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# On choices of iteration parameter in HSS method



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### ABSTRACT

The HSS iteration method is effective to solve non-Hermitian positive definite linear systems, but the choice of its optimal parameter is a difficult and challenging problem in theoretical analysis and practical computations. In this paper, we obtain an accurate estimate to the optimal parameter of the HSS iteration method by adopting a reasonable and simple optimization principle. Numerical experiments show that this principle is feasible to produce an accurate estimate to the optimal parameter of the HSS iteration method.

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#### 1. Introduction

Consider systems of linear equations of the form

$$Ax = b, \quad A \in C^{n \times n} \quad \text{and} \quad x, b \in C^{n}.$$
 (1.1)

This class of linear system often rises in many practical applications. When A is a non-Hermitian and positive definite matrix, the HSS iteration method was proposed to effectively solve this class of linear systems in 2003 [6]. The basic strategies in the construction of the HSS iteration method is matrix splitting and stationary iteration. Any non-Hermitian matrix A can be decomposed into its Hermitian and skew-Hermitian parts as

$$A = H + S$$

where

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

Here,  $A^*$  is used to denote the conjugate transpose of the matrix A. Based on this Hermitian and skew-Hermitian splitting, the HSS iteration method [6] can be described as follows.

**The HSS Iteration Method.** Given an initial guess  $x^{(0)} \in C^n$ , for k = 0, 1, 2, ... until the iteration sequence  $\{x^{(k)}\}$  converges, compute  $x^{(k+1)}$  using the following procedure:

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

where  $\alpha$  is a given positive constant, and I is the identity matrix.

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From the viewpoint of splitting, the nature of the HSS iteration method is that the coefficient matrix A has the splitting

$$A = \frac{1}{2\alpha}(F(\alpha) - G(\alpha)),$$

where

$$\begin{cases} F(\alpha) = (\alpha I + H)(\alpha I + S), \\ G(\alpha) = (\alpha I - H)(\alpha I - S). \end{cases}$$

The HSS iteration method has the following convergence property; see [6].

**Theorem 1.1** [6]. Let  $A \in C^{n \times n}$  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, and  $\alpha$  be a positive constant. Then the iteration matrix  $M(\alpha)$  of the HSS iteration method is given by

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

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

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

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

$$\rho(M(\alpha)) \leq \delta(\alpha) < 1, \quad \forall \alpha > 0,$$

i.e., the HSS iteration method unconditionally converges to the unique solution  $x_* \in C^n$  of the system of linear Eq. (1.1).

The HSS iteration method has been generalized to various forms and applied in many fields. Based on the HSS iteration method, many matrix splitting iteration methods such as PSS, MHSS, GHSS have been proposed [2,5,7]. In addition, the HSS iteration method has been developed to the saddle-point problems and the Toeplitz linear systems [3,8,10,11,14]. To further expand the applications of the HSS iteration method, we need to determine or estimate its optimal parameter  $\alpha_* = \arg\min_{\alpha} \rho(M(\alpha))$ . However, this is unfortunately a very difficult problem. As we have known, till now there is no substantial progress on this topic. Although we can compute an experimentally optimal parameter, it usually costs much time. Many researchers have devoted to estimate  $\alpha_*$  and have obtained many valuable results. In [4] the authors analyzed two-by-two real matrices in detail and obtained an analytical formula for the optimal parameter  $\alpha_*$ . In general, in [6] the authors adopted  $a_{up} = \sqrt{\lambda_{min}\lambda_{max}}$  that minimizes the upper bound  $\delta(\alpha)$  instead of using the experimental optimal parameter. By imposing the HSS iteration matrix  $F(\alpha)^{-1}G(\alpha)$  to approach to zero, in [13] the author solved the minimization problem  $\min_{\alpha} ||G(\alpha)||_F^2$  to obtain an estimated parameter for  $\alpha_*$ . And in [9] by using various matrix traces and error minimizations the authors obtained an estimated parameter for  $\alpha_*$ , too. In this paper, utilizing the Euclidean norm we analyze the condition number of the coefficient matrices  $\alpha I + H$  and  $\alpha I + S$  and obtain an accurate estimate to the optimal parameter  $\alpha_*$  of the HSS iteration method.

