An implicitly-restarted Krylov subspace method for real symmetric/skew-symmetric eigenproblems

V. Simoncini

Dipartimento di Matematica, Università di Bologna
and CIRSA, Ravenna, Italy
valeria@dm.unibo.it

Joint work with
V. Mehrmann and C. Schröder (TU-Berlin)

The problem

Given

$M \in \mathbb{R}^{n\times n}$ symmetric ($M = M^\top$)

$N \in \mathbb{R}^{n\times n}$ skew-symmetric ($N = -N^\top$)

approximate selected (finite) eigenpairs

$$Mx = \lambda N x$$

Problem's features:

- Large dimension
- N may be singular
- The pencil $M - \lambda N$ is regular

Problem in context

Nomenclature and related problems:

alternating eigenproblem

generalized (or extended) Hamiltonian eigenproblem

skew-Hamiltonian / Hamiltonian eigenproblem

even / odd eigenproblem

Application problems:

Quadratic optimal or robust control problems

Passivity analysis

Model reduction

....

General characterization

$$Mx = \lambda N x$$

$\star$ Small scale problem well studied:

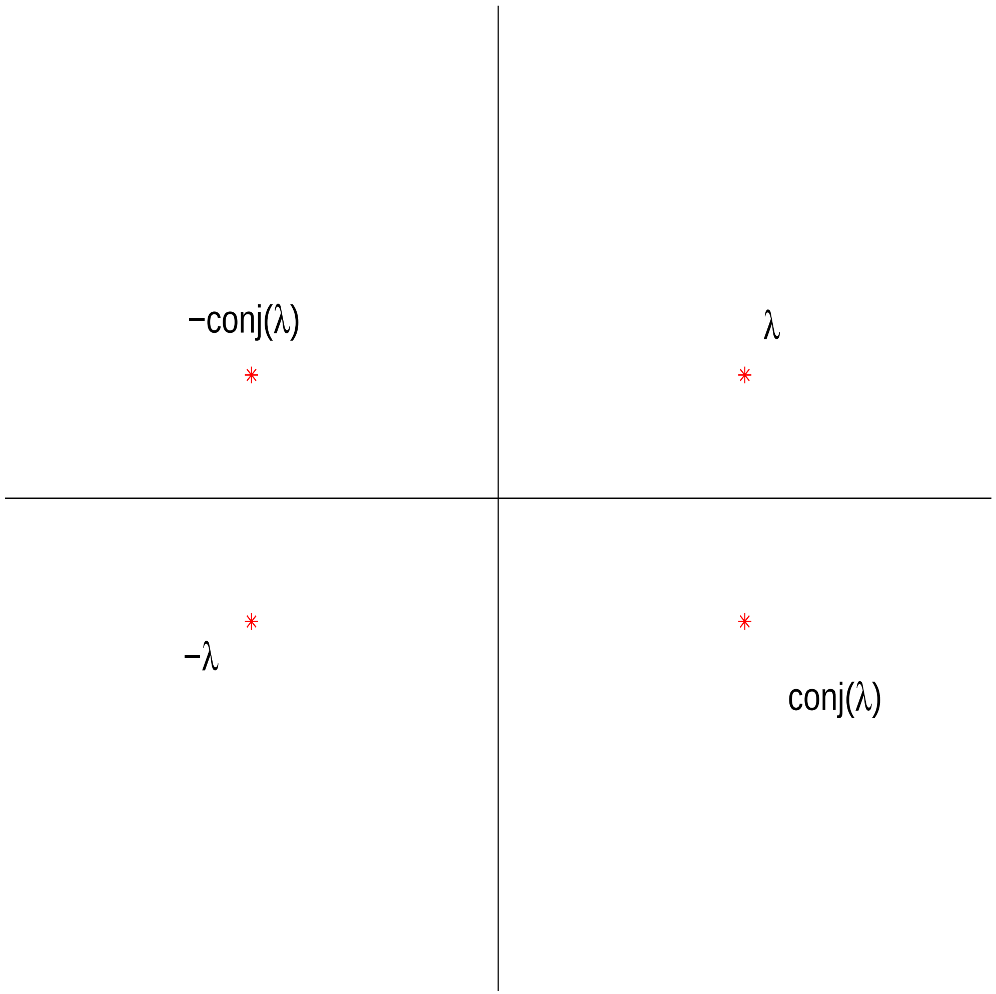
analysis, perturbation theory, software

(cf. Byers, Mehrmann, Xu, Benner, Kressner, Schröder, Watkins, etc.)

