Splitting Iteration Methods for Positive Definite Linear Systems

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1. The Problem

We consider the system of linear equations

$$Ax = b, \quad A \in \mathbb{C}^{n\times n} \quad \textbf{nonsingular}. \tag{1}$$

The matrix A satisfies the following:

- **Large sparse**
- **Non-Hermitian: ($A \neq A^*$)**
- **Positive definite (or real positive):**
  the real part $\Re(x^* A x) > 0$ for any nonzero $x \in \mathbb{C}^n$.

Example 1   A Convection-Diffusion Problem

$$-\nu\Delta u + q(x,y,z)\cdot\nabla u = f(x,y,z)$$

on $\Omega = (0,1)\times(0,1)\times(0,1)$, with zero Dirichlet boundary condition.

Applying the standard centered difference scheme on a uniform grid, we obtain (1).

Example 2 A Complex Symmetric System

$$A = H + \imath W,$$

where H and W are real and symmetric, i.e.,

$$H = H^T, \qquad W = W^T.$$

Therefore, A is complex and symmetric.

But A is not Hermitian as

$$A^* \neq A.$$

This kind of linear systems may arise from areas such as electromagnetics and chemistry.

Example 3 A Regularized KKT System

$$A = \begin{pmatrix} B & E \\ -E^* & C \end{pmatrix},$$

where $B \in \mathbb{C}^{m\times m}$ and $C \in \mathbb{C}^{\ell\times\ell}$ are both symmetric positive definite matrices.

This kind of linear systems may arise from areas such as fluid flow(Stokes, Navier-Stokes), mixed FEM or elliptic PDE's, structural analysis, electrical networks, image processing, $\cdots$.

2. Typical Iteration Methods

Classical Splitting Iteration Methods

The splitting

$$A = M - N; \qquad Mx = Nx + b$$

leads to the "fundamental" iteration scheme:

$$Mx^{(k+1)} = Nx^{(k)} + b. \tag{2}$$

Defining the error and the iteration matrix

$$e^{(k)} = x_* - x^{(k)}; \qquad L = M^{-1}N,$$

we obtain $e^{(k)} \to 0$ **as** $k \to \infty$ **if** $\rho(L) < 1$**.**

Typical splittings are:

$$
\begin{aligned}
A &= D - (D - A) \\
&\qquad \text{— Jacobi splitting} \\
&= (D - L) - U \\
&\qquad \text{— Gauss-Seidel splitting} \\
&= \frac{1}{\omega}(D - \omega L) - \frac{1}{\omega}[(1-\omega)D + \omega U] \\
&\qquad \text{— SOR splitting}
\end{aligned}
$$

The resulting iteration methods only converge when the matrix A is strictly diagonally dominant or Hermitian positive definite.

Krylov Subspace Iteration Methods

- **Split A into its Hermitian and skew-Hermitian parts as $A = H + S$, where**

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

- **Transform $Ax \equiv (H + S)x = b$ into**

$$\begin{aligned} (I + H^{-1}S)x &= H^{-1}b \quad \textbf{or} \\ (I + H^{-1/2}SH^{-1/2})H^{1/2}x &= H^{-1/2}b. \end{aligned}$$

- **Apply CG or Lanczos**

Then we obtain the generalized CG or Lanczos method.

Requirements:

H is strongly dominant over S:
$\|H^{-1}S\|$ or $\|H^{-1/2}SH^{-1/2}\|$ is quite small !

In general, we can apply the Krylov subspace methods (e.g., GMRES, etc.) to the linear system (1).

But now good preconditioners (or splitting matrices) are usually needed !

3. Hermitian/skew-Hermitian splitting (HSS)

Any $A \in \mathbb{C}^{n \times n}$ naturally possesses the splitting

$$A = H + S,$$

where

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

We call this splitting the Hermitian and skew-Hermitian (HS) splitting (HSS) of the matrix A.

And we will study efficient iterative methods based on this particular HS splitting for solving the linear system.

HSS As Preconditioners

- H **is dominant:**

$$A = H(I + H^{-1}S), \quad \textbf{thus} \quad A^{-1} = (I + H^{-1}S)^{-1}H^{-1}.$$

Replace $(I + H^{-1}S)^{-1}$ **by** $I - H^{-1}S$**.**
Then $(I - H^{-1}S)H^{-1}$ **is a preconditioner to** A**.**

- S **is dominant:**
Invert the shifted skew-Hermitian matrix $\alpha I + S$**.**
Then employ $(I - (S + \alpha I)^{-1}(H - \alpha I))(S + \alpha I)^{-1}$ **as a preconditioner to** A**.**

Drawbacks:

- **Require either** H **or** S **be strongly dominant;**
- **Need exact inverses of** H **or** $\alpha I + S$**;**
- **Need to estimate the optimal parameter** α**.**

HSS Iteration [B./Golub/Ng SIMAX(2003)]

Given initial guess $x^{(0)}$.
For $k = 0, 1, 2, \ldots$ until $\{x^{(k)}\}$ converges, compute

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

where $\alpha > 0$ is a given parameter.