The remainder of the paper organized is as follows. We describe our original idea of estimating the optimal parameter of the HSS iteration method and obtain an estimated optimal parameter by using the Euclidean norm in Section 2. Numerical results are given in Section 3 to show the accuracy of our results. At last, in Section 4 we draw some remarks.

#### 2. Parameter estimation using Euclidean norm

We need to solve two sub-systems of linear equations in the HSS iteration method, which have coefficient matrices  $\alpha I + H$  and  $\alpha I + S$ , respectively. If either of these two linear sub-systems are solved inefficiently, then the convergence speed of the HSS iteration method will be deteriorated. Hence, the HSS iteration method may have fast convergence rate if  $\alpha$  minimizes the function

$$\varphi(\alpha) := |(\kappa(\alpha I + H) - \kappa(\alpha I + S))|,$$

where  $\kappa(\cdot)$  denotes the Euclidean condition number of the corresponding matrix.

By direct calculations, we have

$$\varphi(\alpha) = |||(\alpha I + H)^{-1}||\cdot||\alpha I + H|| - ||(\alpha I + S)^{-1}||\cdot||\alpha I + S|||$$

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

where,  $\lambda_{min}$  and  $\lambda_{max}$  are the minimal and the maximal eigenvalues of the matrix H, and  $\sigma_{min}$  and  $\sigma_{max}$  are the minimal and the maximal singular values of the matrix S, respectively. Here we have used  $||\cdot||$  to denote the Euclidean norm of a matrix.

$$||(\alpha I + H)^{-1}|| \cdot ||\alpha I + H|| = ||(\alpha I + S)^{-1}|| \cdot ||\alpha I + S||,$$

then  $\varphi(\alpha) = 0$ . It follows that

$$\frac{\alpha + \lambda_{max}}{\alpha + \lambda_{min}} = \frac{\sqrt{\alpha^2 + \sigma_{max}^2}}{\sqrt{\alpha^2 + \sigma_{min}^2}}.$$
(2.1)

Define

$$g(\alpha) = 2(\lambda_{max} - \lambda_{min})\alpha^3 + \left(\lambda_{max}^2 - \lambda_{min}^2 - \left(\sigma_{max}^2 - \sigma_{min}^2\right)\right)\alpha^2 + 2\left(\sigma_{min}^2\lambda_{max} - \sigma_{max}^2\lambda_{min}\right)\alpha + \sigma_{min}^2\lambda_{max}^2 - \sigma_{max}^2\lambda_{min}^2$$

Then we know that the equation in (2.1) is equivalent to  $g(\alpha) = 0$ .

Now, we discuss the roots of the equation  $g(\alpha) = 0$  in two cases.

Case I.  $\lambda_{max} \neq \lambda_{min}$ , i.e.,  $\lambda_{max} > \lambda_{min}$ . For this case, we let

$$\upsilon = \frac{\sigma_{max}^2 - \sigma_{min}^2}{\lambda_{max} - \lambda_{min}} \tag{2.2}$$

and

$$f(\alpha) = 2\alpha^3 + (\lambda_{max} + \lambda_{min} - \upsilon)\alpha^2 + 2(\sigma_{min}^2 - \lambda_{min}\upsilon)\alpha + \sigma_{min}^2(\lambda_{max} + \lambda_{min}) - \lambda_{min}^2\upsilon.$$
 (2.3)

Then  $g(\alpha) = 0$  is equivalent to  $f(\alpha) = 0$ . We easily know that  $f(\alpha) = 0$  has at least one real root.

If

$$\sigma_{min}^2(\lambda_{max}+\lambda_{min})-\lambda_{min}^2\upsilon<0,$$

then the equation  $\varphi(\alpha) = 0$  has at least one positive solution. And if

$$\sigma_{min}^2(\lambda_{max} + \lambda_{min}) - \lambda_{min}^2 \upsilon = 0,$$

then

$$\sigma_{min}\lambda_{max} = \sigma_{max}\lambda_{min}$$

and

$$f(\alpha) = \alpha \left( 2\alpha^2 + (\lambda_{max} + \lambda_{min}) \left( 1 - \frac{\sigma_{max}^2}{\lambda_{max}^2} \right) \alpha - 2 \frac{\sigma_{max}^2}{\lambda_{max}} \lambda_{min} \right).$$

So the equation  $f(\alpha) = 0$  has a root zero, a positive root and a negative root.