$\star$ Large scale problem less exercised, in particular for N singular

Peculiarity of the problem: spectrum has special symmetry wrto origin

General spectral characterization



Quadruples $(\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda})$

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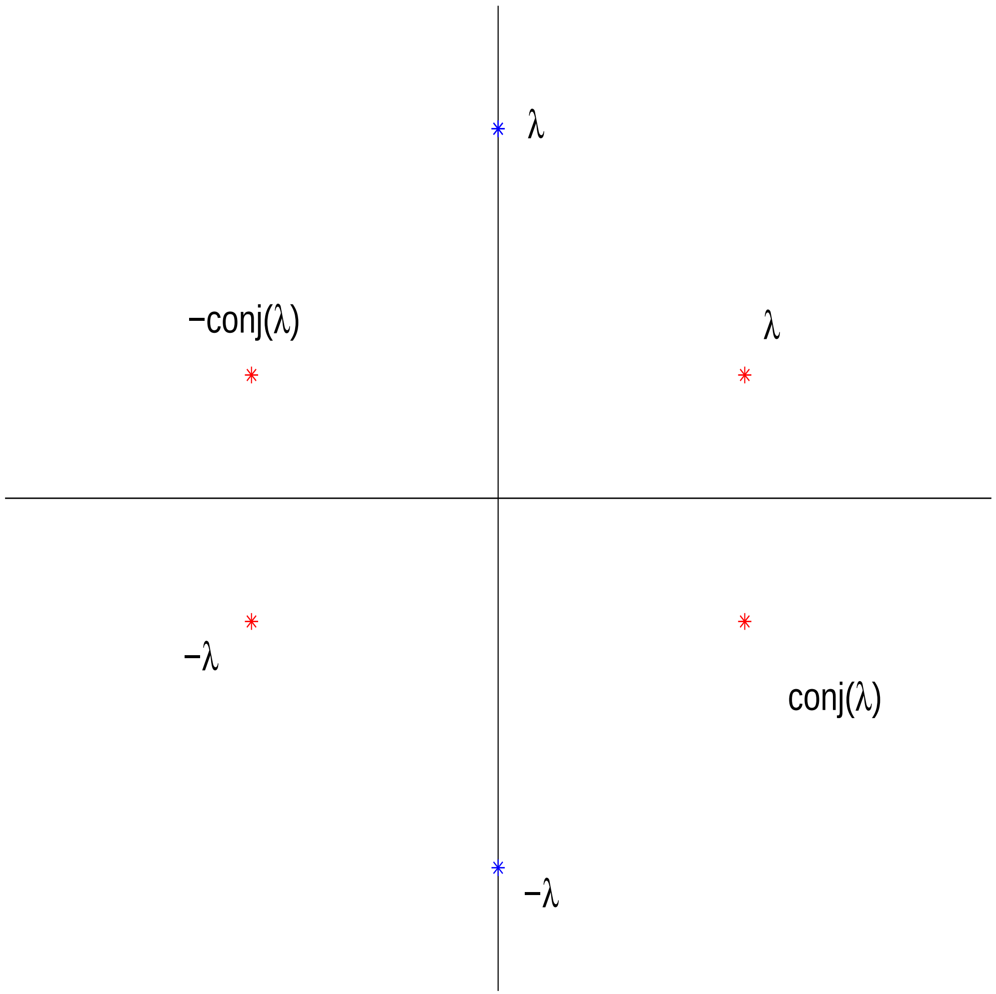

Quadruples $(\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda})$ Purely imaginary pairs $(\lambda, -\lambda)$

More details on structure

- For $N = -N^\top$, $M = M^\top$, the pencil

$$\alpha N - \beta M$$

is even: (α, β) same as $(-\alpha, \beta)$ + transposition

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(H is Hamiltonian if $(HJ)^\top = HJ$, with $J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$)

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(H is Hamiltonian if $(HJ)^\top = HJ$, with $J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$)