Properties of HSS:

- **Alternates between H and S, analog. to ADI for PDE;**
- **Converges unconditionally;**
- **Upper bound of the contraction factor is dependent on the spectrum of H, but is independent of the spectrum of S as well as the eigenvectors of H, S and A;**
- **Optimal α for the upper bound of the contraction factor can be determined by the lower and the upper eigenvalue bounds of H.**

Convergence Theorem of HSS

Theorem. $A \in \mathbb{C}^{n\times n}$ **is positive definite,** $\alpha > 0$**. Then the iteration matrix** $M(\alpha)$ **of HSS is:**

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

and $\rho(M(\alpha))$ **is bounded by**

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

where $\lambda(H)$ **is the spectral set of** H**.**

Therefore,

$$\rho(M(\alpha)) \le \sigma(\alpha) < 1, \quad \forall \alpha > 0,$$

i.e., HSS converges unconditionally to x_* **of** $Ax = b$**.**

Corollary. **Let $\gamma_{\min}$ and $\gamma_{\max}$ be the minimum and the maximum eigenvalues of H, resp., and $\alpha > 0$. Then**

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

and

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

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

Remarks for the Corollary

- **The optimal α^* only minimizes the upper bound $\sigma(\alpha)$, not the spectral radius itself;**
- **When the α^* is employed, the upper bound of the convergence rate of HSS is about the same as that of CG, and it does become the same when, in particular, A is Hermitian;**
- **When A is normal, $HS = SH$, and hence,**

$$\rho(M(\alpha)) = \sigma(\alpha).$$

  The optimal α^* then minimizes both of these quantities.

Application to Model Convection-Diffusion Equation

Consider the 3D convection-diffusion equation:

$$-(u_{xx}+u_{yy}+u_{zz})+q(u_x+u_y+u_z)=f$$

on the unit cube $\Omega = [0,1]\times[0,1]\times[0,1]$**, with constant coefficient** q**, and subject to Dirichlet-type boundary conditions.**

For the classical 7-point centered difference scheme with equidistant step-size $h = \frac{1}{m+1}$, the coefficient matrix satisfies

$$A = T_x \otimes I \otimes I + I \otimes T_y \otimes I + I \otimes I \otimes T_z,$$

where

$$\begin{aligned} T_x &= \textbf{tridiag}(-1-r, 6, -1+r), \\ T_y &= \textbf{tridiag}(-1-r, 0, -1+r), \\ T_z &= \textbf{tridiag}(-1-r, 0, -1+r), \end{aligned}$$

with $r = \frac{qh}{2}$.

Theorem. **If** $\{x^{(k)}\}$ **is generated by HSS, then it satisfies**

$$|||x^{(k+1)} - x_*||| \leq \left[1 - \pi h + \frac{1}{2}\pi^2 h^2 + \mathcal{O}(h^3)\right] \cdot |||x^{(k)} - x_*|||,$$

where $|||\cdot|||$ **is defined by**

$$|||x||| = \|(\alpha I + S)x\|_2.$$

4. Normal/Skew-Hermitian Splitting (NSS)

HSS can be extended to the NSS [B./Golub/Ng (2002)]

$$A = N + S_o,$$

where

N : **normal**, S_o : **skew-Hermitian**.

Theorems are similar but choice of α is more delicate.

5. Positive-Definite/Skew-Hermitian Splitting(PSS)

Further extension:

$$A = P + S,$$

where

$P:$ **positive-definite**, $S:$ **skew-Hermitian**.

PSS Iteration Method **[B./Golub/Lu/Yin SISC(2005)]**

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

where $\alpha > 0$ **is given positive constant.**

Convergence Theorem of PSS

Theorem. **Let $A \in \mathbb{C}^{n\times n}$ be a positive definite matrix. Then the iteration matrix $M(\alpha)$ of PSS is:**

$$M(\alpha) = (\alpha I + S)^{-1}(\alpha I - P)(\alpha I + P)^{-1}(\alpha I - S).$$

Define

$$V(\alpha) = (\alpha I - P)(\alpha I + P)^{-1}.$$

Then $\rho(M(\alpha))$ is bounded by $\|V(\alpha)\|_2$. Therefore,

$$\rho(M(\alpha)) \le \|V(\alpha)\|_2 < 1, \quad \forall \alpha > 0,$$

i.e., the PSS converges unconditionally to the exact solution of (1).

Choices of P:

If

$$A = H + \widetilde{S} = (D + L_H + L_H^*) + \widetilde{S},$$

where L_H is the strictly (block) lower triangular matrix of H, then we can choose

$$P = D + 2L_H \quad \textbf{and} \quad S = L_H^* - L_H + \widetilde{S},$$

or

$$P = D + 2L_H^* \quad \textbf{and} \quad S = L_H - L_H^* + \widetilde{S}.$$

P is (block) triangular !

