Optimal Parameter in Hermitian and Skew-Hermitian Splitting Method for Certain Two-by-Two Block Matrices

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Abstract

The optimal parameter of the Hermitian/skew-Hermitian splitting (HSS) iteration method for a real 2-by-2 linear system is obtained. The result is used to determine the optimal parameters for linear systems associated with certain 2-by-2 block matrices, and to estimate the optimal parameters of the HSS iteration method for linear systems with n-by-n real coefficient matrices. Numerical examples are given to illustrate the results.

Keywords: Non-Hermitian matrix, Hermitian matrix, skew-Hermitian matrix, splitting iteration method, optimal iteration parameter.

AMS(MOS) Subject Classifications: 65F10, 65F50; CR: G1.3.

1 Introduction

To solve the large sparse non-Hermitian and positive definite system of linear equations

$$Ax = f, \; A \in \mathbb{C}^{n\times n} \text{ positive definite}, \; A \neq A^*, \text{ and } x, f \in \mathbb{C}^n, \tag{1.1}$$

Bai, Golub and Ng[2] recently proposed the *Hermitian/skew-Hermitian splitting* **(HSS)** iteration method based on the fact that the coefficient matrix A naturally possesses the *Hermitian/skew-Hermitian* **(HS)** splitting[10, 19]

$$A = H + S,$$

where

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

with A^* being the conjugate transpose of the matrix A. They showed that this HSS iteration converges unconditionally to the exact solution of the system of linear equations (1.1), with the upper bound on convergence speed about the same as that of the conjugate gradient method when applied to Hermitian matrices. Moreover, the upper bound of the contraction factor is dependent on the spectrum of the Hermitian part H, but is independent of the spectrum of the skew-Hermitian part S as well as the eigenvalues of the matrices H, S and A. Numerical experiments have shown that the HSS iteration method is very efficient and robust both as a solver and as a preconditioner (to Krylov subspace methods such as GMRES and BiCGSTAB; see [15, 18]) for solving non-Hermitian and positive definite linear systems.

To further improve the efficiency of the method, it is desirable to determine or find a good estimate for the optimal parameter α^*. Unfortunately, there is no good method in doing that. In this paper, we analyze 2-by-2 real matrices in detail, and obtain the optimal parameter α^* that minimizes the spectral radius of the iteration matrix of the corresponding HSS method. We then use the results to determine the optimal parameters for linear systems associated with certain 2-by-2 block matrices, and to estimate the optimal parameter α^* of the HSS method for general n-by-n nonsymmetric positive definite system of linear equations (1.1). Numerical examples are given to show that our estimations improve previous results and are close to the values of the optimal parameters.

Unless specified otherwise, we assume throughout the paper that the non-Hermitian matrix $A \in \mathbb{C}^{n\times n}$ is positive definite, i.e., $A \neq A^*$ and its Hermitian part $H = \frac{1}{2}(A + A^*)$ is Hermitian positive definite.

2 The HSS Iteration

Let us first review the HSS iteration method presented in Bai, Golub and Ng[2].

The HSS Iteration Method. `Given an initial guess` $x^{(0)} \in \mathbb{C}^n$, `compute` $x^{(k)}$ `for` $k = 0, 1, 2, \ldots$ `using the following iteration scheme until` $\{x^{(k)}\}$ `satisfies the stopping criterion:`

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

where α is a given positive constant.

In matrix-vector form, the above HSS iteration method can be equivalently rewritten as

$$x^{(k+1)} = \mathcal{M}(\alpha)x^{(k)} + \mathcal{G}(\alpha)f, \qquad k = 0, 1, 2, \ldots, \tag{2.1}$$

where

$$\mathcal{M}(\alpha) = (\alpha I + S)^{-1}(\alpha I - H)(\alpha I + H)^{-1}(\alpha I - S) \tag{2.2}$$

and

$$\mathcal{G}(\alpha) = 2\alpha(\alpha I + S)^{-1}(\alpha I + H)^{-1}.$$

Here, $\mathcal{M}(\alpha)$ is the iteration matrix of the HSS method. In fact, (2.1) may also result from the splitting

$$A = B(\alpha) - C(\alpha)$$

of the coefficient matrix A, with

$$\begin{cases} B(\alpha) &= \frac{1}{2\alpha}(\alpha I + H)(\alpha I + S), \\ C(\alpha) &= \frac{1}{2\alpha}(\alpha I - H)(\alpha I - S). \end{cases}$$

The following theorem established in [2] describes the convergence property of the HSS iteration.

Theorem 2.1. *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, respectively, and α be a positive constant. Then the spectral radius $\rho(\mathcal{M}(\alpha))$ of the iteration matrix $\mathcal{M}(\alpha)$ of the HSS iteration (see (2.2)) is bounded by*

$$\sigma(\alpha) = \max_{\lambda_j \in \lambda(H)} \frac{|\alpha - \lambda_j|}{|\alpha + \lambda_j|},$$

where $\lambda(\cdot)$ represents the spectrum of the corresponding matrix. Consequently, we have

$$\rho(\mathcal{M}(\alpha)) \leq \sigma(\alpha) < 1, \qquad \forall \alpha > 0,$$

i.e., the HSS iteration converges to the exact solution $x^* \in \mathbb{C}^n$ of the system of linear equations (1.1).

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

$$\tilde{\alpha} \equiv \arg\min_{\alpha} \left\{ \max_{\gamma_{\min} \leq \lambda \leq \gamma_{\max}} \left| \frac{\alpha - \lambda}{\alpha + \lambda} \right| \right\} = \sqrt{\gamma_{\min}\gamma_{\max}}$$

and

$$\sigma(\tilde{\alpha}) = \frac{\sqrt{\gamma_{\max}} - \sqrt{\gamma_{\min}}}{\sqrt{\gamma_{\max}} + \sqrt{\gamma_{\min}}} = \frac{\sqrt{\kappa(H)} - 1}{\sqrt{\kappa(H)} + 1},$$

where $\kappa(H)$ is the spectral condition number of H.

Of course, $\tilde{\alpha}$ is usually different from the optimal parameter

$$\alpha^* = \arg\min_{\alpha} \rho(\mathcal{M}(\alpha)),$$

and it always holds that

$$\rho(\mathcal{M}(\alpha^*)) \leq \sigma(\tilde{\alpha}).$$

Numerical experiments in [2] have confirmed that in most situation, $\rho(\mathcal{M}(\alpha^*)) \ll \sigma(\tilde{\alpha})$. See [3, 12, 6, 16, 1, 13, 8, 14, 11, 7] for further applications and generalizations of the HSS iteration method.

3 The Real Two-By-Two Case

In this section, we study linear systems associated with a real 2-by-2 matrix A with positive definite symmetric part. We first determine the eigenvalues of $\mathcal{M}(\alpha)$ defined in (2.2). The following theorem is stated in general terms so that it can be used more conveniently for future discussion.

Theorem 3.1. *Let $A = H + S \in \mathbb{R}^{2\times 2}$ be such that H is symmetric positive definite and S is skew-symmetric. Suppose H has eigenvalues $\lambda_1 \geq \lambda_2 > 0$ and $\det(S) = q^2$ with $q \in \mathbb{R}$. Then the two eigenvalues of the iteration matrix $\mathcal{M}(\alpha)$ defined in (2.2) are*

$$\lambda_{\pm} = \frac{(\alpha^2 - \lambda_1\lambda_2)(\alpha^2 - q^2) \pm \sqrt{(\alpha^2 - \lambda_1\lambda_2)^2(\alpha^2 - q^2)^2 - (\alpha^2 - \lambda_1^2)(\alpha^2 - \lambda_2^2)(\alpha^2 + q^2)^2}}{(\alpha + \lambda_1)(\alpha + \lambda_2)(\alpha^2 + q^2)}.$$

As a result, if

$$(\alpha^2 - \lambda_1\lambda_2)^2(\alpha^2 - q^2)^2 \geq (\alpha^2 - \lambda_1^2)(\alpha^2 - \lambda_2^2)(\alpha^2 + q^2)^2,$$

then $\rho(\mathcal{M}(\alpha))$ equals to

$$\frac{|\alpha^2 - \lambda_1\lambda_2||\alpha^2 - q^2| + \sqrt{(\alpha^2 - \lambda_1\lambda_2)^2(\alpha^2 - q^2)^2 - (\alpha^2 - \lambda_1^2)(\alpha^2 - \lambda_2^2)(\alpha^2 + q^2)^2}}{(\alpha + \lambda_1)(\alpha + \lambda_2)(\alpha^2 + q^2)};$$

if

$$(\alpha^2 - \lambda_1\lambda_2)^2(\alpha^2 - q^2)^2 < (\alpha^2 - \lambda_1^2)(\alpha^2 - \lambda_2^2)(\alpha^2 + q^2)^2,$$

then $\rho(\mathcal{M}(\alpha))$ equals to

$$\sqrt{\frac{(\alpha - \lambda_1)(\alpha - \lambda_2)}{(\alpha + \lambda_1)(\alpha + \lambda_2)}}.$$

Proof. Let $A = H + S \in \mathbb{R}^{2\times 2}$, where H is symmetric positive definite, and S is skew-symmetric. Then there is an orthogonal matrix $Q \in \mathbb{R}^{2\times 2}$ such that Q^tHQ is a diagonal matrix with diagonal entries λ_1 and λ_2, where Q^t denotes the transpose matrix of Q. We may replace A by Q^tAQ without changing the assumptions and conclusions of our theorem. So, assume that

$$H = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \quad \text{and} \quad S = \begin{bmatrix} 0 & q \\ -q & 0 \end{bmatrix} \quad \text{with } q \in \mathbb{R}.$$