- If the pb dimension is $2k$ (even) then $\alpha N - \beta M$ is equivalent to the *skew-Hamiltonian / Hamiltonian* pencil

$$\alpha \mathcal{N} - \beta \mathcal{M}, \qquad \mathcal{N} = NJ^\top, \quad \mathcal{M} = MJ^\top$$

What may go wrong with an out-of-the-shelf solver

Approximate eigenpairs around selected value σ:

"shift-and-invert" Krylov subspace method: solve

$$(M - \sigma N)^{-1} N x = \eta x, \qquad \eta = \frac{1}{\lambda - \sigma}$$

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`eigs(M,N,10 i, tol)`, tol$=10^{-12}$ $(m = 20)$

After 5 cycles:

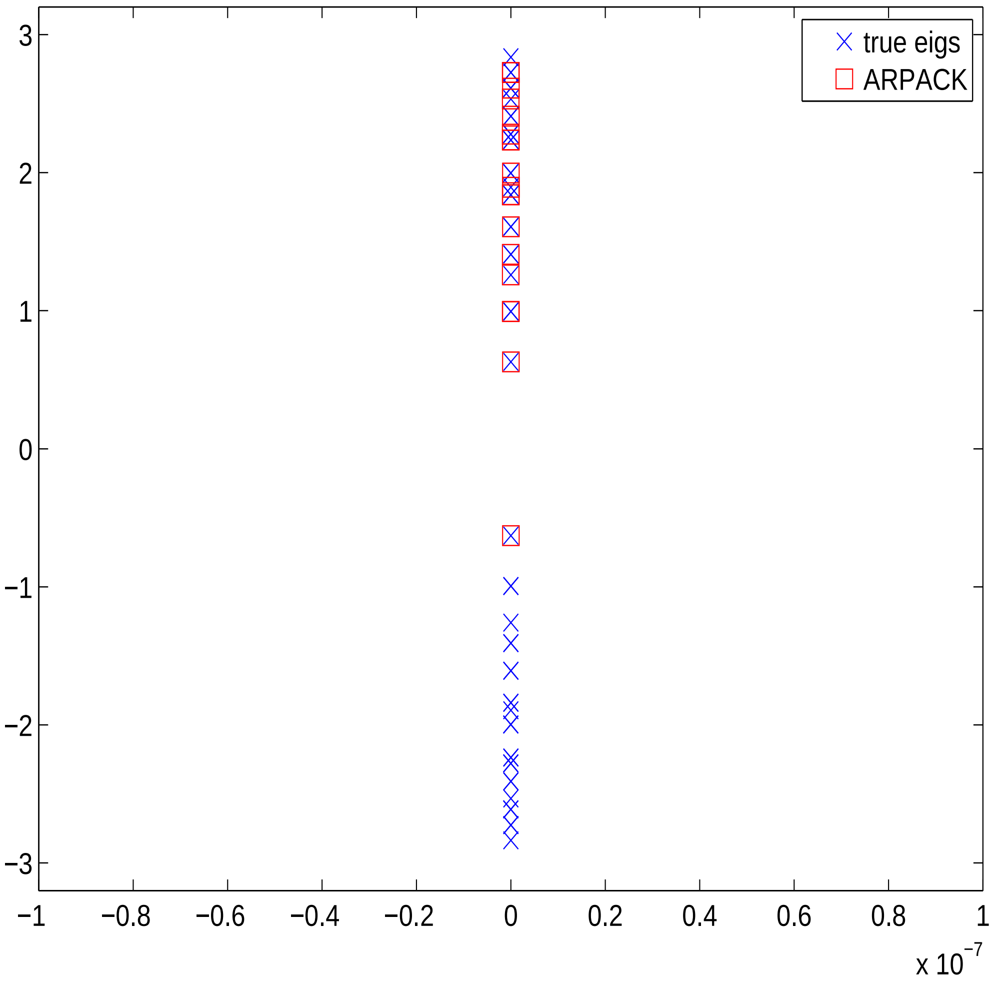
$$\begin{array}{rr} 10.544 + i2.2318 \cdot 10^{-10} & \text{residual} : 1.0013 \cdot 10^{-13} \\ -10.544 + i2.5349 \cdot 10^{-12} & \text{residual} : 5.7810 \cdot 10^{-14} \end{array}$$

both imaginary parts are small, but above residual norm !