6. Block Triangular/Skew-Hermitian Splitting(BTSS)

Assume that A is a block matrix, and D, L and U are its block diagonal, strictly block lower triangular and strictly block upper triangular parts.

$$A = T + S,$$

$$T = T_\ell, \quad S = S_\ell, \qquad \ell = 1, 2, 3, 4.$$

$$
\begin{aligned}
A &= (L + D + U^*) + (U - U^*) \equiv T_1 + S_1 \\
&= (L^* + D + U) + (L - L^*) \equiv T_2 + S_2 \\
&= \left(L + \frac{1}{2}(D + D^*) + U^*\right) + \left(\frac{1}{2}(D - D^*) + U - U^*\right) \\
&\equiv T_3 + S_3 \\
&= \left(L^* + \frac{1}{2}(D + D^*) + U\right) + \left(\frac{1}{2}(D - D^*) + L - L^*\right) \\
&\equiv T_4 + S_4
\end{aligned}
$$

Applying PSS to these splittings we obtain the BTSS iteration methods.

Properties of BTSS:

- **Only need to solve block-triangular linear sub-systems, rather than to invert a shifted positive-definite matrix as in PSS or shifted Hermitian (normal) positive-definite matrix as in HSS (NSS);**
- **The block-triangular linear sub-systems can be solved recursively;**
- **The matrices T_ℓ, $\ell = 1, 2, 3, 4$, may be much more sparse than the matrices H and N involved in HSS and NSS.**

Specialization to Block 2-by-2 Matrices:

$$A = \begin{bmatrix} W & F \\ E & N \end{bmatrix} \quad \textbf{positive definite},$$

where

$$W \in \mathbb{C}^{q\times q} \quad \textbf{and} \quad N \in \mathbb{C}^{(n-q)\times(n-q)}$$

are both positive definite.

$$
\begin{aligned}
A &= \begin{bmatrix} W & 0 \\ E + F^* & N \end{bmatrix} + \begin{bmatrix} 0 & F \\ -F^* & 0 \end{bmatrix} \equiv T_1 + S_1 \\
&= \begin{bmatrix} W & E^* + F \\ 0 & N \end{bmatrix} + \begin{bmatrix} 0 & -E^* \\ E & 0 \end{bmatrix} \equiv T_2 + S_2
\end{aligned}
$$

$$
\begin{aligned}
A &= \begin{bmatrix} \frac{1}{2}(W+W^*) & 0 \\ E+F^* & \frac{1}{2}(N+N^*) \end{bmatrix} \\
&\qquad + \begin{bmatrix} \frac{1}{2}(W-W^*) & F \\ -F^* & \frac{1}{2}(N-N^*) \end{bmatrix} \equiv T_3 + S_3 \\
&= \begin{bmatrix} \frac{1}{2}(W+W^*) & E^*+F \\ 0 & \frac{1}{2}(N+N^*) \end{bmatrix} \\
&\qquad + \begin{bmatrix} \frac{1}{2}(W-W^*) & -E^* \\ E & \frac{1}{2}(N-N^*) \end{bmatrix} \equiv T_4 + S_4.
\end{aligned}
$$

The first half-step of BTSS can be easily solved as T is block triangular.

The second half-step of BTSS requires the solution of linear systems of the form

$$\left\{\begin{array}{lcl} \alpha u^{(k+1)} + F p^{(k+1)} & = & (\alpha I - W) u^{(k+\frac{1}{2})} + f, \\ -F^* u^{(k+1)} + \alpha p^{(k+1)} & = & -(E + F^*) u^{(k+\frac{1}{2})} \\ & & +(\alpha I - N) p^{(k+\frac{1}{2})} + g. \end{array}\right.$$

When $n \leq 2q$, we may first solve the Hermitian positive definite system of linear equations

$$
\begin{aligned}
(\alpha^2 I + F^* F) p^{(k+1)} = & -(\alpha E + F^* W) u^{(k+\frac{1}{2})} \\
& + \alpha(\alpha I - N) p^{(k+\frac{1}{2})} + F^* f + \alpha g,
\end{aligned}
$$

and then compute

$$
u^{(k+1)} = \frac{1}{\alpha}\left(-F p^{(k+1)} + (\alpha I - W) u^{(k+\frac{1}{2})} + f\right).
$$

And when $n \geq 2q$, we may first solve the Hermitian positive definite system of linear equations

$$(\alpha^2 I + FF^*)u^{(k+1)} = (\alpha(\alpha I - W) + F(E + F^*))u^{(k+\frac{1}{2})}$$

$$-F(\alpha I - N)p^{(k+\frac{1}{2})} + \alpha f - Fg,$$

and then compute

$$p^{(k+1)} = \frac{1}{\alpha}\Big(F^* u^{(k+1)} - (E + F^*)u^{(k+\frac{1}{2})}$$

$$+ (\alpha I - N)p^{(k+\frac{1}{2})} + g\Big).$$

7. Numerical Results

Example A

$A \in \mathbb{R}^{n\times n}$ **is the upwind difference matrix of the 2D convection-diffusion equation**