Case II.  $\lambda_{max} = \lambda_{min}$ . For this case, we know

$$\begin{split} g(\alpha) &= - \left( \sigma_{max}^2 - \sigma_{min}^2 \right) \alpha^2 - 2 \lambda_{max} \left( \sigma_{max}^2 - \sigma_{min}^2 \right) \alpha - \lambda_{max}^2 \left( \sigma_{max}^2 - \sigma_{min}^2 \right) \\ &= - \left( \sigma_{max}^2 - \sigma_{min}^2 \right) \left( \alpha^2 + 2 \lambda_{max} \alpha + \lambda_{max}^2 \right). \end{split}$$

So the equation  $g(\alpha) = 0$  has not any positive root. Now, we go back to minimize the function

$$\varphi(\alpha) = |\kappa(\alpha I + H) - \kappa(\alpha I + S)|.$$

In fact,  $\lambda_{max} = \lambda_{min}$  leads to

$$\varphi(\alpha) = \left| \frac{\alpha + \lambda_{max}}{\alpha + \lambda_{min}} - \frac{\sqrt{\alpha^2 + \sigma_{max}^2}}{\sqrt{\alpha^2 + \sigma_{min}^2}} \right|$$
$$= \frac{\sqrt{\alpha^2 + \sigma_{max}^2}}{\sqrt{\alpha^2 + \sigma_{min}^2}} - 1$$
$$= \sqrt{1 + \frac{\sigma_{max}^2 - \sigma_{min}^2}{\alpha^2 + \sigma_{min}^2}} - 1.$$

Hence  $\varphi(\alpha)$  is decreasing in  $(0,+\infty)$ . If we choose  $\frac{\sigma_{\max}^2 - \sigma_{\min}^2}{\alpha^2 + \sigma_{\min}^2} = \theta$ , with  $\theta > 0$ , then it holds that

$$\varphi(\alpha) = \sqrt{1+\theta} - 1.$$

So, when  $\theta$  is smaller,  $\varphi(\alpha)$  will be close to 0. To make  $\varphi(\alpha)$  be as small as possible, we may choose  $\theta$  to approach zero. In this manner, we can obtain specific value of the parameter  $\alpha$  by numerical experiments.

According to the above analysis, we have the following theorem.

**Theorem 2.1.** Let  $A \in C^{n \times n}$  be a positive definite matrix, and  $H = \frac{1}{2}(A + A^*)$  and  $S = \frac{1}{2}(A - A^*)$ . Assume that  $\lambda_{min}$  and  $\lambda_{max}$  are the minimal and the maximal eigenvalues of the matrix H, and  $\sigma_{min}$  and  $\sigma_{max}$  are the minimal and the maximal singular values of the

matrix S, respectively. If  $\sigma_{min}^2(\lambda_{max} + \lambda_{min}) - \lambda_{min}^2 \upsilon \le 0$ , then the equation  $f(\alpha) = 0$  has at least one positive root, where  $f(\alpha)$  and  $\upsilon$  are defined in (2.3) and (2.2).

Next, we analyze the special situation  $\sigma_{min} = 0$ . We have

$$\varphi(\alpha) = \left| ||(\alpha I + H)^{-1}|| \cdot ||\alpha I + H|| - ||(\alpha I + S)^{-1}|| \cdot ||\alpha I + S|| \right|$$
$$= \left| \frac{\alpha + \lambda_{max}}{\alpha + \lambda_{min}} - \frac{\sqrt{\alpha^2 + \sigma_{max}^2}}{\alpha} \right|$$

and  $\varphi(\alpha) = 0$  is equivalent to the formula

$$\frac{\alpha + \lambda_{max}}{\alpha + \lambda_{min}} = \frac{\sqrt{\alpha^2 + \sigma_{max}^2}}{\alpha}.$$
 (2.4)

Let

$$\tilde{g}(\alpha) = 2(\lambda_{max} - \lambda_{min})\alpha^3 + \left(\lambda_{max}^2 - \lambda_{min}^2 - \sigma_{max}^2\right)\alpha^2 - 2\sigma_{max}^2\lambda_{min}\alpha - \sigma_{max}^2\lambda_{min}^2$$

Then the formula (2.4) is equivalent to  $\tilde{g}(\alpha) = 0$ . Similarly, we discuss the roots of this cubic equation in two cases.