Then $(\alpha I+H)^{-1}(\alpha I-H)(\alpha I+S)^{-1}(\alpha I-S)$ equals

$$\frac{1}{\alpha^2+q^2}\cdot\begin{bmatrix} \frac{(\alpha^2-q^2)(\alpha-\lambda_1)}{\alpha+\lambda_1} & -\frac{2q\alpha(\alpha-\lambda_1)}{\alpha+\lambda_1} \\ \frac{2q\alpha(\alpha-\lambda_2)}{\alpha+\lambda_2} & \frac{(\alpha^2-q^2)(\alpha-\lambda_2)}{\alpha+\lambda_2} \end{bmatrix}.$$

The formula for $\lambda_\pm$ and the assertion on $\rho(\mathcal{M}(\alpha))$ follow. $\square$

One may want to use the formula of $\rho(\mathcal{M}(\alpha))$ in Theorem 3.1 to determine the optimal choice of α. It turns out that the analysis is very complicated and not productive. The main difficulty is the expression

$$\sqrt{(\alpha^2-\lambda_1\lambda_2)^2(\alpha^2-q^2)^2-(\alpha^2-\lambda_1^2)(\alpha^2-\lambda_2^2)(\alpha^2+q^2)^2} \tag{3.1}$$

in the formula of $\rho(\mathcal{M}(\alpha))$. For example, one may see [5] for the analysis of a similar and simpler problem. Here, we use a different approach that allows us to avoid the complicated expression (3.1).

For notational simplicity, we write

$$\rho(\alpha)=\rho(\mathcal{M}(\alpha)).$$

Define

$$\phi(\alpha)=\left\{\frac{\operatorname{trace}(\mathcal{M}(\alpha))}{2}\right\}^2=\left\{\frac{(\alpha^2-q^2)(\alpha^2-\lambda_1\lambda_2)}{(\alpha^2+q^2)(\alpha+\lambda_1)(\alpha+\lambda_2)}\right\}^2,$$

$$\psi(\alpha)=\det(\mathcal{M}(\alpha))=\frac{(\alpha-\lambda_1)(\alpha-\lambda_2)}{(\alpha+\lambda_1)(\alpha+\lambda_2)},$$

and

$$\omega(\alpha)=\max\{\phi(\alpha),\ |\psi(\alpha)|\}.$$

Evidently,

$$\rho(\alpha)^2\ge\omega(\alpha).$$

Moreover,

$$1=\phi(0)=\lim_{\alpha\to+\infty}\phi(\alpha) \quad\text{ and }\quad 1=\psi(0)=\lim_{\alpha\to+\infty}\psi(\alpha).$$

Thus,

$$\lim_{\alpha\to+\infty}\omega(\alpha)=\omega(0)=1>\omega(\xi)\quad\text{ for all } \xi>0.$$

Since $\omega(\alpha)$ is continuous and nonnegative, there exists $\alpha^*>0$ such that

$$\omega(\alpha^*)=\min\{\omega(\alpha)\mid\alpha>0\}.$$

We will show that

$$\phi(\alpha^*)=|\psi(\alpha^*)|. \tag{3.2}$$

As a result, the eigenvalues of $\mathcal{M}(\alpha^*)$ have the same modulus, and thus

$$\rho(\alpha)^2\ge\omega(\alpha)\ge\omega(\alpha^*)=\rho(\alpha^*)^2,\quad\text{ for all } \alpha>0.$$

By the above discussion, establishing (3.2) will lead to the following theorem.

Theorem 3.2. *Let the assumptions of Theorem* 3.1 *be satisfied and define the functions* ϕ *and* ψ *as above. Then the optimal* $\alpha^* > 0$ *satisfying*

$$\rho(\mathcal{M}(\alpha^*)) = \min\{\rho(\mathcal{M}(\alpha)) \mid \alpha > 0\}$$

lies in the finite set

$$\mathbf{S} = \{\alpha > 0 \mid \phi(\alpha) = |\psi(\alpha)|\},$$

which consists of numbers $\alpha > 0$ *satisfying*

$$(\alpha^2 + q^2)^2(\alpha^2 - \lambda_1^2)(\alpha^2 - \lambda_2^2) = (\alpha^2 - q^2)^2(\alpha^2 - \lambda_1\lambda_2)^2 \tag{3.3}$$

or

$$(\alpha^2 + q^2)^2(\lambda_1^2 - \alpha^2)(\alpha^2 - \lambda_2^2) = (\alpha^2 - q^2)^2(\alpha^2 - \lambda_1\lambda_2)^2. \tag{3.4}$$

Proof. We only need to demonstrate the validity of (3.2), i.e.,

$$\phi(\alpha^*) = |\psi(\alpha^*)|.$$

Note that $\phi(\alpha)$ is continuously differentiable for $\alpha > 0$, and $|\psi(\alpha)|$ is continuous for $\alpha > 0$ and differentiable except for $\alpha = \lambda_1$ and λ_2. Since $\omega(\alpha) = \max\{\phi(\alpha),\ |\psi(\alpha)|\}$, if α^* satisfies

$$\omega(\alpha^*) = \min\{\omega(\alpha) \mid \alpha > 0\},$$

then one of the following holds.

(i) $\phi(\alpha^*) = |\psi(\alpha^*)|$;

(ii) $\phi(\alpha^*) > |\psi(\alpha^*)|$ and $\phi(\alpha^*)$ is a local minimum of $\phi(\alpha)$;

(iii) $|\psi(\alpha^*)| > \phi(\alpha^*)$ and $|\psi(\alpha^*)|$ is a local minimum of $|\psi(\alpha)|$.

First, we claim that (iii) cannot happen. To see this, note that

$$\psi'(\alpha) = \frac{2(\lambda_1 + \lambda_2)(\alpha^2 - \lambda_1\lambda_2)}{[(\alpha + \lambda_1)(\alpha + \lambda_2)]^2},$$

which is positive or negative according to $\alpha > \sqrt{\lambda_1\lambda_2}$ or $\alpha < \sqrt{\lambda_1\lambda_2}$, respectively, and $\psi'\left(\sqrt{\lambda_1\lambda_2}\right) = 0$. Because $\lambda_1 \geq \sqrt{\lambda_1\lambda_2} \geq \lambda_2$, we see that $|\psi(\alpha)| = \psi(\alpha)$ is differentiable and decreasing on $(0, \lambda_2)$, and $|\psi(\alpha)| = \psi(\alpha)$ is differentiable and increasing on $(\lambda_1, +\infty)$. Thus, there cannot be α^* in $(0, \lambda_2) \cup (\lambda_1, +\infty)$ satisfying (iii). Furthermore, $|\psi(\lambda_j)| = 0$ for $j = 1, 2$; so, it is impossible to have $\alpha^* = \lambda_j$ satisfying (iii). Finally, $|\psi(\alpha)| = -\psi(\alpha)$ is differentiable on (λ_2, λ_1) with a local maximum at $\sqrt{\lambda_1\lambda_2}$. Thus, there cannot be α^* in (λ_2, λ_1) satisfying (iii).

Next, we show that (ii) cannot happen. The analysis is more involved. Instead of $\phi(\alpha)$, we consider its square root

$$F(\alpha) = \frac{(\alpha^2 - q^2)(\alpha^2 - \lambda_1\lambda_2)}{(\alpha^2 + q^2)(\alpha + \lambda_1)(\alpha + \lambda_2)} = \left(1 - \frac{2q^2}{\alpha^2 + q^2}\right)\left(1 - \frac{\lambda_1}{\alpha + \lambda_1} - \frac{\lambda_2}{\alpha + \lambda_2}\right).$$

Then

$$\begin{aligned} F'(\alpha) &= \frac{4q^2\alpha}{(\alpha^2+q^2)^2}\frac{(\alpha^2-\lambda_1\lambda_2)}{(\alpha+\lambda_1)(\alpha+\lambda_2)} + \frac{(\alpha^2-q^2)}{(\alpha^2+q^2)}\left(\frac{\lambda_1}{(\alpha+\lambda_1)^2}+\frac{\lambda_2}{(\alpha+\lambda_2)^2}\right) \\ &= \frac{\lambda_1+\lambda_2}{(\alpha^2+q^2)^2(\alpha+\lambda_1)^2(\alpha+\lambda_2)^2}\cdot P(\alpha), \end{aligned}$$

where

$$\begin{aligned} P(\alpha) &= \alpha^6 + \frac{4(\lambda_1\lambda_2+q^2)}{\lambda_1+\lambda_2}\alpha^5 + (\lambda_1\lambda_2+4q^2)\alpha^4 \\ &\quad -q^2(q^2+4\lambda_1\lambda_2)\alpha^2 - \frac{4q^2\lambda_1\lambda_2(q^2+\lambda_1\lambda_2)}{\lambda_1+\lambda_2}\alpha - \lambda_1\lambda_2 q^4. \end{aligned}$$

Suppose $q \le \sqrt{\lambda_1\lambda_2}$. Then $F'(\alpha) < 0$ for $\alpha \in (0,q)$, and $F'(\alpha) > 0$ for $\alpha \in (\sqrt{\lambda_1\lambda_2}, +\infty)$. So, $F(\alpha)$ is decreasing on $(0,q)$ and increasing on $[\sqrt{\lambda_1\lambda_2}, +\infty)$. Hence, $\phi(\alpha) = F(\alpha)^2$ cannot have a local minimum in these two intervals. Thus, there cannot be an α^* in these intervals satisfying (ii). Because $\phi(q) = \phi\left(\sqrt{\lambda_1\lambda_2}\right) = 0$, we cannot have $\alpha^* = q$ or $\sqrt{\lambda_1\lambda_2}$ satisfying (ii).