$$-(u_{xx}+u_{yy})+q\cdot\exp(x+y)(xu_x+yu_y)=f(x,y)$$

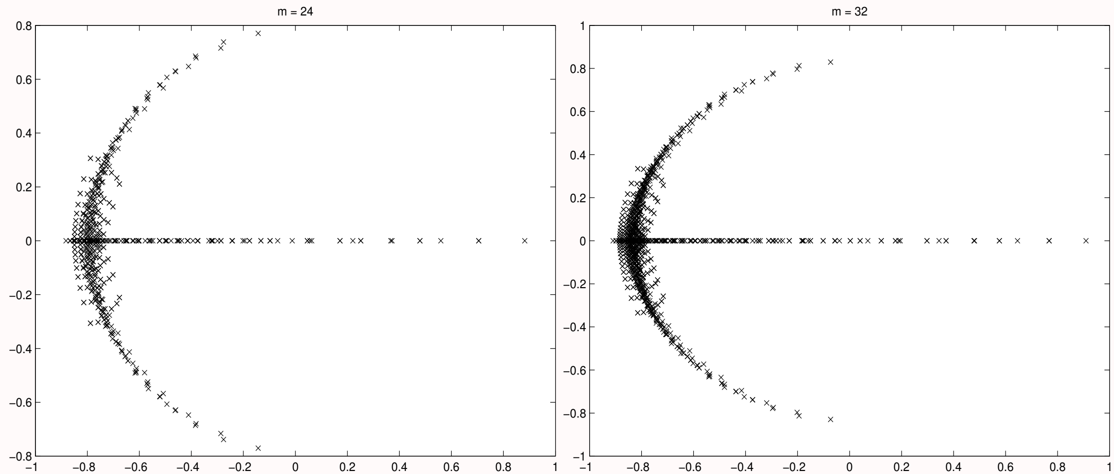
on the unit square $\Omega=[0,1]\times[0,1]$**, with zero Dirichlet boundary conditions. The stepsizes along both** x **and** y **directions are the same, i.e.,** $h=\frac{1}{m+1}$**.**

α_{exp} versus $\rho(M(\alpha_{\text{exp}}))$ when $q = 1$ for Example A

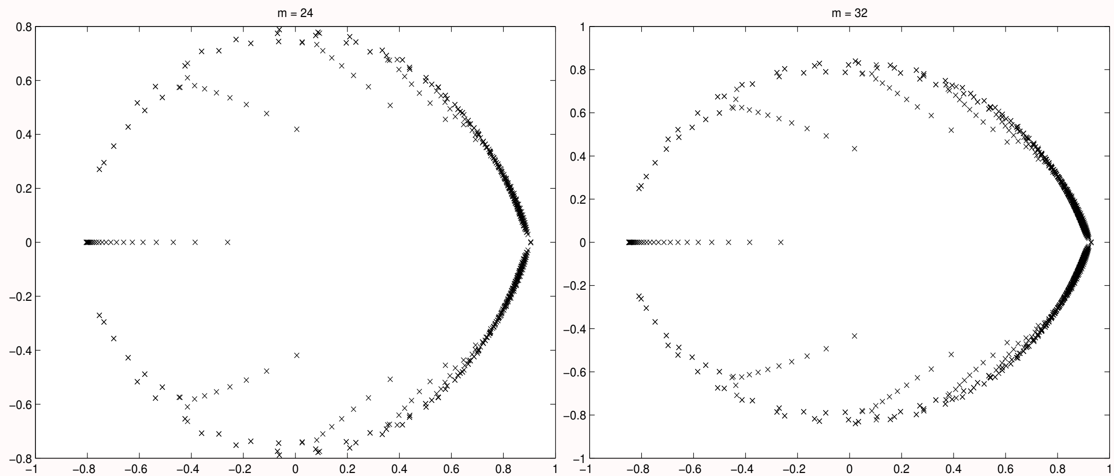
m		**8**	**16**	**24**	**32**	**64**
TSS	α_{exp}	**1.118**	**0.619**	**0.424**	**0.322**	**0.163**
	$\rho(M(\alpha_{\text{exp}}))$	**0.723**	**0.858**	**0.905**	**0.929**	**0.964**
HSS	α_{exp}	**1.054**	**0.595**	**0.413**	**0.316**	**0.163**
	$\rho(M(\alpha_{\text{exp}}))$	**0.706**	**0.837**	**0.882**	**0.909**	**0.953**