Case I.  $\lambda_{max} \neq \lambda_{min}$ , i.e.,  $\lambda_{max} > \lambda_{min}$ . For this case, we let

$$\tilde{v} = \frac{\sigma_{max}^2}{\lambda_{max} - \lambda_{min}}$$

and

$$\tilde{f}(\alpha) = 2\alpha^3 + (\lambda_{max} + \lambda_{min} - \tilde{v})\alpha^2 - 2\tilde{v}\lambda_{min}\alpha - \tilde{v}\lambda_{min}^2. \tag{2.5}$$

Then  $\tilde{g}(\alpha) = 0$  can be rewritten as  $\tilde{f}(\alpha) = 0$ . By straightforward computations we obtain

$$\tilde{f}'(\alpha) = 6\alpha^2 + 2(\lambda_{max} + \lambda_{min} - \tilde{\upsilon})\alpha - 2\tilde{\upsilon}\lambda_{min}.$$

Hence  $\tilde{f}'(\alpha)$  has two roots: one positive root  $\alpha_1$  and one negative root  $\alpha_2$ . As a result,  $\tilde{f}(\alpha)$  is increasing in  $(-\infty, \alpha_2) \cup (\alpha_1, +\infty)$  and decreasing in  $(\alpha_2, \alpha_1)$ . In addition, it is obvious that  $\tilde{f}(0) < 0$ . So  $\tilde{f}(\alpha)$  has a positive root in  $(0, +\infty)$ .

Case II.  $\lambda_{max} = \lambda_{min}$ . For this case, we can similarly obtain

$$\begin{split} \tilde{g}(\alpha) &= -\sigma_{max}^2 \left(\alpha^2 + 2\lambda_{min}\alpha + \lambda_{min}^2\right) \\ &= -\sigma_{max}^2 (\alpha + \lambda_{min})^2. \end{split}$$

So  $\tilde{g}(\alpha)$  has no positive root.

Because  $\lambda_{max} = \lambda_{min}$ , the original minimization problem becomes

$$\varphi(\alpha) = |\kappa(\alpha I + H) - \kappa(\alpha I + S)|$$

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

$$= \frac{\sqrt{\alpha^2 + \sigma_{max}^2}}{\alpha} - 1$$

$$= \sqrt{1 + \frac{\sigma_{max}^2}{\alpha^2}} - 1.$$

Evidently,  $\varphi(\alpha)$  is decreasing in  $(0, +\infty)$ . By choosing  $\tilde{\theta} = \frac{\sigma_{\max}^2}{\alpha^2}$  with  $\tilde{\theta} > 0$ , we obtain

$$\varphi(\alpha) = \sqrt{1 + \tilde{\theta}} - 1.$$

So, to make  $\varphi(\alpha)$  be as small as possible, we may choose  $\tilde{\theta}$  to be close to 0. Straightforwardly, we can obtain specific values of the parameter  $\alpha$  by numerical experiments.

According to the above analysis, we have the following corollary.

**Corollary 2.1.** Let  $A \in C^{n \times n}$  be a positive definite matrix, and  $H = \frac{1}{2}(A + A^*)$  and  $S = \frac{1}{2}(A - A^*)$ . Assume 0 is an eigenvalue of S,  $\lambda_{min}$  and  $\lambda_{max}$  are the minimal and the maximal eigenvalues of the matrix S. Then the equation  $\tilde{f}(\alpha) = 0$  has at least one positive root, where  $\tilde{f}(\alpha)$  is defined in (2.5).

Admittedly, optimal choice of the iteration parameter in the HSS iteration method is a difficult and challenging problem. The above analyses give new strategies to estimate this optimal iteration parameter. By numerical experiments we can compare our new estimates and the old ones.

