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Thick-restart Arnoldi methods for the evaluation of matrix functions

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1 Problem

Given: $A \in \mathbb{C}^{n \times n}$, $\boldsymbol{b} \in \mathbb{C}^n$, $\boldsymbol{b} \neq \boldsymbol{0}$, f analytic in neighborhood of $\Lambda(A)$.

Sought: $f(A)\boldsymbol{b}$.

Original Motivation: Numerical simulation of transient electromagnetic (TEM) geophysical exploration (collaboration with Institute of Geophysics):

$$\boldsymbol{u}(t) = \exp(-tA)\boldsymbol{u}_0,$$

where A discretizes $\sigma^{-1}\nabla \times (\mu^{-1}\nabla \times \cdot\,)$ and is large and sparse.

Other Important Applications:
Exponential integrators: $\varphi_0(\lambda) = \exp(-t\lambda)$, $\varphi_{j+1}(\lambda) = \frac{\varphi_j(t\lambda)-\varphi_j(0)}{t\lambda}$.
Lattice quantum chromodynamics: $\operatorname{sign}(\lambda)$.
Time-dependent hyperbolic problems: trigonometric functions.

- The Arnoldi method projects the problem of evaluating $f(A)\boldsymbol{b}$ onto a sequence of m-dimensional Krylov subspaces.
- The cost of storing (and computing) the basis vectors of these spaces increases with m.
- It is possible to restart the Arnoldi method after a fixed dimension m similar to linear systems or eigenproblems.
- Restarting usually results in slower convergence.
- How can we compensate for the loss of information that occurs upon restarting by retaining a judiciously chosen part of the previously generated spaces?

Outline

- Problem
- Three ways to generate Krylov subspace approximations
- Thick restarts
- Convergence
- A numerical example
- Summary

2 Three ways to generate Krylov subspace approximations

- Krylov subspace methods generate approximants $\boldsymbol{y}_m$ of $f(A)\boldsymbol{b}$ with

  $\boldsymbol{y}_m \in \mathscr{K}_m(A, \boldsymbol{b}) := \operatorname{span}\{\boldsymbol{b}, A\boldsymbol{b}, \ldots, A^{m-1}\boldsymbol{b}\} = \{q(A)\boldsymbol{b} \,:\, q \in \mathscr{P}_{m-1}\}.$

- There are usually based on Arnoldi-like decompositions of A,

$$AW_m = W_m H_m + h_{m+1,m}\boldsymbol{w}_{m+1}\boldsymbol{e}_m^T,$$

  where $\operatorname{colspan}(W_m) = \mathscr{K}_m(A, \boldsymbol{b})$, $\beta W_m \boldsymbol{e}_1 = \boldsymbol{b}$, H_m is unreduced upper Hessenberg.

- Most prominent example: (proper) Arnoldi decomposition, $AV_m = V_m H_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^T$, where $V_m^H V_m = I_m$.

- restarted Arnoldi: k standard Arnoldi decompositions of A

$$AV_j = V_j H_j + h_{j+1} \boldsymbol{v}_{jm+1} \boldsymbol{e}_m^T, \quad j = 1, 2, \ldots, k,$$

wrt the m-dim. Krylov spaces $\mathscr{K}_m(A, \boldsymbol{v}_{(j-1)m+1})$, glued together,

$$A\widehat{V}_k = \widehat{V}_k \widehat{H}_k + h_{k+1} \boldsymbol{v}_{km+1} \boldsymbol{e}_{km}^T,$$

where $\widehat{V}_k := [V_1 \, V_2 \, \cdots \, V_k] \in \mathbb{C}^{n \times km}$,

$$\widehat{H}_k := \begin{bmatrix} H_1 & & & \\ E_2 & H_2 & & \\ & \ddots & \ddots & \\ & & E_k & H_k \end{bmatrix} \in \mathbb{C}^{km \times km}, \qquad E_j := h_j \boldsymbol{e}_1 \boldsymbol{e}_m^T \in \mathbb{R}^{m \times m},$$

cf. [E. & Ernst, 2006].

Projection: With $\beta \boldsymbol{w}_1 = \boldsymbol{b}$ set

$$\boldsymbol{y}_m^{(1)} := \beta W_m f(H_m) \boldsymbol{e}_1 \in \mathscr{K}_m(A, \boldsymbol{b}).$$

Cauchy integral: $f(A)\boldsymbol{b} = \frac{1}{2\pi i} \int_\Gamma f(\lambda) \boldsymbol{x}(\lambda)\, d\lambda$. Approximate $\boldsymbol{x}(\lambda) := (\lambda I - A)^{-1} \boldsymbol{b}$ by $\boldsymbol{z}_m(\lambda) = \beta W_m (\lambda I - H_m)^{-1} \boldsymbol{e}_1$ and set

$$\boldsymbol{y}_m^{(2)} := \frac{1}{2\pi i} \int_\Gamma f(\lambda) \boldsymbol{z}_m(\lambda)\, d\lambda.$$