IT and CPU when $q = 1$ for Example A

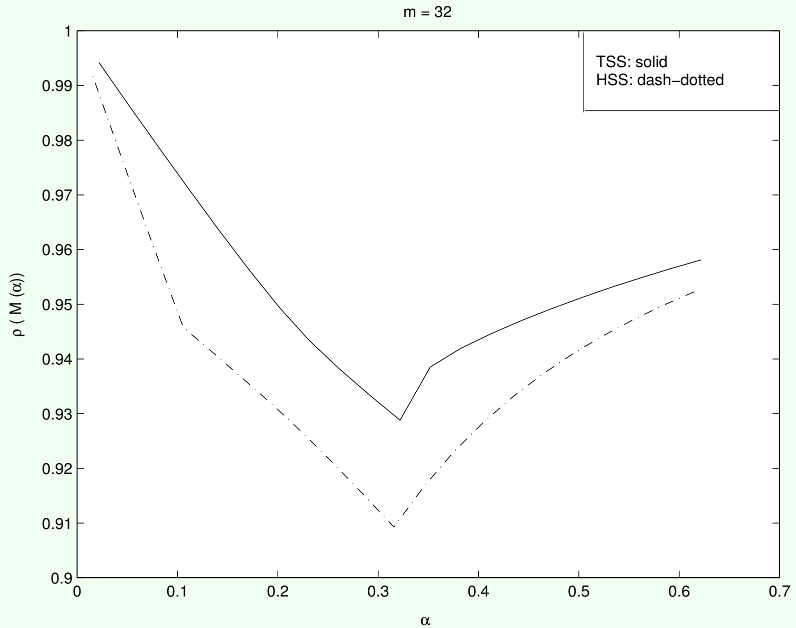
m		8	16	24	32	64
TSS	IT	31	56	83	113	234
	CPU	0.009	0.453	4.78	48.095	75.948
HSS	IT	24	51	82	108	214
	CPU	0.019	0.825	17.954	87.906	115.606
speed-up		2.11	1.82	3.76	1.83	1.52



The eigenvalue distributions of the HSS iteration matrices when $q = 1$, and $m = 24$ (left) and $m = 32$ (right)



The eigenvalue distributions of the TSS iteration matrices when $q = 1$, and $m = 24$ (left) and $m = 32$ (right)



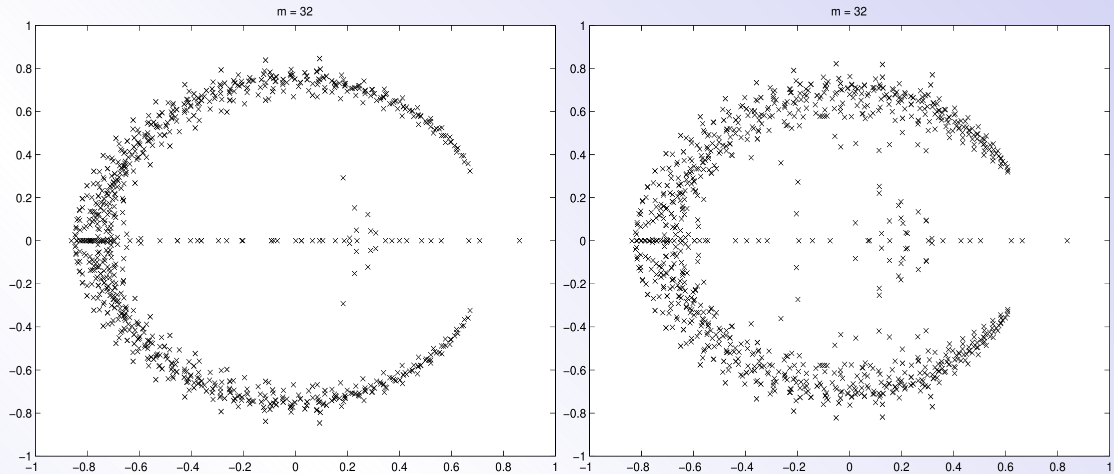
Curves of $\rho(M(\alpha))$ versus α with $q = 1$

α_{exp} **versus** $\rho(M(\alpha_{\text{exp}}))$ **when** $m = 32$ **for Example A**

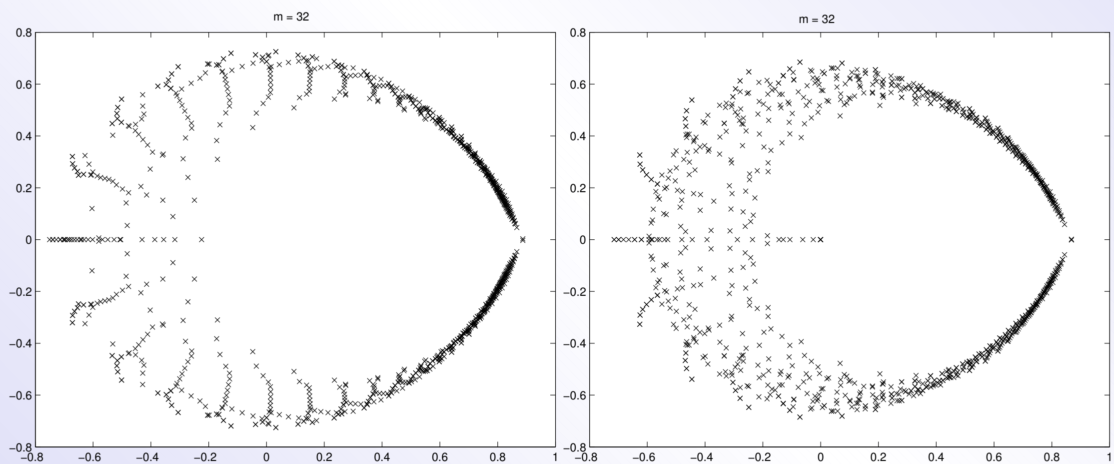
q		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
TSS	α_{exp}	**0.322**	**0.379**	**0.430**	**0.474**	**0.512**	**0.546**	**0.576**	**0.605**	**0.630**
	$\rho(M(\alpha_{\text{exp}}))$	**0.929**	**0.921**	**0.912**	**0.903**	**0.895**	**0.887**	**0.880**	**0.874**	**0.868**
HSS	α_{exp}	**0.316**	**0.286**	**0.285**	**0.298**	**0.315**	**0.331**	**0.346**	**0.360**	**0.373**
	$\rho(M(\alpha_{\text{exp}}))$	**0.909**	**0.903**	**0.892**	**0.882**	**0.871**	**0.862**	**0.853**	**0.845**	**0.837**