Next, we **claim** that $F(\alpha)$ has only one critical point in $\left(q, \sqrt{\lambda_1\lambda_2}\right)$, which is a local minimum. This point will be the unique critical point for $\phi(\alpha) = F(\alpha)^2$ on $\left(q, \sqrt{\lambda_1\lambda_2}\right)$, which is a local maximum. Thus, there cannot be an α^* in this interval satisfying (ii).

To prove our claim, note that $\alpha > 0$ is a critical point of $F(\alpha)$ if and only if α is a zero of $P(\alpha)$. So, it suffices to show that $P(\alpha)$ only has one positive zero. Now,

$$P''(\alpha) = 30\alpha^4 + \frac{80(\lambda_1\lambda_2+q^2)}{\lambda_1+\lambda_2}\alpha^3 + 12(\lambda_1\lambda_2+4q^2)\alpha^2 - 2q^2(q^2+4\lambda_1\lambda_2).$$

Since $P''(0) < 0$ and $\lim_{\alpha\to+\infty} P''(\alpha) = +\infty$, we see that $P''(\alpha)$ has a positive zero. However, $P''(\alpha)$ cannot have two or more positive zeros (counting multiplicity). Otherwise,

$$P'''(\alpha) = 120\alpha^3 + \frac{240(\lambda_1\lambda_2+q^2)}{\lambda_1+\lambda_2}\alpha^2 + 24(\lambda_1\lambda_2+4q^2)\alpha$$

has a positive zero, which is impossible. Next, we argue that

$$\begin{aligned} P'(\alpha) &= 6\alpha^5 + \frac{20(\lambda_1\lambda_2+q^2)}{\lambda_1+\lambda_2}\alpha^4 + 4(\lambda_1\lambda_2+4q^2)\alpha^3 \\ &\quad -2q^2(q^2+4\lambda_1\lambda_2)\alpha - \frac{4q^2\lambda_1\lambda_2(q^2+\lambda_1\lambda_2)}{\lambda_1+\lambda_2} \end{aligned}$$

has exactly one positive zero. Since $P'(0) < 0$ and $\lim_{\alpha\to+\infty} P'(\alpha) = +\infty$, we see that $P'(\alpha)$ has a positive zero. Since $P''(0) < 0$ and $P''(\alpha)$ only has one positive zero α_1, we see that $P'(\alpha)$ is decreasing on $(0,\alpha_1)$ and increasing on $(\alpha_1,+\infty)$. So, $P'(\alpha)$ can only have one positive zero $\alpha_2 > \alpha_1$.

We can apply the same argument to $P(\alpha)$. Since $P(0) < 0$ and $\lim_{\alpha\to+\infty} P(\alpha) = +\infty$, we see that $P(\alpha)$ has a positive zero. Since $P'(0) < 0$ and $P'(\alpha)$ only has one positive zero α_2, we see that $P(\alpha)$ is decreasing on $(0,\alpha_2)$ and increasing on $(\alpha_2,+\infty)$. So, $P(\alpha)$ can only have one positive zero $\alpha_3 > \alpha_2$, and our claim is proved.

One can use a similar argument to get the desired conclusion if $q > \sqrt{\lambda_1\lambda_2}$. We omit the discussion. □

Remark 3.3. Using the absolute value function, we can combine (3.3) and (3.4) to a single equation

$$|(\alpha^2+q^2)^2(\lambda_1^2-\alpha^2)(\alpha^2-\lambda_2^2)| = [(\alpha^2-q^2)(\alpha^2-\lambda_1\lambda_2)]^2.$$

Nonetheless, the polynomial equations are easier to solve and use. In fact, if $\lambda_1=\lambda_2=\lambda^*$, then (3.3) and (3.4) only has one positive solution, namely, $\alpha=\lambda^*$. Suppose $\lambda_1>\lambda_2$. If we use the substitution $\beta=\alpha^2$, then (3.3) reduces to the quadratic equation

$$[(\lambda_1-\lambda_2)^2-4q^2]\beta^2+2q^2(\lambda_1+\lambda_2)^2\beta+q^2[q^2(\lambda_1-\lambda_2)^2-4\lambda_1^2\lambda_2^2]=0,$$

which has solutions

$$\frac{q(2\lambda_1\lambda_2-q\lambda_1+q\lambda_2)}{\lambda_1-\lambda_2+2q} \quad \text{and} \quad \frac{-q(2\lambda_1\lambda_2+q\lambda_1-q\lambda_2)}{\lambda_1-\lambda_2-2q}$$

if $|\lambda_1-\lambda_2|\neq 2q$. Otherwise, the equation is linear and has a solution

$$\beta=\frac{2(q^4-\lambda_1^2\lambda_2^2)}{(\lambda_1+\lambda_2)^2}=\frac{2(q^2+\lambda_1\lambda_2)(q^2-\lambda_1\lambda_2)}{(\lambda_1+\lambda_2)^2}=\frac{(\lambda_1+\lambda_2)^2(q^2-\lambda_1\lambda_2)}{2(\lambda_1+\lambda_2)^2}=\frac{1}{2}(q^2-\lambda_1\lambda_2).$$

Of course, these solutions will be useful only if they are positive and lie outside the interval $[\lambda_2^2,\lambda_1^2]$. Similarly, by the substitution $\beta=\alpha^2$, (3.4) reduces to the quartic equation

$$2\beta^4-(\lambda_1+\lambda_2)^2\beta^3+2[\lambda_1^2\lambda_2^2-q^2(\lambda_1-\lambda_2)^2+q^4]\beta^2-q^4(\lambda_1+\lambda_2)^2\beta+2q^4\lambda_1^2\lambda_2^2=0, \quad (3.5)$$

which has exactly two solutions μ_1 and μ_2 with $\mu_1\in[\lambda_2^2,\lambda_1\lambda_2)$ and $\mu_2\in((\lambda_1^2+\lambda_2^2)/2,\lambda_1^2]$. Furthermore, if $q^2\in[\lambda_2^2,\lambda_1^2]$ then $\mu_1\le q^2$ and $\mu_2\ge q^2$. In particular, if $q=\lambda_i$ for $i\in\{1,2\}$ then $\beta=\lambda_i^2$ is a solution. The verification of the above statements will be given in the last section.

As an illustration of Theorems 3.1 and 3.2 as well as Remark 3.3, we consider a simple example for which $\lambda_1=2$, $\lambda_2=1$ and $q=1$. By straightforward computations, we know that the only positive roots of the equation (3.3) are $\alpha_1^*=1$ and $\alpha_2^*=\sqrt{5}$, and those of the equation (3.4) are $\alpha_3^*=1$ and

$$\alpha_4^*=\frac{\sqrt{6}}{6}\sqrt{\left(7+\sqrt[3]{712+9\sqrt{5277}}+\frac{43}{\sqrt[3]{712+9\sqrt{5277}}}\right)}\approx 1.914.$$

We remark that now equation (3.4) is equivalent to $(\beta-1)(2\beta^3-7\beta^2+\beta-8)=0$. Based on Theorem 3.1, from direct calculations we have

$$\rho(\mathcal{M}(\alpha_1^*))=\rho(\mathcal{M}(\alpha_3^*))=0, \quad \rho(\mathcal{M}(\alpha_2^*))=\frac{\sqrt{3}(7-3\sqrt{5})}{6}\approx 0.0842$$

and

$$\rho(\mathcal{M}(\alpha_4^*))\approx 0.201.$$

Therefore, for the HSS iteration method, the optimal parameter is $\alpha^*=1$ and the corresponding optimal convergence factor is $\rho(\mathcal{M}(\alpha^*))=0$. On the other hand, from Theorem 2.1 we can easily obtain

$$\tilde{\alpha}=\sqrt{2}\approx 1.414 \quad \text{and} \quad \sigma(\tilde{\alpha})=3-2\sqrt{2}\approx 0.172.$$

Obviously, it holds that $\rho(\mathcal{M}(\alpha^*))<\sigma(\tilde{\alpha})$.

Remark 3.4. Note that in our proof of Theorem 3.2, we get much information for the function $\omega(\alpha) = \max\{\phi(\alpha),\ |\psi(\alpha)|\}$ with $\alpha > 0$. In particular, we show that all the local minima of $\omega(\alpha)$ satisfy

$$\phi(\alpha) = |\psi(\alpha)|,$$

and they are the roots of (3.3) and (3.4). Moreover, the local minima of $\omega(\alpha)$ are also local minima of $\rho(\alpha)$, and that the global minimum of $\rho(\alpha)$ and $\omega(\alpha)$ occur at the same α^*. If one can prove independently that the local minima $\rho(\alpha)$ always occur when the eigenvalues of $\mathcal{M}(\alpha)$ have the same magnitude, then one can conclude that the functions $\omega(\alpha)$ and $\rho(\alpha)$ have the same local and global minima. Once again, this is difficult to do because of the expression (3.1) in $\rho(\alpha) = \rho(\mathcal{M}(\alpha))$.