Interpolation: Let $p_{m-1} \in \mathscr{P}_{m-1}$ be the interpolating polynomial (in Hermite's sense) for f at the eigenvalues of H_m and set

$$\boldsymbol{y}_m^{(3)} := p_{m-1}(A) \boldsymbol{b}.$$

Theorem 1 $\boldsymbol{y}_m^{(1)} = \boldsymbol{y}_m^{(2)} = \boldsymbol{y}_m^{(3)}$

cf. [Hochbruck & Hochstenbach, 2005]

- Arnoldi approximation [Druskin & Knizhnerman, 1989], [Saad, 1992]

$$\boldsymbol{f}_m = p_{m-1}(A)\boldsymbol{b} = \frac{1}{2\pi i}\int_\Gamma f(\lambda)\boldsymbol{z}_m(\lambda)\,d\lambda = \beta V_m f(H_m)\boldsymbol{e}_1,$$

where $p_{m-1} \in \mathscr{P}_{m-1}$ interpolates f at the Ritz values of A wrt $\mathscr{K}_m(A, \boldsymbol{b})$, where $\boldsymbol{z}_m(\lambda)$ is the FOM approximation to $(\lambda I_n - A)\boldsymbol{x}(\lambda) = \boldsymbol{b}$.

- Restarted Arnoldi approximation [E. & Ernst, 2006], [Niehoff, 2006]

$$\widehat{\boldsymbol{f}}_k = \widehat{p}_k(A)\boldsymbol{b} = \frac{1}{2\pi i}\int_\Gamma f(\lambda)\widehat{\boldsymbol{z}}_k(\lambda)\,d\lambda = \beta \widehat{V}_k f(\widehat{H}_k)\boldsymbol{e}_1,$$

where $\widehat{p}_k \in \mathscr{P}_{km-1}$ interpolates f at the Ritz values of A wrt $\mathscr{K}_m(A, \boldsymbol{v}_{(j-1)m+1})$ $(j = 1, 2, \ldots, k)$, where $\widehat{\boldsymbol{z}}_k(\lambda)$ is the FOM(m) approximation (after k cycles) to $(\lambda I_n - A)\boldsymbol{x}(\lambda) = \boldsymbol{b}$.

3 Thick restarts

- Compensate for the deterioration of convergence of Krylov subspace methods due to restarting by using nearly invariant subspaces to augment the Krylov subspace.
- Identify a subspace which slows convergence, approximate this space and eliminate its influence from the iteration process.
- In practice: Approximate eigenspaces which belong to eigenvalues close to singularities of f (for $f = \exp$, approximate eigenspaces which belong to "large" eigenvalues).
- Well known for eigenproblems [Wu & Simon, 2000], [Stewart, 2001] and linear systems [Morgan, 2002]. For matrix functions, first proposed by [Niehoff, 2006].

Thick-restart procedure

- Starting point: $\mathscr{K}_m(A, \boldsymbol{b})$ with Arnoldi decomposition

$$AV_1 = V_1 H_1 + h_2 \boldsymbol{v}_{m+1} \boldsymbol{e}_m^T.$$

- Compute ℓ-dimensional H_1-invariant subspace,

$$H_1 \, [X_1 \; *] = [X_1 \; *] \begin{bmatrix} U_1 & * \\ O & * \end{bmatrix}$$

(partial Schur decomposition), i.e., $U_1 \in \mathbb{C}^{\ell \times \ell}$ is upper triangular, $X_1 \in \mathbb{C}^{m \times \ell}$ has orthonormal columns.
Set $Y_1 := V_1 X_1$. Then

$$AY_1 = Y_1 U_1 + h_2 \boldsymbol{v}_{m+1} \boldsymbol{u}_1^T, \text{ where } \boldsymbol{u}_1 = X_1^T \boldsymbol{e}_\ell \in \mathbb{C}^\ell \text{ (dense!)}.$$

- Extend by m Arnoldi steps

$$A\,[Y_1\ V_2] = [Y_1\ V_2] \begin{bmatrix} U_1 & G_2 \\ h_2\,\boldsymbol{e}_1\,\boldsymbol{u}_1^T & H_2 \end{bmatrix} + h_3\,\boldsymbol{v}_{2m+1}\,\boldsymbol{e}_{\ell+m}^T,$$

where $[Y_1\ V_2\ \boldsymbol{v}_{2m+1}]$ has orthonormal columns, $V_2\,\boldsymbol{e}_1 = \boldsymbol{v}_{m+1}$, $H_2 \in \mathbb{C}^{m\times m}$ is upper Hessenberg.

