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

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The HSS Iteration

Let $A = H + S \in \mathbb{C}^{n \times n}$ be a sparse matrix, where

$$H = (A + A^*)/2 \qquad \text{and} \qquad S = (A - A^*)/2,$$

so that H is positive definite and $S \neq 0$. To solve the linear system

$$Ax = b,$$

consider the following HSS (Hemitian and Skew-Hermitian Spliting) iteration scheme proposed in [Bai,Golub,Ng, 2003].

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consider the following HSS (Hemitian and Skew-Hermitian Spliting) iteration scheme proposed in [Bai,Golub,Ng, 2003].

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:

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

where α is a given positive constant.

In matrix-vector form, we have

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

where

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

and

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

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Note that (1) may also result from the splitting

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

of the coefficient matrix A, with

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

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Furthermore, $\widetilde{\mathcal{M}}(\alpha)$ has singular values

$$\frac{1 - \lambda_j(H)}{1 + \lambda_j(H)}, \qquad j = 1, \ldots, n.$$

So, the spectral radius $\rho(\mathcal{M}(\alpha)) = \rho(\widetilde{\mathcal{M}}(\alpha))$ is bounded above by

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Problem How to find the optimal α^* so that

$$\rho(\mathcal{M}(\alpha^*)) \leq \rho(\mathcal{M}(\alpha)) \qquad \text{for all } \alpha > 0.$$

Let λ_1 and λ_2 be the maximum and minumum eigenvalues of H. If $\tilde{\alpha} = \sqrt{\lambda_1 \lambda_2}$, then

$$\frac{\sqrt{\lambda_1} - \sqrt{\lambda_2}}{\sqrt{\lambda_1} + \sqrt{\lambda_2}} = \|\widetilde{\mathcal{M}}(\tilde{\alpha})\| \leq \|\widetilde{\mathcal{M}}(\alpha)\|, \qquad \alpha > 0.$$

Thus,

$$\rho(\mathcal{M}(\alpha^*)) \leq \rho(\mathcal{M}(\tilde{\alpha})) \leq \frac{\sqrt{\lambda_1} - \sqrt{\lambda_2}}{\sqrt{\lambda_1} + \sqrt{\lambda_2}}.$$

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Problem Can we do better?

The two-by-two real case

Theorem 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* $\mathcal{M}(\alpha)$ *are*

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

where

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

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As a result,

$$\rho(\mathcal{M}(\alpha)) = \frac{|(\alpha^2 - \lambda_1\lambda_2)(\alpha^2 - q^2)| + \sqrt{\Delta(\alpha)}}{(\alpha + \lambda_1)(\alpha + \lambda_2)(\alpha^2 + q^2)} \qquad \text{if } \Delta(\alpha) \geq 0;$$

$$\rho(\mathcal{M}(\alpha)) = \sqrt{\frac{(\alpha - \lambda_1)(\alpha - \lambda_2)}{(\alpha + \lambda_1)(\alpha + \lambda_2)}} \qquad \text{if } \Delta(\alpha) < 0.$$

Proof. Apply an orthogonal similarity, and 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 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

$$\sqrt{\Delta(\alpha)} = \sqrt{(\alpha^2 - \lambda_1\lambda_2)^2(\alpha^2 - q^2)^2 - (\alpha^2 - \lambda_1^2)(\alpha^2 - \lambda_2^2)(\alpha^2 + q^2)^2} \quad (3)$$

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If X has eigenvalues γ_1, γ_2 then $\rho(X) = \max\{|\gamma_1|, |\gamma_2|\}$ so that

$$\rho(X) \geq |(\gamma_1 + \gamma_2)/2| = |(\mathrm{tr}\, X)/2|$$

and

$$\rho(X)^2 \geq |\gamma_1\gamma_2| = |\det(X)|.$$

For notational simplicity, write

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

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

$$\delta(\alpha) = |\det\,(\mathcal{M}(\alpha))| = \left|\frac{(\alpha - \lambda_1)(\alpha - \lambda_2)}{(\alpha + \lambda_1)(\alpha + \lambda_2)}\right|,$$

and

$$\omega(\alpha) = \max\{\tau(\alpha), \delta(\alpha)\}.$$

Then

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

Note that

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

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

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

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

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

Theorem 2 *Let the assumptions of Theorem 1 be satisfied and define the functions τ and δ as above. Then the optimal $\alpha^* > 0$ satisfying*

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

lies in the finite set

$$\mathbf{S} = \{\alpha > 0 : \tau(\alpha) = \delta(\alpha)\},$$

which consists of numbers $\alpha > 0$ satisfying

$$(\alpha^2 + q^2)^2(\alpha^2 - \lambda_1^2)(\alpha^2 - \lambda_2^2) = (\alpha^2 - q^2)^2(\alpha^2 - \lambda_1\lambda_2)^2 \tag{5}$$

or

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Remark Use the substitution $\beta = \alpha^2$ in (5) and (6) to get degree two/three polynomial equations!

Applications to two-by-two block matrices

Theorem 3 *Suppose* $A = H + S \in \mathbb{C}^{n\times n}$ *such that*

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

where $\lambda_1 > \lambda_2 > 0$, *and the nonzero matrix* $E \in \mathbb{C}^{r\times s}$ *has nonzero singular values* $q_1 \geq q_2 \geq \cdots \geq q_k$. *Then the spectral radius of the iteration matrix*

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

attains the minimum at α^*, *which is* $\sqrt{\lambda_1\lambda_2}$, $\sqrt{q_1 q_k}$, *or a root of one of the following equations:*

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

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where $j = 1, k$.

Estimation of optimal parameters for n-by-n matrices

In general, for a nonsymmetric and positive definite system of linear equations $Ax = b$, the eigenvalues of its coefficient matrix A lies in

$$\mathbf{D} = \{x + iy : \lambda_1 \geq x \geq \lambda_2,\ -q \leq y \leq q\},$$

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A reduced (simpler and lower-dimensional) matrix A_R whose eigenvalues possess the same contour as the domain $\mathbf{D}$ is used to approximate the matrix A. For instance, a simple choice of the reduced matrix is given by

$$A_R = \begin{bmatrix} \lambda_1 & q \\ -q & \lambda_2 \end{bmatrix} \qquad \text{with} \quad q = \|S\| \quad \text{or} \quad q = \rho(H^{-1}S)\sqrt{\lambda_1 \lambda_2}.$$

We then use our results to estimate the optimal parameter α^* of the HSS iteration method as follows.

Eestimation 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 λ_1 and λ_2 be the largest and smallest eigenvalues of H. Suppose

$$q = \|S\| \qquad \text{or} \qquad q = \rho(H^{-1}S)\sqrt{\lambda_1\lambda_2}.$$

Then one can use the positive roots of the equation

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Numerical examples were given to illustate that the estimations are useful.

Further research

Determine the optimal parameters for other classes of matrices A.

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Thank you for your attention!!!