IT and CPU when $m = 32$ for Example A

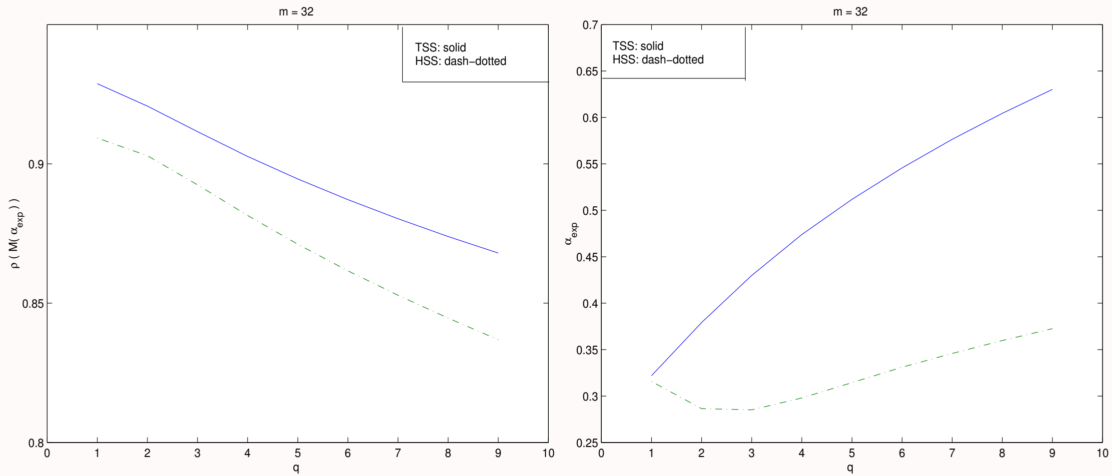
q		1	2	3	4	5	6	7	8	9
TSS	IT	113	98	95	91	88	83	79	79	76
	CPU	48.095	38.567	39.224	35.889	35.161	18.116	17.741	17.379	16.330
HSS	IT	108	106	99	91	82	83	71	72	65
	CPU	87.906	91.372	85.389	72.429	37.056	38.673	32.981	31.427	29.013
speed-up		1.83	2.37	2.18	2.02	1.05	2.13	1.86	1.81	1.78



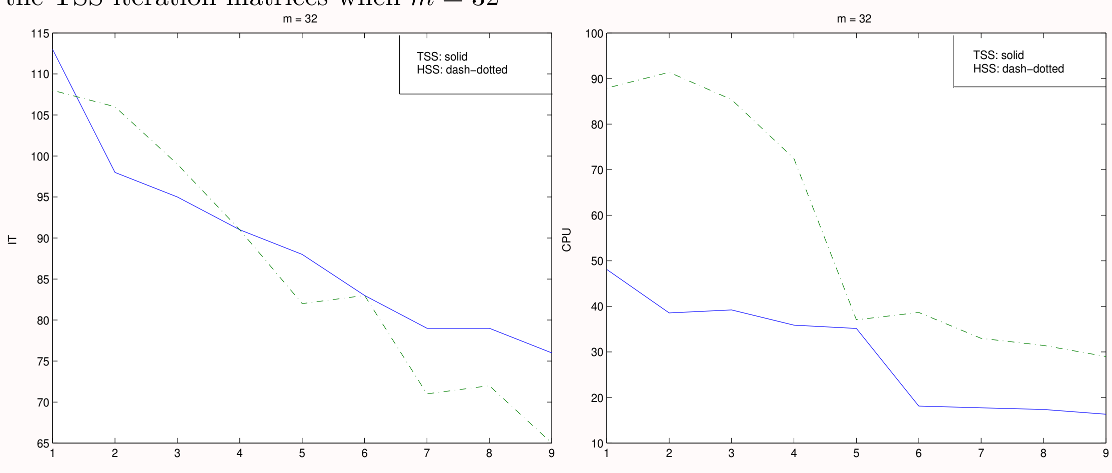
The eigenvalue distributions of the HSS iteration matrices when $m = 32$, and $q = 6$ (left) and $q = 9$ (right)



The eigenvalue distributions of the TSS iteration matrices when $m = 32$, and $q = 6$ (left) and $q = 9$ (right)