- Known [Morgan, 2002]: $\mathrm{colspan}([Y_1\ V_2]) = \mathscr{K}_{\ell+m}(A, s(A)\boldsymbol{b})$, where

$$s(\lambda) = \prod_{\mu\in\Lambda(H_1)\setminus\Lambda(U_1)} (\lambda - \mu) \in \mathscr{P}_{m-\ell}$$

(implicitly restarted Arnoldi [Sorensen, 1992]).

- If $A = A^H$: U_1 is diagonal, H_2 is symmetric tridiagonal, $G_2 = h_2\overline{\boldsymbol{u}}_1\,\boldsymbol{e}_1^T$.

- Second sweep: Compute ℓ-dimensional invariant subspace,

$$\begin{bmatrix} U_1 & G_2 \\ h_2 \boldsymbol{e}_1 \boldsymbol{u}_1^T & H_2 \end{bmatrix} [X_2 \ *] = [X_2 \ *] \begin{bmatrix} U_2 & * \\ O & * \end{bmatrix}.$$

- With $Y_2 := [Y_1 \ V_2] X_2$,

$$AY_2 = Y_2 U_2 + h_3 \boldsymbol{v}_{2m+1} \boldsymbol{u}_2^T, \text{ where } \boldsymbol{u}_2 = X_2^T \boldsymbol{e}_{\ell+m} \in \mathbb{C}^\ell.$$

- Extend by m further Arnoldi steps

$$A [Y_2 \ V_3] = [Y_2 \ V_3] \begin{bmatrix} U_2 & G_3 \\ h_3 \boldsymbol{e}_1 \boldsymbol{u}_2^T & H_3 \end{bmatrix} + h_4 \boldsymbol{v}_{3m+1} \boldsymbol{e}_{\ell+m}^T,$$

where $[Y_2 \ V_3 \ \boldsymbol{v}_{3m+1}]$ has orthonormal columns, $V_3 \boldsymbol{e}_1 = \boldsymbol{v}_{2m+1}$, H_3 is upper Hessenberg.

We glue these decompositions together,

$$A\,[V_1\,Y_1\,V_2\,Y_2\,V_3] = [V_1\,Y_1\,V_2\,Y_2\,V_3]\left[\begin{array}{c||c|c||c|c} H_1 & O & O & O & O \\ \hline\hline O & U_1 & G_2 & O & O \\ \hline E_2 & F_2 & H_2 & O & O \\ \hline\hline O & O & O & U_2 & G_3 \\ \hline O & O & E_3 & F_3 & H_3 \end{array}\right]$$

$$+h_4\,\boldsymbol{v}_{3m+1}\,\boldsymbol{e}_{3m+2\ell}^T.$$

Here $E_j = h_j\,\boldsymbol{e}_1\,\boldsymbol{e}_m^T \in \mathbb{R}^{m\times m}$, $F_j = h_j\,\boldsymbol{e}_1\,\boldsymbol{u}_{j-1}^T \in \mathbb{C}^{m\times \ell}$.

After k sweeps, we arrive at a "thick-restart decomposition"

$$A\widetilde{V}_k = \widetilde{V}_k \widetilde{H}_k + h_{k+1} \boldsymbol{v}_{km+1} \boldsymbol{e}_{\widehat{k}}^T, \text{ where}$$

$$\widetilde{V}_k = [V_1 | Y_1 | V_2 | \cdots | Y_{k-1} | V_k] \in \mathbb{C}^{n \times \widehat{k}} \text{ has linearly dependent columns,}$$

$$\widetilde{H}_k = \left[\begin{array}{c|cc|cc|cc}
H_1 & & & & & & \\ \hline
 & U_1 & G_2 & & & & \\
E_2 & F_2 & H_2 & & & & \\ \hline
 & \ddots & & \ddots & & & \\ \hline
 & & & & & U_{k-1} & G_k \\
 & & & & E_k & F_k & H_k
\end{array}\right] \in \mathbb{C}^{\widehat{k} \times \widehat{k}}$$

is not Hessenberg ($\widehat{k} = km + (k-1)\ell$).

We need km mvm's to construct this decomposition.