$\Rightarrow$ Are these matching eigs?

What may go wrong with an out-of-the-shelf solver. II

Missing some of the requested (unmatching) eigenvalues:



Possible difficulties with spectral preserving solver

Assume for the moment that $N = J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$. Then the matrix

$$K := (M + \sigma J)^{-1} J (M - \sigma J)^{-1} J$$

is skew-Hamiltonian $\qquad (JK = -(JK)^\top)$

(cf. Mehrmann, Watkins, Benner, Faßbender, Stoll, Effenberger)

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$\Rightarrow$ Generate a *tall* matrix V such that

$$T = V^\top JKV$$

is skew-Hamiltonian and of lower dimension

(e.g. V portion of symplectic transf.)

$\Rightarrow$ Compute eig(T) with structure preserving method for dense pbs

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Problem: T is not skew-Hamiltonian to machine precision !

A convenient spectral transformation

$$Mx = \lambda N x$$

Given the target value σ (real or purely imaginary),

$$K := (M + \sigma N)^{-1} N (M - \sigma N)^{-1} N$$

$$Mx = \lambda N x \qquad \Rightarrow \qquad Kx = \theta x, \quad \text{with} \quad \theta = \frac{1}{\lambda^2 - \sigma^2}$$

(cf. SHIRA method, Mehrmann-Watkins '01)

λ close to σ $\qquad \Rightarrow \qquad$ θ large

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Natural search space for approximation:

$$\mathcal{K}_m(K, v_1) = \mathrm{span}\{v_1, K v_1, \ldots, K^{m-1} v_1\}$$

A convenient spectral transformation: basic properties

$$K = (M + \sigma N)^{-1} N (M - \sigma N)^{-1} N$$

i) $M + \sigma N = (M - \sigma N)^\top$

ii) the matrices $(M + \sigma N)^{-1} N$ and $(M - \sigma N)^{-1} N$ commute

iii) the matrix $K = (M + \sigma N)^{-1} N (M - \sigma N)^{-1} N$ satisfies

$$N K^\ell = -(N K^\ell)^\top, \quad \ell \in \mathbb{N},$$

that is, $N K^\ell$ is skew-symmetric for any natural number ℓ

In particular, $K^\top N = N K$

iv) If $\sigma \in \imath\mathbb{R}$, then $M + \sigma N = (M + \sigma N)^*$

A convenient spectral transformation: Pros and Cons

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Pros

- Matching eigs captured: $\pm\lambda = \pm\sqrt{\frac{1}{\theta} + \sigma^2}$, $\theta \in \Lambda(K)$
- Well established recurrence for $\mathcal{K}_m(K, v_1)$
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Cons

- All eigs of K are double! Only one instance should be retained (round-off plays against us)
- Search space with K in general not good for evecs of (M, N)
  x_-, x_+ matched evecs of (M, N) $\Rightarrow$ span$\{x_-, x_+\}$ invariant space of K
  but $\not\Leftarrow$

An important property to be exploited

Let (λ, x_+) be a simple eigenpair of (M, N) $\quad (\lambda \neq 0)$

Let $(-\lambda, x_-)$ be the matched eigenpair of (M, N)

Then

a) $x_+^\top N x_- \neq 0$

b) Let $\mathcal{V}$ be an N-neutral subspace of $\mathbb{C}^n$
   (i.e., $v^\top N w = 0$ for any $v, w \in \mathcal{V}$)
   If $u \in \operatorname{span}\{x_+, x_-\} \cap \mathcal{V}$, then no other linearly independent vector of span$\{x_+, x_-\}$ also belongs to $\mathcal{V}$

Fixing the cons

Pb.: All eigs of K are double!   Only one instance should be retained

Fix: Require that the search space be N-neutral

Arnoldi-type recursion

$$KV_m = V_m H_m + v_{m+1} h_{m+1,m} e_m^\top, \quad V_m^\top N V_m = O_m$$

Thanks to $NK^\ell = -(NK^\ell)^\top$, condition satisfied for free!

explicit enforcement of N-neutrality in finite precision arithm

Fixing the cons

Pb.: Search space with K in general not good for evecs of (M, N)

Fix: Enrich the space

Define $\quad W_m(\sigma) := (M - \sigma N)^{-1} N V_m$

Then

$$
\begin{aligned}
M[V_m, W_m(\sigma)] \begin{bmatrix} O_m & H_m \\ I_m & O_m \end{bmatrix} &= N[V_m, W_m(\sigma)] \begin{bmatrix} I_m & -\sigma H_m \\ \sigma I_m & I_m \end{bmatrix} \\
& \quad + [O_m, (M + \sigma N) v_{m+1} h_{m+1,m} e_m^\top].
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$\Rightarrow$ $[V_m, W_m(\sigma)]$ contains approximate invariant subspace of (M, N)

$\Rightarrow$ symmetric/ skew-sym structure preserved!