Curves of $\rho(M(\alpha_{\exp}))$ versus q (left) and $\alpha_{\exp}$ versus q (right) for the HSS and the TSS iteration matrices when $m = 32$



Curves of IT versus q (left) and CPU versus q (right) for the HSS and the TSS iteration matrices when $m = 32$

IT, CPU and RES for Example A

q		7		8		9	
m		32	64	32	64	32	64
TSS	$\alpha_{\exp}$	0.5762	0.3072	0.6041	0.3231	0.6303	0.3379
	IT	40	80	38	76	38	73
	CPU	0.35	19.96	0.33	19.00	0.32	18.96
GMRES(5)	IT	201	419	458	309	–	–
	CPU	1.54	65.52	3.51	55.07	–	–
	RES	–	–	–	–	4.32e-2	1.14e-2
GMRES(10)	IT	144	201	181	309	387	–
	CPU	0.95	34.80	1.19	55.07	2.58	–
	RES	–	–	–	–	–	8.76e-3
GMRES(15)	IT	151	178	161	309	200	346
	CPU	0.97	22.47	1.03	55.07	1.25	62.57
	RES	–	–	–	–	–	–
GMRES(20)	IT	120	163	178	231	179	218
	CPU	0.72	20.21	1.08	37.83	1.10	34.48
BiCGSTAB	IT	50	85	53	82	60	86
	CPU	0.54	27.34	0.57	26.67	0.65	25.11

IT and CPU when $q = 7$ for Example A

Methods	m	Preconditioners					
		TSS		ILU		UGS	
		IT	CPU	IT	CPU	IT	CPU
GMRES(5)	32	24	0.18	39	1.78	561	3.45
	64	28	3.66	140	96.70	362	142.74
GMRES(10)	32	22	0.12	27	1.59	410	2.41
	64	28	3.15	100	23.34	335	112.81
GMRES(15)	32	23	0.12	25	0.91	263	1.38
	64	28	2.90	58	32.31	391	123.82
GMRES(20)	32	20	0.09	19	0.65	189	0.97
	64	26	2.73	55	29.73	280	84.91
BiCGSTAB	32	14	0.12	21	1.22	101	0.92
	64	15	2.83	51	11.47	151	87.80

Example B

$$A = \begin{bmatrix} W & F\Omega \\ -F^T & N \end{bmatrix},$$

where

$W \in \mathbb{R}^{q\times q}$ **and** $N, \Omega \in \mathbb{R}^{(n-q)\times(n-q)}$**,**
with $2q > n$**.**

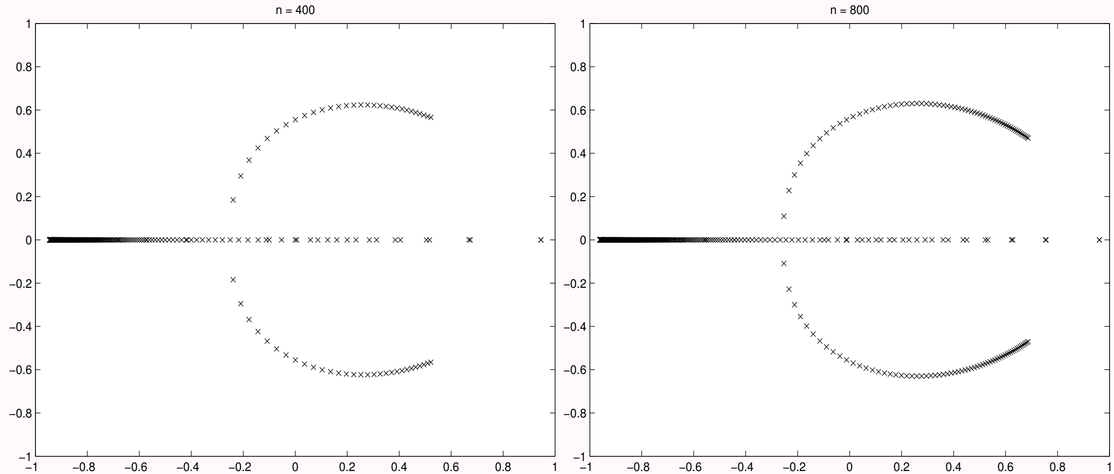
The matrices $W = (w_{k,j})$**,** $N = (n_{k,j})$**,** $F = (f_{k,j})$ **and** $\Omega = \mathbf{diag}(\omega_1, \ldots, \omega_{n-q})$ **are:**

$$w_{k,j} = \begin{cases} k+1, & \textbf{for} \quad j = k, \\ 1, & \textbf{for} \quad |k-j| = 1, \\ 0, & \textbf{otherwise}, \end{cases}$$