From the decomposition $A\widetilde{V}_k = \widetilde{V}_k \widetilde{H}_k + h_{k+1} \boldsymbol{v}_{km+1} \boldsymbol{e}_{\widehat{k}}^T$, we define

$$\widetilde{\boldsymbol{f}}_k := \beta \widetilde{V}_k f(\widetilde{H}_k) \boldsymbol{e}_1.$$

Since $Y_1 = V_1 X_1$ and $Y_j = [Y_{j-1}\ V_j]\, X_j$ $(j = 2, \ldots, k)$, we write

$$\widetilde{V}_k = [V_1\, Y_1\, V_2\, \cdots\, Y_{k-1}\, V_k] = [V_1\, V_2\, \cdots\, V_k]\; C =: \widehat{V}_k C,$$

where $C \in \mathbb{C}^{mk \times \widehat{k}}$ has full row rank.
We have $CC^\dagger = I_{km}$ and $\boldsymbol{e}_{\widehat{k}}^T C^\dagger = \boldsymbol{e}_{km}$. Thus, by inserting

$$A\widehat{V}_k C = \widehat{V}_k C \widetilde{H}_k + h_{k+1} \boldsymbol{v}_{km+1} \boldsymbol{e}_{\widehat{k}}^T$$

or $$A\widehat{V}_k = \widehat{V}_k \left(C \widetilde{H}_k C^\dagger \right) + h_{k+1} \boldsymbol{v}_{km+1} \boldsymbol{e}_{\widehat{k}}^T C^\dagger =: \widehat{V}_k \widehat{H}_k + h_{k+1} \boldsymbol{v}_{km+1} \boldsymbol{e}_{km}^T$$

which is a valid Arnoldi-like decomposition, i.e., $\widehat{H}_k$ is upper Hessenberg and the columns of $\widehat{V}_k$ are linearly independent.

Theorem 2 *Given the thick-restart decomposition*

$$A\widetilde{V}_k = \widetilde{V}_k \, \widetilde{H}_k + h_{k+1} \boldsymbol{v}_{km+1} \boldsymbol{e}_{\widehat{k}}^T$$

(k-th sweep, i.e., after $k-1$ restarts, ℓ Ritz vectors per restart, m mvm per sweep) and the associated Arnoldi-like decomposition

$$A\widehat{V}_k = \widehat{V}_k \, \widehat{H}_k + h_{k+1} \boldsymbol{v}_{km+1} \boldsymbol{e}_{km}^T.$$

Then

$$\widetilde{\boldsymbol{f}}_k = \beta \, \widetilde{V}_k \, f(\widetilde{H}_k) \boldsymbol{e}_1 = \beta \, \widehat{V}_k \, f(\widehat{H}_k) \boldsymbol{e}_1.$$

Three interpretations:

Theorem 3 *For the thick-restart approximation there holds*

$$\widetilde{\boldsymbol{f}}_k = \beta \widetilde{V}_k f(\widetilde{H}_k)\boldsymbol{e}_1 = \widehat{p}_k(A)\boldsymbol{b} = \frac{1}{2\pi i}\int_\Gamma f(\lambda)\widehat{\boldsymbol{z}}_k^{(m,\ell)}(\lambda)\,d\lambda,$$

where $\widehat{p}_k \in \mathscr{P}_{km-1}$ *interpolates* f *in*

$$\Lambda(\widehat{H}_k) = \Lambda(\widetilde{H}_k) \setminus \left(\cup_{j=1}^{k-1}\Lambda(U_j)\right),$$

and where $\widehat{\boldsymbol{z}}_k^{(m,\ell)}(\lambda)$ *is the approximate solution of* $(\lambda I - A)\boldsymbol{x}(\lambda) = \boldsymbol{b}$ *which is generated by* k *sweeps of* $FOM(m,\ell)$ *(cf. [Morgan, 2002]).*

cf. [Niehoff, 2006]