Using the notations defined in Theorem 3.1, we immediately get the following conclusion from Theorem 3.2.

Corollary 3.5. *Let the assumptions of Theorem* 3.1 *be satisfied. Then the optimal* $\alpha^* > 0$ *satisfying*

$$\rho(\mathcal{M}(\alpha^*)) = \min\{\rho(\mathcal{M}(\alpha)) \mid \alpha > 0\}$$

is a positive root of the equation

$$(\alpha^2 + q^2)^2(\alpha^2 - \lambda_1^2)(\alpha^2 - \lambda_2^2) = (\alpha^2 - q^2)^2(\alpha^2 - \lambda_1\lambda_2)^2$$

or

$$(\alpha^2 + q^2)^2(\lambda_1^2 - \alpha^2)(\alpha^2 - \lambda_2^2) = (\alpha^2 - q^2)^2(\alpha^2 - \lambda_1\lambda_2)^2.$$

Remark 3.6. The first equation in Corollary 3.5 can be reduced to a quadratic equation and the second one can be reduced to a quartic equation with respect to $\beta = \alpha^2$, respectively, analogously to those in Remark 3.3.

Remark 3.7. Note that the results in this section are also valid if $\lambda_1 > 0 = \lambda_2$ and $q \neq 0$.

Remark 3.8. We should point out again that Theorem 3.2 has been established only for real matrices. For complex matrices, how to determine the optimal iteration parameter of the HSS iteration method is still an open problem.

4 Two-By-Two Block Matrices

In this section, we determine the optimal parameter α^* for a 2-by-2 block matrix of the form

$$A = \begin{bmatrix} \lambda_1 I_r & E \\ -E^* & \lambda_2 I_s \end{bmatrix}, \tag{4.1}$$

where $\lambda_1 > \lambda_2 > 0$. Note that the case when $\lambda_1 = \lambda_2$ is trivial [1]. Systems of linear equations with the 2-by-2 block matrices (4.1) arise in many applications; for details we

[1] If $\lambda_1 = \lambda_2 \equiv \lambda^*$, then the iteration matrix of the HSS iteration method is given by $\mathcal{M}(\alpha) = \frac{\alpha-\lambda^*}{\alpha+\lambda^*}Q(\alpha)$, where $Q(\alpha) := (\alpha I + S)^{-1}(\alpha I - S)$ is a Cayley transform of S and is, thus, unitary, and $S = \begin{bmatrix} 0 & E \\ -E^* & 0 \end{bmatrix}$; see (2.2). Obviously, it holds that $\rho(\mathcal{M}(\alpha)) = \frac{|\alpha-\lambda^*|}{\alpha+\lambda^*}$. Therefore, for the HSS iteration method applied to this special linear system, the optimal parameter is $\alpha^* = \lambda^*$ and the corresponding optimal convergence factor is $\rho(\mathcal{M}(\alpha^*)) = 0$.

refer the readers to [17, Chapter 6], [9, Chapters 4, 5 and 10], [20, 10, 4, 5] and references therein. According to Young[20] and Varga[17], the matrix A in (4.1) is called a 2-cyclic matrix, and is connected with property A.

Theorem 4.1. *Suppose that the matrix $A \in \mathbb{C}^{n\times n}$ defined in (4.1) satisfies $\lambda_1 > \lambda_2 > 0$, and the nonzero matrix $E \in \mathbb{C}^{r\times s}$ has nonzero singular values $q_1 \geq q_2 \geq \cdots \geq q_k$. Let*

$$H = \frac{1}{2}(A + A^*) = \begin{bmatrix} \lambda_1 I_r & 0 \\ 0 & \lambda_2 I_s \end{bmatrix} \quad \text{and} \quad S = \frac{1}{2}(A - A^*) = \begin{bmatrix} 0 & E \\ -E^* & 0 \end{bmatrix}$$

be the Hermitian and the skew-Hermitian parts of the matrix A, respectively. Then, for the correspondingly induced HSS iteration method, the spectral radius $\rho(\mathcal{M}(\alpha))$ of its iteration matrix $\mathcal{M}(\alpha)$ (see (2.2)) attains the minimum at α^*, which is a root of one of the following equations:

$$(\alpha - \sqrt{\lambda_1\lambda_2})(\alpha - \sqrt{q_1 q_k}) = 0,$$

$$(\alpha^2 + q_j^2)^2(\alpha^2 - \lambda_1^2)(\alpha^2 - \lambda_2^2) = (\alpha^2 - q_j^2)^2(\alpha^2 - \lambda_1\lambda_2)^2$$

or

$$(\alpha^2 + q_j^2)^2(\lambda_1^2 - \alpha^2)(\alpha^2 - \lambda_2^2) = (\alpha^2 - q_j^2)^2(\alpha^2 - \lambda_1\lambda_2)^2,$$

where $j = 1, k$.

Proof. Suppose A satisfies the hypotheses of the theorem. Then A is unitarily similar to $A_1 \oplus \cdots \oplus A_k \oplus \lambda_1 I_u \oplus \lambda_2 I_v$, where $\oplus$ denotes the matrix direct sum, $A_j = \begin{bmatrix} \lambda_1 & q_j \\ -q_j & \lambda_2 \end{bmatrix}$, $u = r - k$ and $v = s - k$. For $\alpha > 0$, define

$$\rho(\alpha) = \rho(\mathcal{M}(\alpha)) \quad \text{and} \quad \rho_j(\alpha) = \rho(\mathcal{M}_j(\alpha)),$$

where $\mathcal{M}(\alpha)$ is unitarily similar to $\mathcal{M}_1(\alpha) \oplus \cdots \oplus \mathcal{M}_k(\alpha) \oplus \frac{\alpha-\lambda_1}{\alpha+\lambda_1} I_u \oplus \frac{\alpha-\lambda_2}{\alpha+\lambda_2} I_v$, with $\mathcal{M}_j(\alpha)$ being the HSS iteration matrix associated with A_j for $j = 1, 2, \ldots, k$. Furthermore, define

$$f_j(\alpha) = |\alpha - \lambda_j|/|\alpha + \lambda_j| \quad \text{for } j = 1, 2.$$

Consider four cases.

Case 1. If $r > k$ and $s > k$, then $f_1(\alpha)$ and $f_2(\alpha)$ are eigenvalues of $\mathcal{M}(\alpha)$ and

$$\rho(\alpha) = \max\{|f_1(\alpha)|,\ |f_2(\alpha)|\}$$

is the largest singular value of $\mathcal{M}(\alpha)$. Thus,

$$\rho(\alpha^*) = \rho\left(\sqrt{\lambda_1\lambda_2}\right) = \frac{\sqrt{\lambda_1} - \sqrt{\lambda_2}}{\sqrt{\lambda_1} + \sqrt{\lambda_2}}.$$

Case 2. Suppose $r > k$ and $s = k$. Let $\rho_0(\alpha) = f_1(\alpha)$. Then

$$\rho(\alpha) = \max\{\rho_j(\alpha) \mid 0 \leq j \leq k\}.$$

For $\alpha \in \left(0, \sqrt{\lambda_1\lambda_2}\right]$,

$$\rho(\alpha) = \rho_0(\alpha) = f_1(\alpha)$$

is the largest singular value of $\mathcal{M}(\alpha)$. If $\alpha \geq (\lambda_1^3/\lambda_2)^{1/2}$, then

$$f_1(\alpha) = \left|\frac{\alpha-\lambda_1}{\alpha+\lambda_1}\right| = \left|1 - \frac{2\lambda_1}{\alpha+\lambda_1}\right| \geq \left|1 - \frac{2\lambda_1}{\sqrt{\lambda_1\lambda_2}+\lambda_1}\right| = \rho\left(\sqrt{\lambda_1\lambda_2}\right).$$

Thus, $\rho(\alpha) \geq \rho\left(\sqrt{\lambda_1\lambda_2}\right)$ if $\alpha \in \left[0, (\lambda_1\lambda_2)^{1/2}\right] \cup \left[(\lambda_1^3/\lambda_2)^{1/2}, +\infty\right)$. So, we focus on the interval

$$J = \left((\lambda_1\lambda_2)^{1/2},\ (\lambda_1^3/\lambda_2)^{1/2}\right).$$

For $\alpha \in J$, let

$$\phi_j(\alpha) = \left\{\frac{\mathrm{trace}\,(\mathcal{M}_j(\alpha))}{2}\right\}^2 = \left\{\frac{(\alpha^2-q_j^2)(\alpha^2-\lambda_1\lambda_2)}{(\alpha^2+q_j^2)(\alpha+\lambda_1)(\alpha+\lambda_2)}\right\}^2$$

and

$$\psi(\alpha) = \det(\mathcal{M}_j(\alpha)) = \frac{(\alpha-\lambda_1)(\alpha-\lambda_2)}{(\alpha+\lambda_1)(\alpha+\lambda_2)}, \qquad j = 1, 2, \ldots, k.$$

