0$. Then

$$d_k = \alpha + \alpha_k - \beta_k^2/d_{k-1} = ib + \alpha_k - \frac{\beta_k^2 \bar{d}_{k-1}}{|d_{k-1}|^2},$$

where $\bar{d}_{k-1}$ is the conjugate of d_{k-1}. Thus

$$Re(d_k) = \alpha_k - \frac{\beta_k^2 Re(d_{k-1})}{|d_{k-1}|^2},$$

$$Re(d_k) - d_k^0 = \beta_k^2 \left(\frac{1}{d_{k-1}^0} - \frac{Re(d_{k-1})}{|d_{k-1}|^2} \right) = \beta_k^2 \left(\frac{|d_{k-1}|^2 - Re(d_{k-1}) d_{k-1}^0}{d_{k-1}^0 |d_{k-1}|^2} \right) > 0.$$

This completes the proof of the lemma. □

We have the following convergence property of the method for solving the CSH linear system (1.1).

Theorem 2.2. *Suppose that the matrix* H *is Hermitian, and the complex shift* α *satisfies* $Re(\alpha) + \lambda_{min}(H) > 0$. *Then the Lanczos method for the CSH linear system* $(\alpha I + H)x = f$ *converges faster than that for the linear system* $(Re(\alpha)I + H)x = f$.

The faster convergence factor is dependent on the colinear coefficient $|c_m|$, or equivalently, on the ratio $|d_m^0|/|d_m|$; see the figures in the next section.

3. Numerical Experiments

Theorem 2.2 shows that the Lanczos method for the CSH linear system $(\alpha I + H)x = f$ converges faster than that for the real shifted Hermitian linear system $(Re(\alpha)I + H)x = f$. In this section, we report on two experiments to reveal such convergence property.

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

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

$$A = W + iZ \tag{3.1}$$

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 [3,14]) 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 tested, and in such case, the Hermitian matrix H is positive definite.

In this experiment, we reveal the convergence property of the Lanczos method for the linear system (1.1) with zero and nonzero imaginary part of the shift α by showing convergence curves for norm of residuals and the colinear coefficient $|c_m|$ curves of the residual r_m and r_m^0 (see (2.11)). We test two groups of values for the shift α: one is with $Re(\alpha) = 0$ (see Fig. 3.1) and another is with $Re(\alpha) = 0.3$ (see Fig. 3.2). Note that $|c_m| = \frac{|d_m^0 \cdots d_1^0|}{|d_m \cdots d_1|}$ and $|d_k| > |d_k^0|$, $\forall k$. We also show the ratio curve $\frac{|d_m^0|}{|d_m|}$ (see Fig. 3.3).

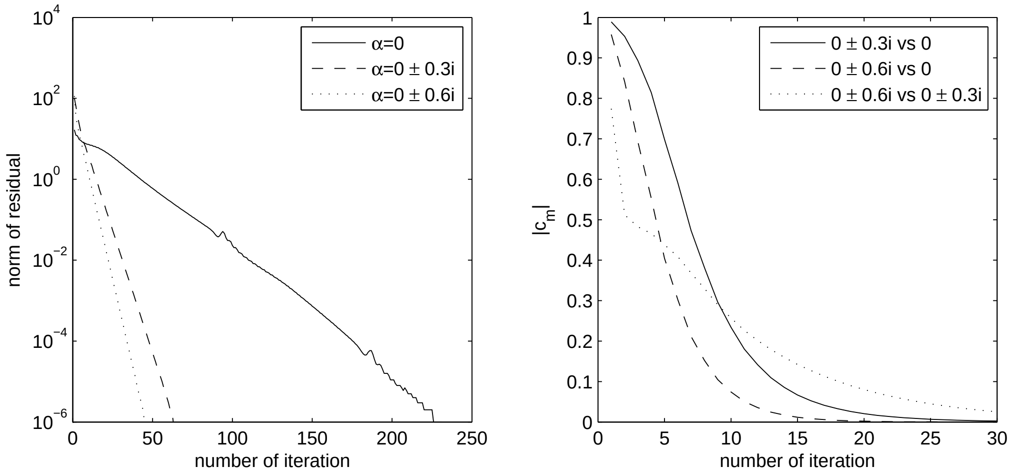

Fig. 3.1. The first group with $Re(\alpha) = 0$. Left: norm of residuals with different shift α. Right: colinear coefficient $|c_m|$ of r_m and r_m^0.

The curves in the Figures show the following facts:

1. the Lanczos method for the linear system (1.1) converges faster than that for the linear system (1.2); *e.g.*, the method converges after 66 iteration (IT) steps for the linear system (1.1) with the shift $\alpha = 0 + 0.3i$; however it converges after IT=231 for the linear system (1.2) with the real shift $Re(\alpha) = 0$;
2. for the complex shifted linear system, the larger the imaginary part of the shift α is, the better convergence property the methods will be; *e.g.*, IT=66 with $\alpha = 0 + 0.3i$ and IT=46 with $\alpha = 0 + 0.6i$, and thus confirm the theoretical analysis in [17];
3. the convergence property is irrelevant to the sign of the imaginary of the shift;
4. the curve of $|c_m|$ decreases quickly from 1 to 0 with respect to the iteration step m;