4 Convergence

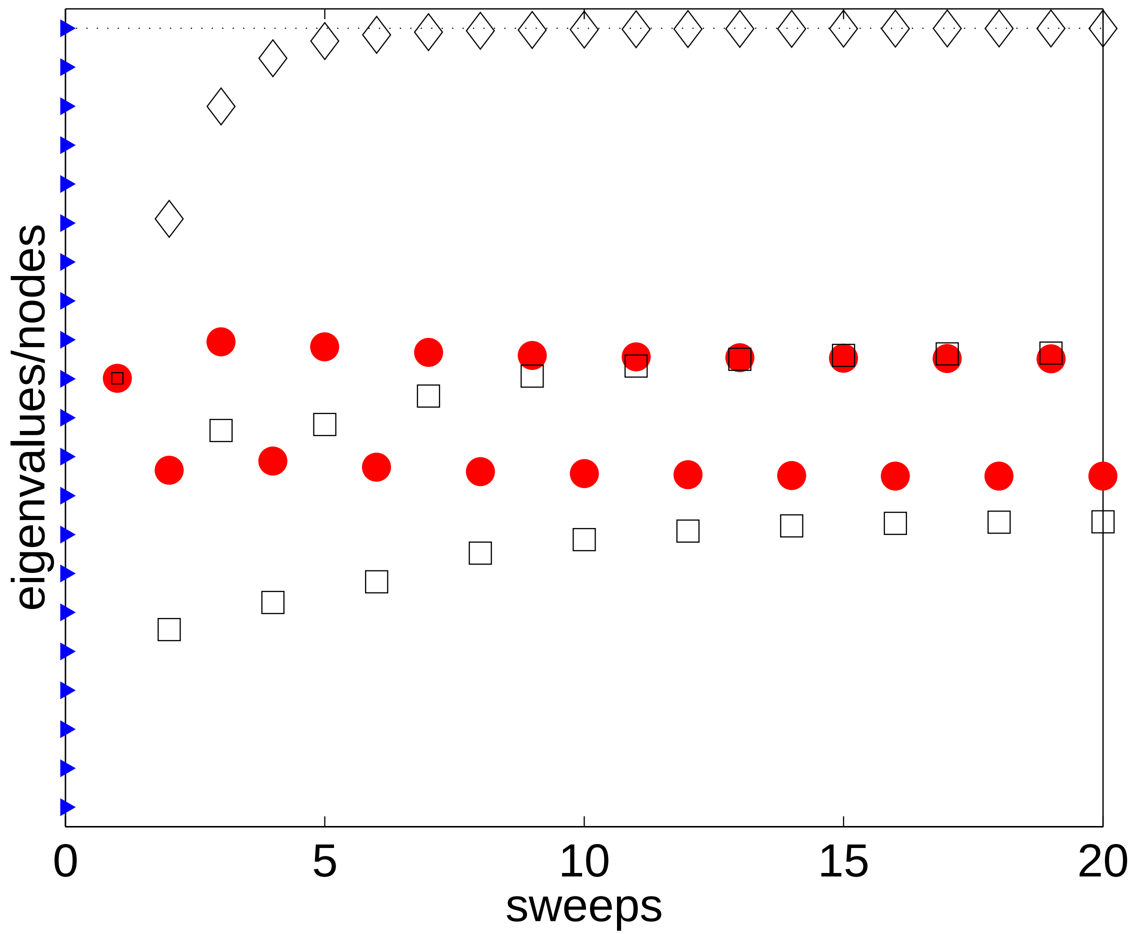
Use the interpretation as an interpolation procedure.

Programm:

1. Where in the complex plane is $\Lambda(\widehat{H}_k)$, the set of interpolation points, located?
2. For which $\lambda \in \mathbb{C}$ do the corresponding interpolation polynomials converge to $f(\lambda)$?

Remarks:

1. This approach works only for (nearly) normal A.
2. The second question is answered, e.g., by [Walsh, 1969].

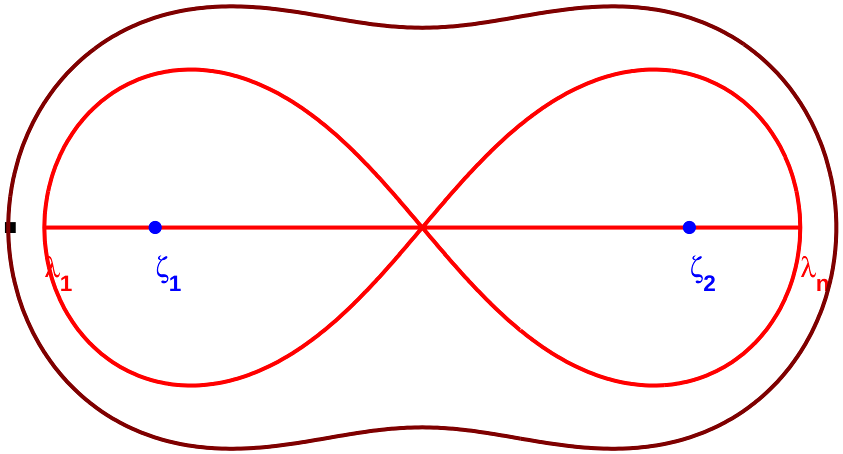


A Hermitian with eigenvalues $\lambda_1 < \lambda_2 < \cdots < \lambda_n$: ▶
Nodes for standard restarted Arnoldi $(m = 1)$: ●
Nodes for thick-restart Arnoldi $(m = 1, \ell = 1)$: $\square$ + last $\diamondsuit$

Theorem 4 (Afanasjew et al., 2008) *Let A be Hermitian. Consider the restarted Arnoldi method with restart length $m = 1$: $\Lambda(\widehat{H}_k) = \{\eta_1, \ldots, \eta_k\}$ and $\Lambda(\widehat{H}_{k+1}) = \{\eta_1, \ldots, \eta_k, \eta_{k+1}\}$. There exists $\alpha \in (0,1)$ (which depends on $\boldsymbol{b}$ and $\Lambda(A)$) such that*

$$\lim_{j\to\infty} \eta_{2j+1} = \zeta_1 = \alpha\lambda_1 + (1-\alpha)\lambda_n,$$

$$\lim_{j\to\infty} \eta_{2j} = \zeta_2 = (1-\alpha)\lambda_1 + \alpha\lambda_n.$$