Clearly, $\psi(\alpha)$ is independent of the index j. By Theorem 3.1, if $\phi_j(\alpha) \geq \psi(\alpha)$, then

$$\rho_j(\alpha) = \sqrt{\phi_j(\alpha)} + \sqrt{\phi_j(\alpha) - \psi(\alpha)};$$

otherwise,

$$\rho_j(\alpha) = \sqrt{\frac{(\alpha-\lambda_1)(\alpha-\lambda_2)}{(\alpha+\lambda_1)(\alpha+\lambda_2)}}.$$

We claim that

$$\max\{\rho_j(\alpha) : 1 \leq j \leq k\} = \max\{\rho_1(\alpha),\ \rho_k(\alpha)\}, \qquad \alpha \in J.$$

Suppose $1 < j < k$. If $\phi_j(\alpha) < \psi(\alpha)$ then

$$\rho_j(\alpha) = \sqrt{\frac{(\alpha-\lambda_1)(\alpha-\lambda_2)}{(\alpha+\lambda_1)(\alpha+\lambda_2)}},$$

and $\min\{\phi_1(\alpha), \phi_k(\alpha)\} \leq \phi_j(\alpha) < \psi(\alpha)$. It follows that $\rho_1(\alpha) = \rho_j(\alpha)$ or $\rho_k(\alpha) = \rho_j(\alpha)$. If $\phi_j(\alpha) \geq \psi(\alpha)$ and $\alpha \geq q_j^2$, then

$$0 \leq \phi_j(\alpha) \leq \phi_k(\alpha),$$

and hence

$$\rho_j(\alpha) = \sqrt{\phi_j(\alpha)} + \sqrt{\phi_j(\alpha) - \psi(\alpha)} \leq \sqrt{\phi_k(\alpha)} + \sqrt{\phi_k(\alpha) - \psi(\alpha)} = \rho_k(\alpha);$$

if $\phi_j(\alpha) \geq \psi(\alpha)$ and $\alpha < q_j^2$, then

$$0 < \phi_j(\alpha) \leq \phi_1(\alpha)$$

and hence

$$\rho_j(\alpha) = \sqrt{\phi_j(\alpha)} + \sqrt{\phi_j(\alpha) - \psi(\alpha)} \leq \sqrt{\phi_1(\alpha)} + \sqrt{\phi_1(\alpha) - \psi(\alpha)} = \rho_1(\alpha).$$

Thus, our claim is proved.

For each $\alpha \in J$, we have

$$\sqrt{|\alpha-\lambda_1|/|\alpha+\lambda_1|} \le \sqrt{|\alpha-\lambda_2|/|\alpha+\lambda_2|},$$

and hence

$$\rho_0(\alpha) = \left|\frac{\alpha-\lambda_1}{\alpha+\lambda_1}\right| \le \sqrt{\left|\frac{(\alpha-\lambda_1)(\alpha-\lambda_2)}{(\alpha+\lambda_1)(\alpha+\lambda_2)}\right|} \le \max\{\rho_1(\alpha),\ \rho_k(\alpha)\}.$$

Combining the above, we see that

$$\rho(\alpha) = \max\{\rho_1(\alpha),\ \rho_k(\alpha)\}, \quad \alpha \in J.$$

Let

$$\Omega(\alpha) = \max\{\phi_1(\alpha),\ \phi_k(\alpha),\ |\psi(\alpha)|\}.$$

Then

$$\Omega(\alpha) \le \max\{\rho_1(\alpha)^2,\ \rho_k(\alpha)^2\}.$$

If $\alpha^* \in J$ is such that $\Omega(\alpha^*) \le \Omega(\alpha)$ for all $\alpha \in J$, then one of the following holds.

(1) $\phi_1(\alpha^*) = \phi_k(\alpha^*) = |\psi(\alpha^*)|$;

(2.a) $\phi_1(\alpha^*) = \phi_k(\alpha^*) > |\psi(\alpha^*)|$, α^* is a local minimum of the function $\max\{\phi_1(\alpha),\ \phi_k(\alpha)\}$,

(2.b) $\phi_1(\alpha^*) = |\psi(\alpha^*)| > \phi_k(\alpha^*)$, α^* is a local minimum of the function $\max\{\phi_1(\alpha),\ |\psi(\alpha)|\}$,

(2.c) $\phi_k(\alpha^*) = |\psi(\alpha^*)| > \phi_1(\alpha^*)$, α^* is a local minimum of the function $\max\{\phi_k(\alpha),\ |\psi(\alpha)|\}$;

(3.a) $\max\{\phi_1(\alpha^*),\ \phi_k(\alpha^*)\} < |\psi(\alpha^*)|$ and α^* is a local minimum of the function $|\psi(\alpha^*)|$,

(3.b) $\max\{\phi_1(\alpha^*),\ |\psi(\alpha^*)|\} < \phi_k(\alpha^*)$ and α^* is a local minimum of the function $\phi_k(\alpha^*)$,

(3.c) $\max\{\phi_k(\alpha^*),\ |\psi(\alpha^*)|\} < \phi_1(\alpha^*)$ and α^* is a local minimum of the function $\phi_1(\alpha^*)$.

By the proof of Theorem 3.2, we see that the function $|\psi(\alpha)|$ has a differentiable local maximum at $\alpha > 0$, and two non-differentiable local minima at λ_2 and λ_1, where $\psi(\lambda_1) = \psi(\lambda_2) = 0$. Thus, condition (3.a) cannot hold. Similarly, for $j = 1, k$, the proof of Theorem 3.2 shows that the function $\phi_j(\alpha)$ has a local maximum at $\alpha > 0$, and two local minima at $|q_j|$ and $\sqrt{\lambda_1\lambda_2}$, where $\phi_j(|q_j|) = \phi_j(\sqrt{\lambda_1\lambda_2}) = 0$. Thus, none of conditions (3.b) or (3.c) holds.

Now suppose that (1) or (2.a) holds. Then $\phi_1(\alpha^*) = \phi_k(\alpha^*)$ implies that $\alpha^* = \sqrt{q_1 q_k}$. In both cases, we have

$$\rho_1(\alpha^*) = \sqrt{\phi_1(\alpha^*)} + \sqrt{\phi_1(\alpha^*) - \psi(\alpha^*)} = \sqrt{\phi_k(\alpha^*)} + \sqrt{\phi_k(\alpha^*) - \psi(\alpha^*)} = \rho_k(\alpha^*),$$

and $\Omega(\alpha^*) = \max\{\rho_1(\alpha^*)^2,\ \rho_k(\alpha^*)^2\}$.

Suppose that (2.b) holds. If $\phi_k(\alpha^*) \ge \psi(\alpha^*)$, then

$$\rho_k(\alpha^*) = \sqrt{\phi_k(\alpha^*)} + \sqrt{\phi_k(\alpha^*) - \psi(\alpha^*)} < \sqrt{\phi_1(\alpha^*)} + \sqrt{\phi_1(\alpha^*) - \psi(\alpha^*)} = \rho_1(\alpha^*);$$

otherwise,

$$\rho_k(\alpha^*) = \sqrt{\frac{(\alpha^* - \lambda_1)(\alpha^* - \lambda_2)}{(\alpha^* + \lambda_1)(\alpha^* + \lambda_2)}} \le \rho_1(\alpha^*).$$

Thus, $\Omega(\alpha^*) = \rho_1(\alpha^*)^2 = \max\{\rho_1(\alpha^*)^2,\ \rho_k(\alpha^*)^2\}$. Moreover, since α^* is a local minimum of the function $\max\{\phi_1(\alpha),\ |\psi(\phi)|\}$, by Remark 3.4 we see that α^* is a root of the equation

$$(\alpha^2 + q_1^2)^2(\alpha^2 - \lambda_1^2)(\alpha^2 - \lambda_2^2) = (\alpha^2 - q_1^2)^2(\alpha^2 - \lambda_1\lambda_2)^2$$

or

$$(\alpha^2 + q_1^2)^2(\lambda_1^2 - \alpha^2)(\alpha^2 - \lambda_2^2) = (\alpha^2 - q_1^2)^2(\alpha^2 - \lambda_1\lambda_2)^2.$$

Suppose that (2.c) holds. We can use an argument similar to the case of (2.b) to conclude that $\Omega(\alpha^*) = \rho_k(\alpha^*)^2 = \max\{\rho_1(\alpha^*)^2,\ \rho_k(\alpha^*)^2\}$ and that α^* is a root of the equation

$$(\alpha^2 + q_k^2)^2(\alpha^2 - \lambda_1^2)(\alpha^2 - \lambda_2^2) = (\alpha^2 - q_k^2)^2(\alpha^2 - \lambda_1\lambda_2)^2$$

or

$$(\alpha^2 + q_k^2)^2(\lambda_1^2 - \alpha^2)(\alpha^2 - \lambda_2^2) = (\alpha^2 - q_k^2)^2(\alpha^2 - \lambda_1\lambda_2)^2.$$

Note that in all the cases (1), (2.a), (2.b), and (2.c), we have

$$\Omega(\alpha^*) = \max\{\rho_1(\alpha^*)^2,\ \rho_k(\alpha^*)^2\}.$$

Consequently, if $\alpha^* \in J$ yields the smallest $\Omega(\alpha)$, then

$$\rho(\alpha)^2 = \max\{\rho_1(\alpha)^2,\ \rho_k(\alpha)^2\} \ge \Omega(\alpha) \ge \Omega(\alpha^*) = \max\{\rho_1(\alpha^*)^2,\ \rho_k(\alpha^*)^2\} = \rho(\alpha^*)^2.$$

So, we only need to consider those α satisfying the specified equations in the theorem to determine the optimal parameter α^*.