**Table 1**  $\alpha$  and  $\rho(M(\alpha))$  for Example 3.1 when n = 16.

β	80	90	100	110
$\alpha_{opt}$	7.8271	7.5920	7.2970	7.0148
$\rho(M(\alpha_{opt}))$	0.5065	0.5107	0.5169	0.5247
$\alpha_{est}$	92.5767	92.1013	91.5640	90.9627
$\rho(M(\alpha_{est}))$	0.9172	0.9168	0.9163	0.9158
$\alpha_{sug}$	1.8501	3.1853	4.7489	6.5055
$\rho(M(\alpha_{sug}))$	0.6197	0.5495	0.5152	0.5237

**Table 2** IT and CPU for Example 3.1 when n = 16.

	β	80	90	100	110
opt	IT	33	32	32	31
	CPU	0.0083	0.0079	0.0082	0.0077
est	IT	277	254	236	221
	CPU	0.0531	0.0458	0.0432	0.0420
sug	IT	29	25	27	30
	CPU	0.0087	0.0073	0.0087	0.0184

## 3. Numerical experiments

We use an example to show that our choices of the iteration parameter of the HSS iteration method are feasible and effective in practical computations. In the following, "sug" represents the estimated parameter by using our suggestion, "opt" denotes the estimated optimal parameter in [4], and "est" indicates the estimated parameter in [13]. Furthermore, all numerical results are computed by using these three choices of the iteration parameter  $\alpha$ .

In our implementations, the initial guess is chosen to be  $x^{(0)} = 0$  and the iteration is terminated once the current iterate  $x^{(k)}$  satisfies

$$\frac{\|b-Ax^{(k)}\|_2}{\|b-Ax^{(0)}\|_2} \leq 10^{-6}.$$

In addition, all codes are run in MATLAB (R2009a) with a machine precision  $10^{-16}$ , and all experiments are performed on a personal computer with 1.86 GHz central processing unit (Intel(R) Core(TM) 2Duo L9400), 2.96 G memory. The exact solution of the system of linear equations is set to be  $(1, 1, ..., 1)^T \in C^n$ . Moreover, In all tables, IT and CPU denote the number of iteration steps and the CPU time, respectively.

**Example 3.1.** [4] Consider the two-dimensional convection-diffusion equation

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

on the unit square  $(0, 1) \times (0, 1)$  with a constant coefficient  $\beta$ . The Dirichlet boundary condition is imposed on the boundary. By using the five-point centered finite difference discretization, we obtain the linear system Ax = b with

$$A = T \otimes I + I \otimes T.$$

Here, the equidistant stepsize  $h = \frac{1}{n+1}$  is used in the discretization on both directions and the natural lexicographic ordering is employed to the unknowns. In addition, we use  $\otimes$  to denote the Kronecker product, T = tridiag(-1 - Re, 2, 1 + Re) the tridiagonal matrix, and  $Re = \frac{1}{2}\beta h$  the mesh Reynolds number.

We list the computing results with respect to different  $\beta$  in Tables 1 and 2 when n = 16.

From Tables 1 and 2, we see that the parameters  $\alpha_{opt}$  and  $\alpha_{est}$  have no significant change with respect to different  $\beta$ . In addition,  $\rho(M(\alpha_{opt}))$  is the least among the three values of the spectral radius computed by using  $\alpha_{opt}$ ,  $\alpha_{est}$  and  $\alpha_{sug}$  when  $\beta=80$  and 90, but the number of iteration steps is not the least. Moreover, when we use  $\alpha_{sug}$  the number of iteration steps is the smallest among those corresponding to the three values  $\alpha_{opt}$ ,  $\alpha_{est}$  and  $\alpha_{sug}$ . In theory, the computations of  $\alpha_{opt}$  and  $\alpha_{sug}$  need the eigenvalues of the matrices H and S, but the computation of  $\alpha_{est}$  needs the traces of these matrices. It is clear that the numerical results computed by using  $\alpha_{opt}$  and  $\alpha_{sug}$  are better than that computed by using  $\alpha_{est}$ .

#### 4. Concluding remarks

By deriving and using a cubic polynomial equation, we propose a new strategy to estimate the optimal parameter for the HSS iteration method. Numerical results show that our new strategy for computing the optimal parameter is feasible and effective in actual implementations. However, this estimate of the optimal parameter may be only appropriate to the HSS iteration method and not appropriate to the HSS preconditioner used to accelerate the convergence rates of the Krylov subspace iteration methods such as GMRES and BiCGSTAB; see [1,12].

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