Theorem 5 (Afanasjew et al., 2008) *Under the conditions of Theorem 4*

$$\limsup_{k\to\infty} \|f(A)\boldsymbol{b} - \widehat{\boldsymbol{f}}_k\|^{1/k} \le \frac{\kappa_A}{\kappa_f}, \text{ where}$$

$$\kappa_A := \min\{\rho > 0 \,:\, \Lambda(A) \subset \operatorname{int}\Gamma_\rho \cup \Gamma_\rho\},$$

$$\kappa_f := \max\{\rho > 0 \,:\, f \text{ analytic in } \operatorname{int}\Gamma_\rho\}.$$

If $f(\lambda) = \exp(\tau\lambda)$, $\tau \ne 0$, *then*

$$\limsup_{k\to\infty} \left[k \|f(A)\boldsymbol{b} - \boldsymbol{f}_k\|^{1/k} \right] \le \kappa_A\, |\tau|\, e.$$

In each case, there exist vectors $\boldsymbol{b}$ *such that equality holds.*

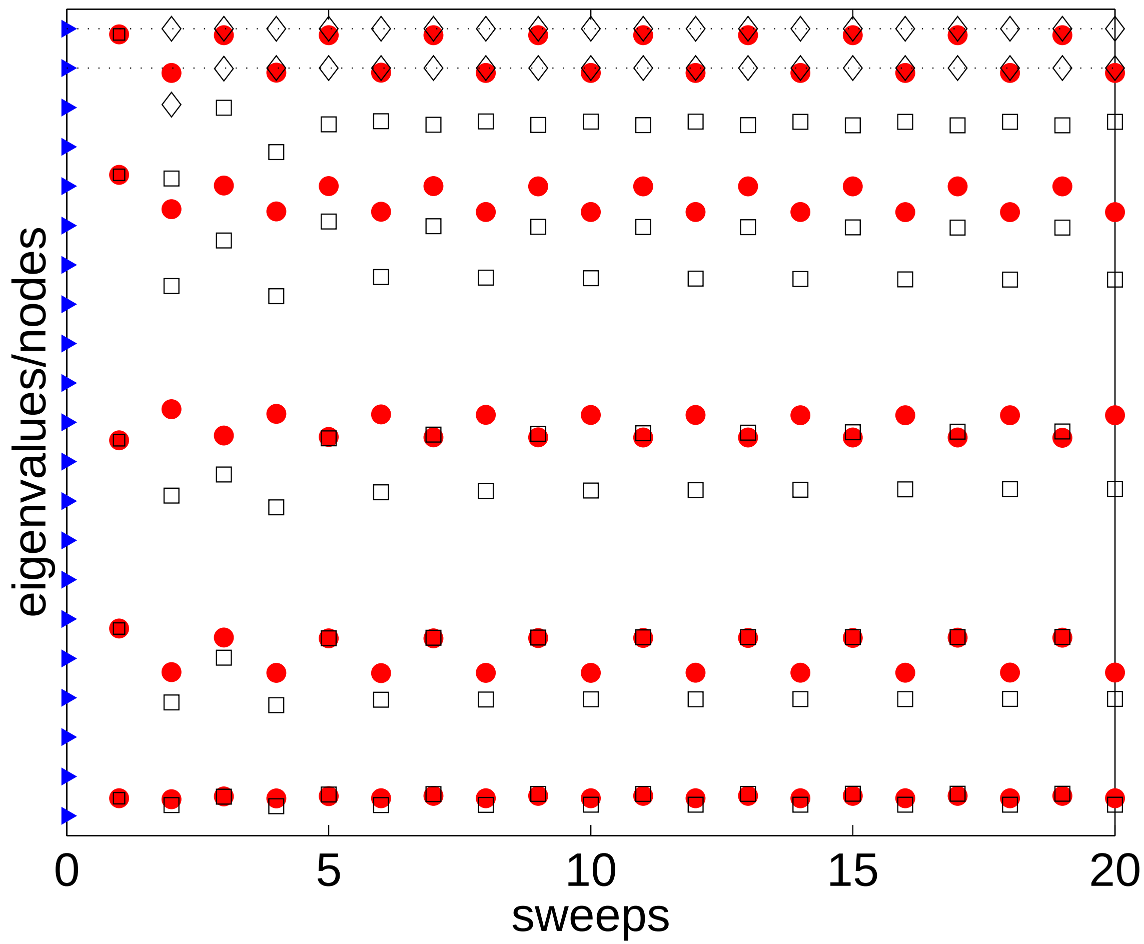
Theorem 6 (E. & Güttel, 2008) *Let A be Hermitian.*
Consider the thick-restarted Arnoldi method with $(m, \ell) = (1, 1)$ with target λ_n.
$\Lambda(\widehat{H}_k) : \eta_1, \eta_2, \ldots, \eta_{k-1}, \eta_k^*$ *and* $\Lambda(\widehat{H}_{k+1}) : \eta_1, \eta_2, \ldots, \eta_{k-1}, \eta_k, \eta_{k+1}^*$.
There exists $\alpha \in (0, 1)$ (which depends on $\boldsymbol{b}$ and $\Lambda(A)$) such that