Case 3. Suppose $r = k$ and $s > k$. Let $\rho_0(\alpha) = f_2(\alpha)$. Then

$$\rho(\alpha) = \max\{\rho_j(\alpha) \mid 0 \le j \le k\}.$$

Similarly to the proof of Case 2, we can show that

$$\rho(\alpha) \ge \rho(\sqrt{\lambda_1\lambda_2})$$

if α is positive and lies outside the interval

$$J = \left((\lambda_2^3/\lambda_1)^{1/2},\ (\lambda_1\lambda_2)^{1/2}\right).$$

So, we can focus on the interval J.

For $\alpha \in J$, we have

$$\rho(\alpha) = \max\{\rho_1(\alpha),\ \rho_k(\alpha)\}.$$

Note that in this case, for each $\alpha \in J$, we have

$$\sqrt{|\alpha - \lambda_2|/|\alpha + \lambda_2|} \le \sqrt{|\alpha - \lambda_1|/|\alpha + \lambda_1|},$$

and hence

$$\rho_0(\alpha) = \left|\frac{\alpha-\lambda_2}{\alpha+\lambda_2}\right| \le \sqrt{\left|\frac{(\alpha-\lambda_1)(\alpha-\lambda_2)}{(\alpha+\lambda_1)(\alpha+\lambda_2)}\right|} \le \max\{\rho_1(\alpha),\ \rho_k(\alpha)\}.$$

Finally, if $\alpha^* \in J$ is such that $\rho(\alpha^*) < \rho(\sqrt{\lambda_1\lambda_2})$, we can show that α^* must satisfy one of the three specified equations using an argument similar to the one in Case 2.

Case 4. Suppose $r = s = k$. Then

$$\rho(\alpha) = \max\{\rho_j(\alpha) \mid 1 \le j \le k\}.$$

Note that if α is positive and lies outside the interval

$$J = \left((\lambda_2^3/\lambda_1)^{1/2},\ (\lambda_1^3/\lambda_2)^{1/2}\right),$$

then each of the singular values of $\mathcal{M}(\alpha)$, which is equal to $|\alpha-\lambda_1|/|\alpha+\lambda_1|$ or $|\alpha-\lambda_2|/|\alpha+\lambda_2|$, has magnitude larger than $\rho(\sqrt{\lambda_1\lambda_2})$. Thus

$$\rho(\alpha) \ge |\det(\mathcal{M}(\alpha))|^{1/n} \ge \rho(\sqrt{\lambda_1\lambda_2}).$$

So, we can focus on those $\alpha \in J$. For each $\alpha \in J$, we can show that

$$\rho(\alpha) = \max\{\rho_1(\alpha),\ \rho_k(\alpha)\}.$$

Moreover, if $\alpha^* \in J$ is such that $\rho(\alpha^*) < \rho(\sqrt{\lambda_1\lambda_2})$, we can show that α^* must satisfy one of the three specified equations. □

Remark 4.2. The second group of equations in Theorem 4.1 can be reduced to a group of quadratic equations and the last one can be reduced to a group of quartic equations with respect to $\beta = \alpha^2$, respectively, analogously to those in Remark 3.3.

As an illustration of Theorem 4.1 and Remark 4.2, we consider a simple example for which $\lambda_1 = 2$, $\lambda_2 = 1$, $q_1 = 1$ and $q_k = 2$. Obviously, $\alpha_0^* = \sqrt{2} \approx 1.414$ is the root of the first equation in Theorem 4.1. In addition, by straightforward computations, we know that the only positive roots of the group of the equations with respect to $q_1 = 1$ in Theorem 4.1 are

$$\alpha_1^* = 1, \quad \alpha_2^* = \sqrt{5} \approx 2.236$$

and

$$\alpha_3^* = \frac{\sqrt{6}}{6}\sqrt{\left(7 + \sqrt[3]{712 + 9\sqrt{5277}} + \frac{43}{\sqrt[3]{712 + 9\sqrt{5277}}}\right)} \approx 1.914,$$

and those with respect to $q_k = 2$ in Theorem 4.1 are

$$\alpha_4^* = 2, \quad \alpha_5^* = \frac{\sqrt{20}}{5} \approx 0.894$$

and

$$\alpha_6^* = \frac{\sqrt{6}}{6}\sqrt{\left(1 + \sqrt[3]{1477 + 36\sqrt{5277}} - \frac{167}{\sqrt[3]{1477 + 36\sqrt{5277}}}\right)} \approx 1.045.$$

We remark that now the second one in the group of equations with respect to $q_1 = 1$ is equivalent to $(\beta-1)(2\beta^3-7\beta^2+\beta-8)=0$, and the second one in the group of equations with respect to $q_k = 2$ is equivalent to $(\beta-4)(2\beta^3-\beta^2+28\beta-32)=0$. Based on Theorem 3.1, from direct calculations we have

$$\rho(\mathcal{M}(\alpha_0^*)) = 3-2\sqrt{2} \approx 0.172, \quad \rho(\mathcal{M}(\alpha_1^*)) = 0, \quad \rho(\mathcal{M}(\alpha_2^*)) = \frac{\sqrt{3}(7-3\sqrt{5})}{6} \approx 0.0842$$

and

$$\rho(\mathcal{M}(\alpha_3^*)) \approx 0.201, \quad \rho(\mathcal{M}(\alpha_4^*)) = 0, \quad \rho(\mathcal{M}(\alpha_5^*)) \approx 0.146, \quad \rho(\mathcal{M}(\alpha_6^*)) \approx 0.0899.$$

Therefore, for the HSS iteration method, the optimal parameter is $\alpha^* = 1$ or $\alpha^* = 2$ and the corresponding optimal convergence factor is $\rho(\mathcal{M}(\alpha^*)) = 0$. On the other hand, from Theorem 2.1 we can easily obtain

$$\tilde{\alpha} = \sqrt{2} \quad \text{and} \quad \sigma(\tilde{\alpha}) = 3-2\sqrt{2} \approx 0.172.$$

Obviously, it holds that $\rho(\mathcal{M}(\alpha^*)) < \sigma(\tilde{\alpha})$.

Remark 4.3. Our proof techniques can be used to handle the case when $\lambda_2 = 0$, which also occur in applications; see [4] and its references. In such case, we may normalize $\lambda_1 = 1$, and we always assume that $s = k$ to ensure that A is invertible. In such case, we can use the analysis of Case 2 and Case 4 in our proof of Theorem 4.1. Note that in this case, we have

$$\psi(\alpha) = \frac{\alpha-1}{\alpha+1}, \qquad \phi_j(\alpha) = \left\{ \frac{(\alpha^2-q_j^2)\alpha}{(\alpha^2+q_j^2)(\alpha+\lambda_1)} \right\}^2 \quad \text{for} \quad j = 1, k.$$

If $q_1 = q_k$, then A is unitarily similar to

$$A_1 \oplus \cdots \oplus A_k \oplus I_u$$

with

$$A_j = \begin{bmatrix} 1 & q_1 \\ -q_1 & 0 \end{bmatrix}, \qquad j = 1, 2, \ldots, k.$$

So, the analysis reduces to the 2-by-2 case, and Theorem 3.2 applies.

Suppose $q_1 > q_k > 0$. Then the optimal value α^* can be easily determined by checking whether $\rho_1(\alpha)$ and $\rho_k(\alpha)$ intersect at a point α^* such that

$$\phi_1(\alpha^*) - \psi(\alpha^*) = \phi_k(\alpha^*) - \psi(\alpha^*) \geq 0.$$

This happens if and only if $q_1 q_k \leq \frac{1}{2}(q_1+q_k)$. In this case, $\alpha^* = \sqrt{q_1 q_k}$ is the optimal parameter, and

$$\rho(\mathcal{M}(\alpha^*)) = \frac{q_1-q_k}{q_1+q_k} \left(\frac{\sqrt{q_1 q_k}}{\sqrt{q_1 q_k}+1} + \frac{\sqrt{(q_1+q_k)^2 - 4q_1^2 q_k^2}}{(\sqrt{q_1 q_k}+1)(q_1-q_k)} \right).$$

Otherwise, $\alpha^* = \frac{q_1}{\sqrt{2q_1-1}}$ is the optimal parameter such that $\phi_1(\alpha^*) = \psi(\alpha^*) > \phi_k(\alpha^*)$ and

$$\rho(\mathcal{M}(\alpha^*)) = \frac{|q_1 - 1|}{q_1 + \sqrt{2q_1 - 1}}.$$

Note that the second case rarely appears in applications and its discussion was not included in [4]. Also, note that there were some typos in the formula of $\rho(\mathcal{M}(\alpha^*))$ for the first case in [4].