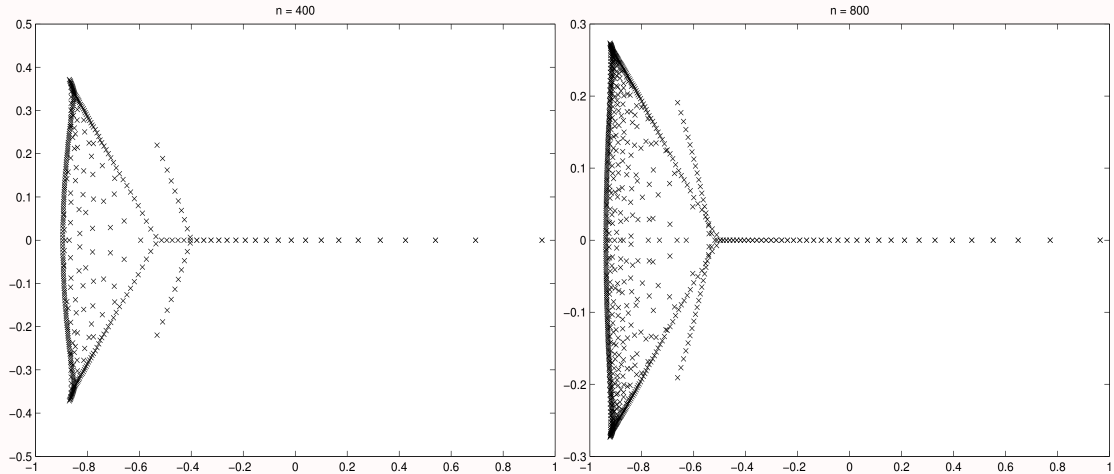
$$n_{k,j} = \begin{cases} k+1, & \textbf{for} \quad j = k, \\ 1, & \textbf{for} \quad |k-j| = 1, \\ 0, & \textbf{otherwise}, \end{cases}$$

$$f_{k,j} = \begin{cases} j, & \textbf{for} \quad k = j + 2q - n, \\ 0, & \textbf{otherwise}, \end{cases}$$

$$\omega_k = \frac{1}{k}.$$



The eigenvalue distributions of the HSS iteration matrices when $n = 400$ (left) and $n = 800$ (right)



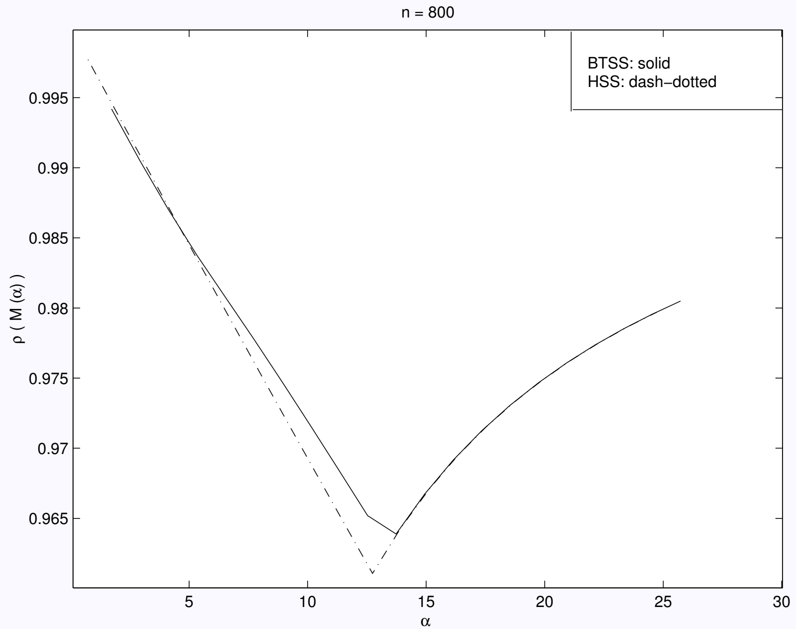
The eigenvalue distributions of the BTSS iteration matrices when $n = 400$ (left) and $n = 800$ (right)

α_{exp} and $\rho(M(\alpha_{exp}))$ for Example B

n		100	200	400	800	1600
BTSS	α_{exp}	4.865	6.874	9.713	13.733	19.418
	$\rho(M(\alpha_{exp}))$	0.901	0.929	0.949	0.964	0.974
HSS	α_{exp}	4.476	6.351	8.999	12.736	18.018
	$\rho(M(\alpha_{exp}))$	0.896	0.924	0.946	0.961	0.972

IT and CPU for Example B

n		100	200	400	800	1600
BTSS	IT	66	101	145	210	293
	CPU	0.064	0.402	2.991	39.869	208.375
HSS	IT	70	97	134	192	269
	CPU	0.133	0.967	6.635	69.744	394.706
speed-up		2.08	2.41	2.22	1.75	1.89



Curves of $\rho(M(\alpha))$ versus α for the HSS and the BTSS iteration matrices when $n = 800$

8. Concluding Remarks

- **We have established a series of unconditionally convergent splitting iteration methods, which present new solvers for non-Hermitian and positive definite linear systems**
- **The splitting iteration methods provide convergent smoothers for multigrid methods for non-Hermitian and positive definite linear systems**
- **Choice of the optimal iteration parameter α and efficient method for the shifted skew-Hermitian subsystem need in-depth study**

Thank you!