(multiply second block by $-H_m^\top$)

Approximate pairs

$$M[V_m, W_m(\sigma)] \begin{bmatrix} O_m & H_m \\ I_m & O_m \end{bmatrix} = N[V_m, W_m(\sigma)] \begin{bmatrix} I_m & -\sigma H_m \\ \sigma I_m & I_m \end{bmatrix} + [O_m, (M + \sigma N) v_{m+1} h_{m+1,m} e_m^\top].$$

Then

$$\left(\pm\hat{\lambda},\ \hat{x}_\pm(\sigma) \right) \qquad \hat{x}_\pm(\sigma) = [V_m, W_m(\sigma)] z_\pm(\sigma)$$

is an approximate eigenpair of (M, N), where

$$\begin{bmatrix} I_m & -\sigma H_m \\ \sigma I_m & I_m \end{bmatrix} z = \mu \begin{bmatrix} O_m & H_m \\ I_m & O_m \end{bmatrix} z$$

so that: $\hat{\lambda}_\pm = \pm\sqrt{\sigma^2 + \frac{1}{\mu}}$, $\qquad \hat{z}_\pm(\sigma) := \begin{bmatrix} I_m & -\sigma H_m \\ \sigma I_m & I_m \end{bmatrix} z(\sigma)$

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⋆ Further saving possible: recover z from evec's of $H_m = V_m^\top K V_m$

Implementation consideration

Problem: If σ is extremely close to $\hat{\lambda}_+$, then $\hat{x}_-(\sigma) \in \mathrm{range}(V_m)$

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In summary, we obtain approx eigenpairs:

$$\Big(+\hat{\lambda},\ [V_m, W_m(\sigma)] z_+(\sigma) \Big), \quad \Big(-\hat{\lambda},\ [V_m, W_m(-\sigma)] z_-(-\sigma) \Big)$$

Implicit restart

Krylov subspace of max size m with regular Arnoldi recursion

$$\Downarrow$$

Standard Krylov-Schur restarting (à la Stewart)

Note. Convergence is the same as that of IRA on matrix K

Algorithm Even-IRA

Require: v_1, maximum dimension m_{max}, restart size m_{res}

$V \leftarrow [v_1]$, $m \leftarrow 0$
while cycle 1,2,3,... **do**
    % Generation of the approximation space
    while $m < m_{max}$ **do**
        $m \leftarrow m + 1$
        $v \leftarrow K v_m$
        Orthogonalize v against V giving $H_{1:m,m}$, and v against NV
        $h_{m+1,m} \leftarrow \|v\|$, $v_{m+1} \leftarrow v/h_{m+1,m}$, $V \leftarrow [V, v_{m+1}]$
    end while
    % Contraction of approximation space and matrix
    $H_{1:m,1:m} \rightarrow QTQ^\top$ (real Schur form)
    Partition $T = \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{bmatrix}$, $Q = [Q_1, Q_2]$,
    $V \leftarrow [V_m Q_1, v_{m+1}]$, $H \leftarrow \begin{bmatrix} T_{11} \\ h_{m+1,m} e_m^\top Q_1 \end{bmatrix}$, $m \leftarrow m_{res}$
    % Eigenpair extraction
    Compute approximate eigenpairs and Check for convergence
end while

Example: linear quadratic optimal control problem

$$\min \int_{t_0}^{t_1} x^\top Q x + 2u^\top S x + u^\top R u \; dt, \qquad Q = Q^\top, R = R^\top$$

subject to the descriptor system

$$\begin{aligned} E\dot{x} &= Ax + Bu, \;\; x(0) = x^0 \\ y &= Cx, \end{aligned}$$