5 Estimation of Optimal Parameters for n-By-n Matrices and Numerical Examples

In general, for a nonsymmetric and positive definite system of linear equations (1.1), the eigenvalues of its coefficient matrix A is evidently contained in the complex domain $\mathcal{D}_A := [\lambda_{\min}, \lambda_{\max}] \times \imath[-q, q]$, where $\imath$ is the imaginary unit, $\lambda_{\min}$ and $\lambda_{\max}$ are, respectively, the smallest and the largest eigenvalues of the Hermitian part H, and q is the largest module of the eigenvalues of the skew-Hermitian part S, of the coefficient matrix A. If a reduced (simpler and lower-dimensional) matrix A_R whose eigenvalues possess the same contour as the domain $\mathcal{D}_A$ is used to approximate the matrix A, then we may expect that the main mathematical and numerical properties of the HSS iteration method for the original linear system with the coefficient matrix A can be roughly preserved by the HSS iteration method applied to the linear system with the reduced coefficient matrix A_R. A simple choice of the reduced matrix is given by

$$A_R = \begin{bmatrix} \lambda_{\max} & q \\ -q & \lambda_{\min} \end{bmatrix}$$

with $q = \|S\|$ or $q = \rho(H^{-1}S)\sqrt{\lambda_{\min}\lambda_{\max}}$. We can then use Theorem 3.2 and Corollary 3.5 to estimate the optimal parameter α^* of the HSS iteration method as follows.

Estimation 5.1. *Let $A \in \mathbb{R}^{n\times n}$ be a positive definite matrix, and $H, S \in \mathbb{R}^{n\times n}$ be its symmetric and skew-symmetric parts, respectively. Let $\lambda_{\min} = \min\{\lambda \mid \lambda \in \lambda(H)\}$ and $\lambda_{\max} = \max\{\lambda \mid \lambda \in \lambda(H)\}$. Suppose*

$$q = \|S\| \quad \text{or} \quad q = \rho(H^{-1}S)\sqrt{\lambda_{\min}\lambda_{\max}}.$$

Then one can use the positive roots of the equation

$$(\alpha^2 + q^2)^2(\alpha^2 - \lambda_{\max}^2)(\alpha^2 - \lambda_{\min}^2) = (\alpha^2 - q^2)^2(\alpha^2 - \lambda_{\min}\lambda_{\max})^2$$

or

$$(\alpha^2 + q^2)^2(\lambda_{\max}^2 - \alpha^2)(\alpha^2 - \lambda_{\min}^2) = (\alpha^2 - q^2)^2(\alpha^2 - \lambda_{\min}\lambda_{\max})^2$$

to estimate the optimal parameter $\alpha^* > 0$ satisfying

$$\rho(\mathcal{M}(\alpha^*)) = \min\{\rho(\mathcal{M}(\alpha)) \mid \alpha > 0\}.$$

Here, $\mathcal{M}(\alpha)$ is the iteration matrix of the HSS iteration method, see (2.2).

We first illustrate our estimates with the following example of a general nonsymmetric positive definite system of linear equations, see [2].

Consider the two-dimensional convection-diffusion equation

$$-(u_{xx} + u_{yy}) + \delta(u_x + u_y) = g(x, y)$$

on the unit square $[0, 1] \times [0, 1]$, with constant coefficient δ and subject to Dirichlet-type boundary conditions. When the five-point centered finite difference discretization is applied to it, we get the system of linear equations (1.1) with the coefficient matrix

$$A = T \otimes I + I \otimes T, \tag{5.1}$$

where the equidistant step-size $h = \frac{1}{m+1}$ is used in the discretization on both directions and the natural lexicographic ordering is employed to the unknowns. In addition, $\otimes$ denotes the Kronecker product, T is a tridiagonal matrix given by

$$T = \mathrm{tridiag}(-1 - R_e, 2, -1 + R_e),$$

and

$$R_e = \frac{\delta h}{2}$$

is the mesh Reynolds number. We remark that here the first-order derivatives are also approximated by the centered difference scheme.

From Lemma A.1 in [2, Appendix], we know that

$$\begin{cases} \gamma_{\min} & \equiv & \lambda_{\min} = \min\limits_{1 \le j,k \le m} \lambda_{j,k}(H) = 4(1 - \cos(\pi h)), \\ \gamma_{\max} & \equiv & \lambda_{\max} = \max\limits_{1 \le j,k \le m} \lambda_{j,k}(H) = 4(1 + \cos(\pi h)) \end{cases}$$

and

$$\min_{1 \le j,k \le m} |\lambda_{j,k}(S)| = 0, \qquad \max_{1 \le j,k \le m} |\lambda_{j,k}(S)| = 4R_e \cos(\pi h).$$

Therefore, the optimal parameter $\tilde{\alpha}$ that minimizes the upper bound $\sigma(\alpha)$ of the convergence factor $\rho(\mathcal{M}(\alpha))$ of the HSS iteration method is given by

$$\tilde{\alpha} \equiv \sqrt{\gamma_{\min}\gamma_{\max}} = \sqrt{\lambda_{\min}\lambda_{\max}} = 4\sin(\pi h),$$

see Theorem 2.1.

In Table 1 we list the experimental optimal parameter α (denoted by α_{exp}), the estimated optimal parameter α (denoted by α_{est}) determined by Estimation 5.1, the upper-bound minimizer $\tilde{\alpha}$, and the corresponding spectral radii $\rho(\mathcal{M}(\alpha))$ of the HSS iteration matrix $\mathcal{M}(\alpha)$ for $\alpha = \alpha_{\mathrm{exp}}, \alpha_{\mathrm{est}}$ and $\tilde{\alpha}$. From this table we see that $\tilde{\alpha}$ always overestimates $\rho(\mathcal{M}(\alpha))$ when compared with α_{est}, and that α_{est} yields quite a good approximation to α_{exp}.

In Table 2 we list the number of iterations (denoted by "IT") and the elapsed CPU time in seconds (denoted by "CPU") of the HSS iteration method when it is applied to the nonsymmetric positive definite system of linear equations (1.1) with coefficient matrix

Table 1: α versus $\rho(\mathcal{M}(\alpha))$ when $m = 32$

δ	10	50	100	500	1000
α_{exp}	0.5195	2.2129	3.5606	12.0063	17.6346
$\rho(\mathcal{M}(\alpha_{\text{exp}}))$	0.7794	0.4414	0.4635	0.6357	0.7161
α_{est}	0.5967	2.7084	5.1536	10.2948	15.0075
$\rho(\mathcal{M}(\alpha_{est}))$	0.8055	0.4582	0.4771	0.6374	0.7179
$\tilde{\alpha}$	0.3802	0.3802	0.3802	0.3802	0.3802
$\rho(\mathcal{M}(\tilde{\alpha}))$	0.8312	0.8702	0.8839	0.8999	0.9030

Table 2: IT and CPU when $m = 32$ and $\varepsilon = 10^{-6}$

δ		10	50	100	500	1000
α_{exp}	IT	70	38	36	58	79
	CPU	0.7414	0.3905	0.6986	1.1147	1.5510
α_{est}	IT	66	44	45	55	72
	CPU	0.6842	0.4568	0.9238	1.0780	1.3991

(5.1). From this table we see that the numerical results produced with α_{est} coincide with those using α_{exp}, and the match is quite pertinent.

Here and in the next example, we choose the right-hand-side vector f such that the exact solution of the system of linear equations is $(1, 1, \ldots, 1)^T \in \mathbb{R}^n$. In addition, all runs are initiated from the initial vector $x^{(0)} = 0$, and terminated if the current iteration satisfy

$$\frac{\|f - Ax^{(k)}\|_2}{\|f - Ax^{(0)}\|_2} \leq \varepsilon.$$

The experiments are run in MATLAB (version 6.1) with a machine precision 10^{-16}. The machine used is a Pentium-III 500 personal computer with 256M memory.

Then, we use the following example of 2-by-2 block system of linear equations to further confirm the above observations.

Consider the system of linear equations (1.1) with the coefficient matrix

$$A = \begin{bmatrix} B & E \\ -E^T & 0.5I \end{bmatrix}, \tag{5.2}$$

where

$$B = \begin{bmatrix} I \otimes T_H + T_H \otimes I & 0 \\ 0 & I \otimes T_H + T_H \otimes I \end{bmatrix} \in \mathbb{R}^{2m^2 \times 2m^2}, \tag{5.3}$$

$$E = \begin{bmatrix} I \otimes F \\ F \otimes I \end{bmatrix} \in \mathbb{R}^{2m^2 \times m^2}, \tag{5.4}$$

and

$$T_H = \text{tridiag}(-1, 2, -1) \in \mathbb{R}^{m\times m}, \qquad F = \delta h \cdot \text{tridiag}(-1, 1, 0) \in \mathbb{R}^{m\times m}, \tag{5.5}$$

with $h = \frac{1}{m+1}$ the discretization meshsize, see [4].

For this example, we have $r = 2m^2$ and $s = m^2$. Hence, the total number of variables is $r + s = 3m^2$.

In Table 3 we list the experimental optimal parameter α_{exp}, the estimated optimal parameter α_{est} determined by Estimation 5.1, and the corresponding spectral radii $\rho(\mathcal{M}(\alpha))$ of the HSS iteration matrix $\mathcal{M}(\alpha)$ for $\alpha = \alpha_{\text{exp}}$ and α_{est}. Here, considering Theorem 4.1 and the two-by-two block structure of the matrix A in (5.2), we may apply the equations in Estimation 5.1 to the q which is either the largest or the smallest singular value (denoted, respectively, by q_1 or q_k) of the matrix E, and also consider the two points $\alpha = \sqrt{\lambda_{\min}\lambda_{\max}}$ and $\alpha = \sqrt{q_1 q_k}$, to obtain a more accurate estimate to the optimal iteration parameter for the HSS iteration method. From this table we can see that α_{est} yields quite a good approximation to α_{exp}.