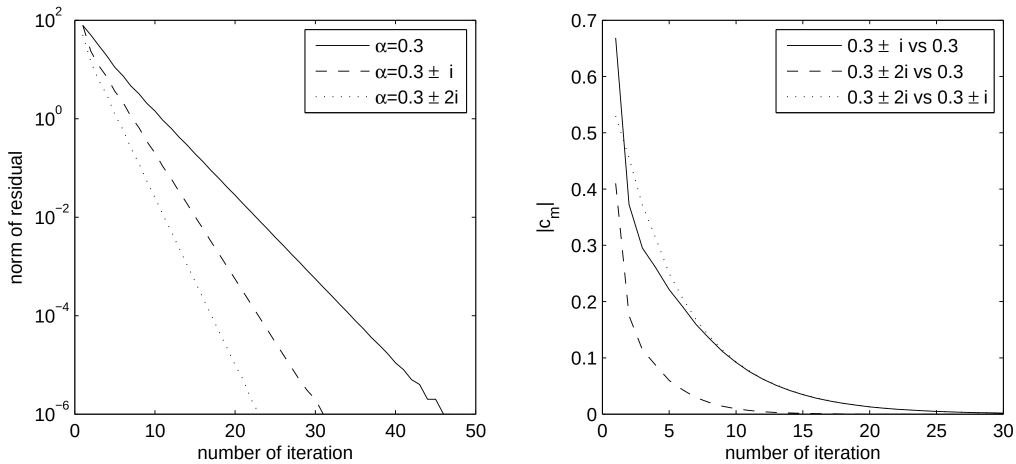

Fig. 3.2. The second group with $Re(\alpha) = 0.3$. Left: norm of residuals with different shift α. Right: colinear coefficient $|c_m|$ of r_m and r_m^0.

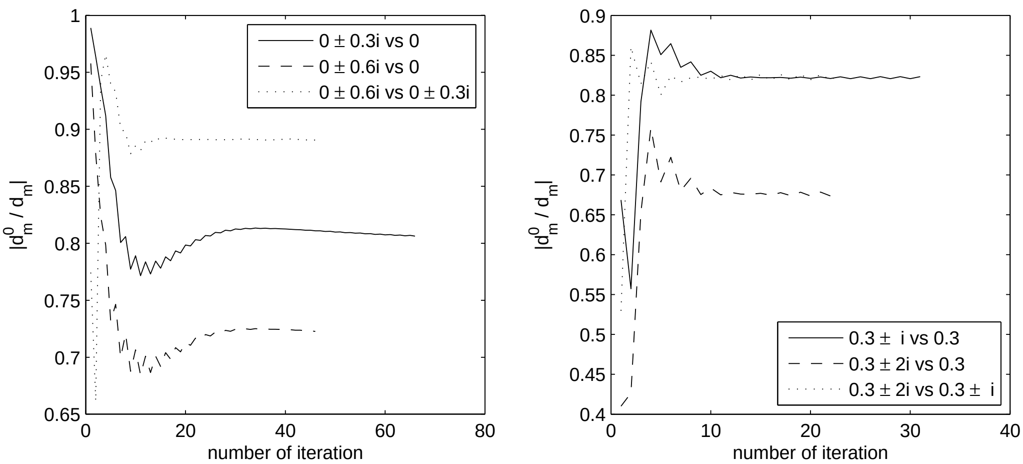

Fig. 3.3. The ratio curve $\frac{|d_m^0|}{|d_m|}$. Left: with $Re(\alpha) = 0$. Right: with $Re(\alpha) = 0.3$.

5. the ratio $\frac{|d_m^0|}{|d_m|}$ nearly tends to a constant less than 1 with respect to the iteration step m. The smaller this constant is, the faster the method converges.

These numerical results illustrate that the method benefits from the imaginary part of a complex shift when solving the CSH linear system (1.1).

Experiment 2. As a source of the shifted Hermitian linear system and also as our motivation to discuss the CSH linear system (1.1), in this experiment we use the HSS iteration method with a complex parameter α (see [14]) to solve the linear system

$$Ax = b, \tag{3.2}$$

with respect to the positive definite complex matrix A of (3.1). The mesh size $m = 32$ and the parameter $\gamma = 2$ are chosen. 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 CSH linear system (1.1) and we use the D-Lanczos method to solve these sub-systems in the HSS iteration method. In [14], 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 (3.2). As a comparison, we also test an experimental optimal real parameter $\alpha = a_{exp} = 0.6819$ in the HSS iteration method, 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 $(j = 1, \cdots, 401)$ is the equally-spaced points in $[0, \lambda_{max}(H)]$. In our test, the eigenvalues of a matrix are solved by the function *eig* in *MATLAB(7.4 ed)*.

In Table 3.1, 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 (3.2) residual $\|r^{(k)}\| < 10^{-6}$. Also, we show IT for convergence of the inner iteration using the D-Lanczos 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 the Table 1 are stable iteration numbers for convergence of the inner iteration after nearly 3 outer iteration steps k.

Table 3.1: - $\rho(T(\alpha))$, IT and CPU Time for convergence of HSS for Experiment 2, and IT for convergence of D-Lanczos 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

The numerical results in Table 1 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-Lanczos 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 CSH linear system (1.1), and also confirm the theoretical analysis in [17].

3. as 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 (3.2) than with an experimental optimal real parameter a_{exp}, in particular, for the $'$dominant$'$ imaginary part of the matrix; see [14].

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