Under further conditions, a necessary condition for the existence of a stabilizing feedback controller requires eigeninfo closest to the imaginary axis of

$$L(\lambda) = \lambda N - M = \lambda \begin{bmatrix} 0 & E & 0 \\ -E^\top & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & A & B \\ A^\top & C^\top Q C & C^\top S \\ B^\top & S^\top C & R \end{bmatrix}.$$

Application problem: `rail_1357`, $R = 0 = Q$, $S = I$, A of size 1357, R of size 7

Example `rail_1357`, tol$=10^{-12}$, 6 matching eigs closest to σ

condest$(M - \sigma N) = 5.5 \cdot 10^{12}$ $m_{max} = 20/2 = 10$, 3 restarts

eigenvalue	residual norm	residual norm
	$\sigma = i10^{-5}$	$\sigma = 10^{-5}$
2.7062e-05	1.1674e-17	3.0662e-17
-2.7062e-05	7.7496e-18	6.7802e-18
8.8841e-05	6.0929e-17	6.2008e-17
-8.8841e-05	6.9922e-17	4.6029e-17
2.2710e-04	5.9494e-16	1.4799e-14
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Imaginary shift:

`eigs`: After 100 cycles ($m = 10$) $\lambda = \pm 2.2710 \cdot 10^{-4}$ with res norm $O(10^{-8})$ and $O(10^{-5})$

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Real shift:

`eigs`: After 1 cycle ($m = 20$) 2.7062e-05 (res norm 8.9218e-13), -2.7063e-05 (res norm 2.2999e-12), 8.8842e-05 (res norm 1.6850e-11)

Passivity test

Under certain conditions, a necessary condition for a control system to be "passive" is that

$$M - \lambda N = \begin{bmatrix} 0 & A & B & 0 \\ A^\top & 0 & 0 & C^\top \\ B^\top & 0 & -I & D^\top \\ 0 & C & D & -I \end{bmatrix} - \lambda \begin{bmatrix} 0 & I & 0 & 0 \\ -I & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

has no purely imaginary eigs

$\Rightarrow$ we will be content with very inaccurate eigenvalues!

coax1 (from Schröder-Stykel,'07)

$\sigma = 6i$, one cheap cycle

Even-IRA: $m = 12$: $\pm 6.0377i$, $\pm 6.0681i$ with res norm below 10^{-5}

Even-IRA: $m = 20$: $\pm 6.0377i$, $\pm 6.0681i$ with res norm below 10^{-8}

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IRA (our implementation of `eigs` with true residual norms):

m (tol)	eigenvalue	residual norm	n. cycles
12 (10^{-5})	9.5567e-09 + 6.0377 i	2.3684e-08	2
	-1.5054e-06 + 6.0681 i	3.9961e-07	2
20 (10^{-8})	3.2863e-13 + 6.0377 i	3.8536e-16	2
	-4.8055e-12 + 6.0681 i	3.9425e-13	2

Appendix: a seemingly related method

The new method seeks evec approximations in

$$\mathrm{range}([V_m, W_m(\sigma)]), \qquad W_m(\sigma) = (M - \sigma N)^{-1} N V_m$$

What about building directly the space $\mathrm{range}([V_m, W_m(\sigma)])$?

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Alternate multiplications by $(M - \sigma N)^{-1}N$ or by $(M + \sigma N)^{-1}N$:

$$\{v_1, (M - \sigma N)^{-1} N v_1, (M + \sigma N)^{-1} N (M - \sigma N)^{-1} N v_1, \ldots,$$
$$(M - \sigma N)^{-1} N \big((M + \sigma N)^{-1} N (M - \sigma N)^{-1} N\big)^{m-1} v_1, \ldots\}$$

$\Rightarrow$ rational Krylov subspace, with shifts $\pm\sigma$ as multiple poles

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$\Rightarrow$ rational Krylov subspace, with shifts $\pm\sigma$ as multiple poles

Note: Performance essentially similar to `eigs` on our problem

Concluding remarks

- "Matching preserving" method
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- Possible problem: ghost eigenvalues detected in certain artificial problem

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Paper:

An Implicitly-restarted Krylov Method for Real Symmetric/Skew-Symmetric Eigenproblems

Volker Mehrmann , Christian Schröder and V. Simoncini

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