Table 3: α versus $\rho(\mathcal{M}(\alpha))$

δ	10			100		
m	16	24	32	16	24	32
α_{exp}	0.7457	0.5087	0.3849	1.0340	0.6553	0.4639
$\rho(\mathcal{M}(\alpha_{\text{exp}}))$	0.8291	0.8812	0.9090	0.7700	0.8490	0.8912
α_{est}	0.7350	0.5013	0.3802	0.7350	0.5013	0.3802
$\rho(\mathcal{M}(\alpha_{est}))$	0.8304	0.8816	0.9091	0.8304	0.8816	0.9091

In Table 4 we list the number of iterations and the elapsed CPU time of the HSS iteration method when it is applied to the 2×2 block system of linear equations (1.1) with the coefficient matrix (5.2)-(5.5). From this table we can see that the numerical results produced with α_{est} coincide with those using α_{exp}, and the match is quite pertinent.

Table 4: IT and CPU when $\varepsilon = 10^{-6}$

δ		10			100		
m		16	24	32	16	24	32
α_{exp}	IT	59	90	117	43	70	97
	CPU	0.4416	3.0069	15.2751	0.3531	2.3821	13.3629
α_{est}	IT	60	90	119	60	92	118
	CPU	0.4250	3.0139	15.2881	0.4617	3.1193	15.6046

6 Proof of Remark 3.3

Here we give the proof of Remark 3.3.

The assertion concerning $\lambda_1 = \lambda_2$ and the assertion concerning equation (3.3) can be readily verified. We consider the equation (3.4) and the reduced equation (3.5). Note that for $\alpha > 0$, the right side of (3.4) is nonnegative, and the left side is nonnegative on the interval $[\lambda_2, \lambda_1]$ only. So, all the positive solutions $\beta = \alpha^2$ of the equation (3.5) lie in $[\lambda_2^2, \lambda_1^2]$. Define

$$f(\beta) = (\lambda_1^2 - \beta)(\beta - \lambda_2^2), \quad g_1(\beta) = (\beta - \lambda_1\lambda_2)^2, \quad g_2(\beta) = \frac{(\beta - q^2)^2}{(\beta + q^2)^2},$$

$$g(\beta) = g_1(\beta)g_2(\beta) \quad \text{and} \quad h(\beta) = f(\beta) - g(\beta),$$

for $\beta > 0$. Then β is a positive solution of (3.5) if and only if β is a positive solution of

$$h(\beta) = 0.$$

Obviously, the graph of $f(\beta)$ is a concave parabola which intersects the β-axis at $\beta = \lambda_2^2$ and λ_1^2, while the graph of $g_1(\beta)$ is a convex parabola touching the β-axis at $\beta = \lambda_1\lambda_2$. Note that $f(\beta) = g_1(\beta)$ has two solutions in the intervals $[\lambda_2^2, \lambda_1\lambda_2)$ and $((\lambda_1^2 + \lambda_2^2)/2, \lambda_1^2]$. The graph of $g(\beta)$ can be obtained from that of $g_1(\beta)$ by reducing the vertical height of each point by the factor $g_2(\beta) \in (0, 1)$. Thus, the solution of $f(\beta) = g_1(\beta)$ nearer to λ_2^2 will move further left to a solution of $f(\beta) = g(\beta)$; the solution of $f(\beta) = g_1(\beta)$ nearer to λ_1^2 will move further right to a solution of $f(\beta) = g(\beta)$.

We claim that $h(\beta)$ cannot have more than 2 positive solutions in $[\lambda_2^2, \lambda_1^2]$, equivalently, (3.5) cannot have more than 2 positive solutions in $[\lambda_2^2, \lambda_1^2]$.

First, we prove the claim if $q^2 < \lambda_2^2$ or $q^2 > \lambda_1^2$. Let $p(\beta)$ be the polynomial on the left side of (3.5) divided by 2. Then the product of the roots of (3.5) is the constant term of $p(\beta)$ and equals the positive number $q^4\lambda_1^2\lambda_2^2$. So, if (3.5) have more than 2 positive roots, then it must have 4 positive roots, say, $\beta_1 \le \beta_2 \le \beta_3 \le \beta_4$. Suppose $p'(\beta)$ has zeros $\beta_1' \le \beta_2' \le \beta_3'$, $p''(\beta)$ has zeros $\beta_1'' \le \beta_2''$, and $p'''(\beta)$ has zero β_1'''. We have $\beta_1' \le \beta_1'' \le \beta_2' \le \beta_2'' \le \beta_3'$ and $\beta_1'' \le \beta_1''' \le \beta_2''$. Thus,

$$\beta_1' \le \beta_1''' \le \beta_3'.$$

Now, examining the constant terms of the polynomials $p'(\beta)/4$ and $p'''(\beta)/24$, we see that

$$\beta_1'\beta_2'\beta_3' = q^4(\lambda_1 + \lambda_2)^2/8 \tag{6.1}$$

and $\beta_1''' = (\lambda_1 + \lambda_2)^2/8$. If $q^2 < \lambda_2^2$, then $q^2 < \beta_1 \le \beta_1' \le \beta_2'$ and hence

$$\beta_1'\beta_2'\beta_3' > (q^2)(q^2)(\beta_1''') = q^4(\lambda_1 + \lambda_2)^2/8,$$

which contradicts (6.1). Similarly, if $q^2 > \lambda_1^2$, then $q^2 > \beta_4 \ge \beta_3' \ge \beta_2'$ and hence

$$\beta_1'\beta_2'\beta_3' < \beta_1'''(q^2)(q^2) = q^4(\lambda_1 + \lambda_2)^2/8,$$

which again contradicts (6.1). Thus, our claim is proved in these cases.

Next, we assume that $q^2 \in [\lambda_2^2, \lambda_1^2]$. Then

$$g(\beta) = \frac{(\beta - q^2)^2(\beta - \lambda_1\lambda_2)^2}{(\lambda_1^2 - \beta)(\beta - \lambda_2^2)}$$

has two zeros in $[\lambda_2^2, \lambda_1^2]$, namely, $\beta = q^2$ and $\beta = \lambda_1\lambda_2$.

If $\lambda_2^2 \leq q^2 \leq \lambda_1\lambda_2$, then f is increasing on $[\lambda_2^2, (\lambda_1^2+\lambda_2^2)/2]$ and $q^2 \leq \lambda_1\lambda_2 \leq (\lambda_1^2+\lambda_2^2)/2$. So, f is increasing on $[\lambda_2^2, q^2]$. Since $g(\beta)$ is decreasing on $[\lambda_2^2, q^2]$, and the function $h(\beta)$ have different signs at λ_2^2 and q^2, it follows that $h(\beta) = 0$ has a root in $[\lambda_2\lambda_1, q^2]$. On $(q^2, (\lambda_1^2 + \lambda_2^2)/2]$, we have $f(\beta) > g_1(\beta) \geq g_1(\beta)g_2(\beta)$. Thus, $f(\beta) = g_1(\beta)g_2(\beta)$ has no root in this interval. Finally, on the interval $[(\lambda_1^2 + \lambda_2^2)/2, \lambda_1^2]$, f is decreasing and $g(\beta)$ is increasing, and the function $h(\beta)$ assume nonzero values with different signs at the end points. Thus, $f(\beta) = g_1(\beta)g_2(\beta)$ has a root in $((\lambda_1^2 + \lambda_2^2)/2, \lambda_1^2)$.

Suppose $\lambda_1\lambda_2 < q^2 \leq \lambda_1^2$. On $[\lambda_2^2, \lambda_1\lambda_2]$, f is increasing and $g(\beta)$ is decreasing. Moreover, the function $h(\beta)$ assume nonzero values with different signs at λ_2^2 and $\lambda_1\lambda_2$, it follows that $h(\beta) = 0$ has a root in $(\lambda_2^2, \lambda_1\lambda_2)$.

Suppose $q^2 < (\lambda_1^2 + \lambda_2^2)/2$. On $(\lambda_1\lambda_2, (\lambda_1^2 + \lambda_2^2)/2]$, we have $f(\beta) > g_1(\beta) \geq g_1(\beta)g_2(\beta)$. Thus, $f(\beta) = g_1(\beta)g_2(\beta)$ has no root in this interval. On the interval $[(\lambda_1^2 + \lambda_2^2)/2, \lambda_1^2]$, f is decreasing and $g(\beta)$ is increasing, and the function $h(\beta)$ assume nonzero values with different signs at the end points. Thus, $f(\beta) = g(\beta)$ has a root in $((\lambda_1^2 + \lambda_2^2)/2, \lambda_1^2)$.

Finally, if $q^2 \in [(\lambda_1^2 + \lambda_2^2)/2, \lambda_1^2]$, then for $\beta \in (\lambda_1\lambda_2, q^2)$ we have

$$(\beta - \lambda_1\lambda_2)^2/(\beta + q)^2 \in (0, 1)$$

and hence

$$f(\beta) > (\beta - q)^2 > g(\beta).$$

Thus, $f(\beta) = g(\beta)$ has no solution in $[(\lambda_1^2 + \lambda_2^2)/2, q^2)$. Now, on the interval $[q^2, \lambda_1^2]$, f is decreasing and $g(\beta)$ is increasing, and the function $h(\beta)$ assume values with different signs at the end points. Thus, $f(\beta) = g(\beta)$ has a root in $[q^2, \lambda_1^2]$.

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