$$\lim_{j\to\infty} \eta_{2j+1} = \widetilde{\zeta}_1 = \alpha\lambda_1 + (1-\alpha)\lambda_{n-1}$$

$$\lim_{j\to\infty} \eta_{2j} = \widetilde{\zeta}_2 = (1-\alpha)\lambda_1 + \alpha\lambda_{n-1}$$

$$\lim_{j\to\infty} \eta_j^* = \lambda_n.$$

Here, the lemniscates with foci $\widetilde{\zeta}_1$, $\widetilde{\zeta}_2$ determine the convergence behavior.

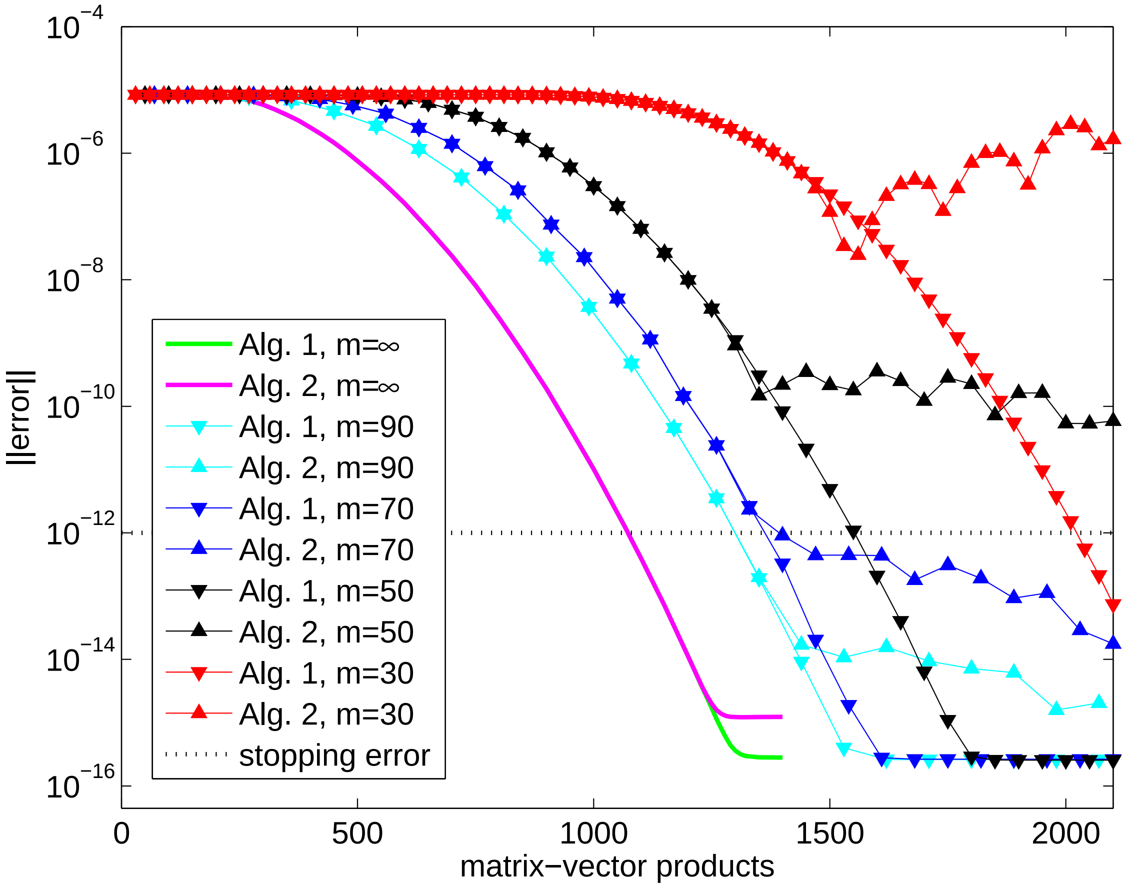


A Hermitian with eigenvalues $\lambda_1 < \lambda_2 < \cdots < \lambda_n$: ▶

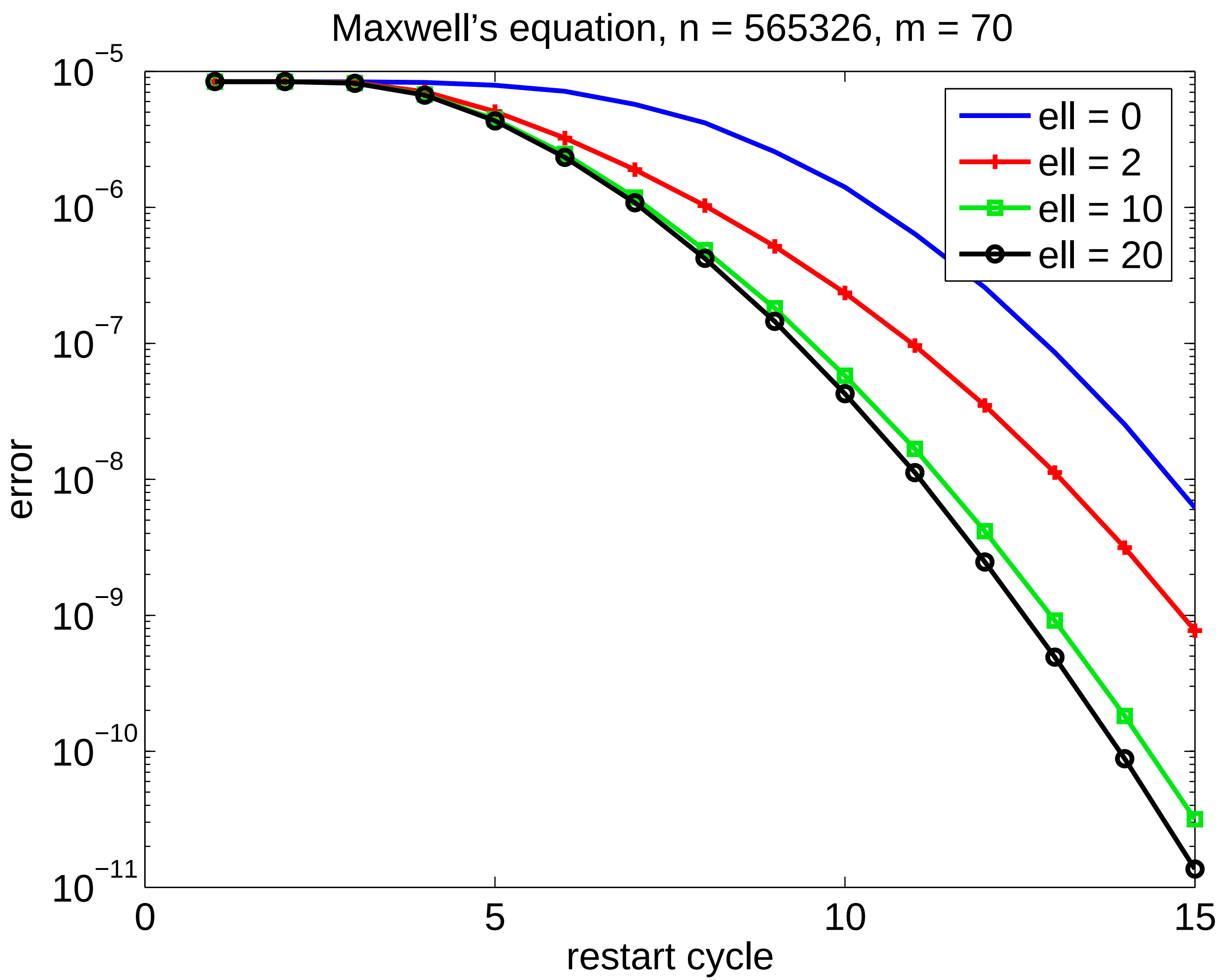
Nodes for standard restarted Arnoldi $(m = 5)$: ●

Nodes for thick-restart Arnoldi $(m = 5, \ell = 2)$: $\square$ + last $\diamondsuit$

5 A numerical example



$\exp(-tA)\boldsymbol{b}$, where $t = 10^{-3}$, A =discrete version of $\sigma^{-1}\nabla\times(\mu^{-1}\nabla\times\dot{\ })$, $\Lambda(A)\in[0,10^8]$, $\dim(A)=565,326$ (see [Afanasjew et al., 2008a])



target = eigenvalues closest to 0

6 Summary

- Restarted Arnoldi methods result in acceptable storage cost even for very large matrices.
- Thick restarts accelerate the convergence.
- There is a stable implementation with constant (low) computational costs per sweep. Necessary: A near best rational approximation to f on $W(A)$ (Faber-Carathéodory-Fejér).
- The asymptotic convergence behavior is (nearly) understood in the Hermitian case.
- Stopping criteria (a posteriori error estimates) are available.