Krylov Subspace Methods for Matrix Functions
Recent Advances and Open Problems

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includes joint work with
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1 Problem

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

Sought: \( f(A)b \).

Original Motivation: Numerical simulation of transient electromagnetic (TEM) geophysical exploration (collaboration with Institute of Geophysics, TU Freiberg):
\[
\mathbf{u}(t) = \exp(-tA)\mathbf{u}_0,
\]
where \( A \) discretizes \( \sigma^{-1}\nabla \times (\mu^{-1}\nabla \times \cdot) \) and is large and sparse.

Other Important Applications:
Exponential integrators: \( \varphi_0(\lambda) = \exp(-t\lambda), \ \varphi_{j+1}(\lambda) = \frac{\phi_j(t\lambda) - \phi_j(0)}{t\lambda}, \ j = 0, 1, \ldots \).
Lattice quantum chromodynamics: \( \text{sign}(\lambda) \).
Time-dependent hyperbolic problems: trigonometric functions, e.g., \( \cos(t\lambda^{1/2}) \).
Outline

1. Krylov subspace methods
2. Restarting
3. Implementation
4. Convergence
generate approximants $y_m$ of $f(A)b$ with

$$y_m \in \mathcal{K}_m(A, b) := \text{span}\{b, Ab, \ldots, A^{m-1}b\} = \{q(A)b : q \in \mathcal{P}_{m-1}\}.$$

Nested bases of $\mathcal{K}_m(A, b)$:

$w_1 = p_0(A)b$, $w_2 = p_1(A)b$, $\ldots$, $w_m = p_{m-1}(A)b$ with $p_k \in \mathcal{P}_k \setminus \mathcal{P}_{k-1}$.

We have

$$\lambda p_{m-1}(\lambda) = h_{m+1,m}p_m(\lambda) + h_{m,m}p_{m-1}(\lambda) + \cdots + h_{m,1}p_0(\lambda),$$

$$A w_m = \eta_{m+1,m} w_{m+1} + \eta_{m,m} w_m + \cdots + \eta_{m,1} w_1,$$

$$A \begin{bmatrix} w_1 & w_2 & \cdots & w_m \end{bmatrix} = \begin{bmatrix} w_1 & w_2 & \cdots & w_m \end{bmatrix} H_m + \eta_{m+1,m} w_{m+1} e_m^T$$

(Arnoldi-like decomposition).
From the Arnoldi-like decomposition $AW_m = W_m H_m + \eta_{m+1,m} w_{m+1} e_m^T$ we define three Krylov approximants to $f(A)b$:

**Projection:** With $\beta w_1 = b$

$$y_m^{(1)} := \beta W_m f(H_m) e_1 \in \mathcal{K}_m(A, b).$$

**Cauchy integral:** There holds $f(A)b = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda) x(\lambda) d\lambda$ if $(\lambda I - A) x(\lambda) = b$. Approximate $x(\lambda)$ by $z_m(\lambda) = \beta W_m (\lambda I - H_m)^{-1} e_1$ and set

$$y_m^{(2)} := \frac{1}{2\pi i} \int_{\Gamma} f(\lambda) z_m(\lambda) d\lambda.$$

**Interpolation:** Let $q_{m-1} \in P_{m-1}$ be the interpolating polynomial (in Hermite’s sense) for $f$ at the zeros of $p_m$.

$$y_m^{(3)} := q_{m-1}(A)b.$$

**Theorem 1**

$$y_m^{(1)} = y_m^{(2)} = y_m^{(3)}.$$
Most popular choice: Proper Arnoldi/Lanczos decomposition
\[ A V_m = V_m H_m + \eta_{m+1,m} v_{m+1} e_m^T, \] i.e., \[ V_m^H V_m = I. \]

Arnoldi approximation [Saad, 1992]:
\[ f_m = \beta V_m f(H_m) e_1 = q_{m-1}(A) b = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda) z_m(\lambda) \, d\lambda, \]
where \( q_{m-1} \) interpolates \( f \) at the Ritz values of \( A \) wrt \( \mathcal{H}_m(A, b) \), and where \( z_m(\lambda) \) is the \( m \)-th FOM iterate for \( (\lambda I - A)x = b \).

**Theorem 2** For the Arnoldi approximation, there holds:
\[ f_L = f(A) b, \] where \( L = L(A, b) = \min\{m \in \mathbb{N} : A \mathcal{H}_m(A, b) \subseteq \mathcal{H}_m(A, b)\}. \)
If \( f(\lambda) = 1/\lambda \), then \( f_m \) is the \( m \)-th FOM-iterate for the solution of \( A x = b \) (if \( x_0 = 0 \)).
If, in addition, \( A \) is Hermitian positive definite, then \( f_m \) is the \( m \)-th CG-iterate.
Alternatives:

**Harmonic Ritz values:** [van den Eshof et al., 2002]

\[ y_m = V_m f(H_m + h_m e_m^T) e_1, \quad \text{where} \quad h_m = \eta_{m+1,m}^2 (H_m - \tau I)^{-H} e_m. \]

(Can be seen as resulting from an Arnoldi-like decomposition with an \((A - \tau I)\)-orthonormal basis \(\tilde{V}_m\).)

Is equivalent to MINRES/GMRES for \(f(\lambda) = 1/\lambda\).

Is there another implementation?

**Two-sided (or nonsymmetric) Lanczos process:** Three-term recurrence for basis vectors. Needs \(A^H\).

**Block orthonormal basis** (see restarts).
3 Restarting

Why is restarting necessary?

Arnoldi approximation:

\[ f_m = q_{m-1}(A)b = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda)\beta V_m(\lambda I - H_m)^{-1}e_1 \, d\lambda = \beta V_m f(H_m)e_1. \]

**Advantage:** avoids \( A \) (except for Arnoldi process, where only matrix-vector multiplications with \( A \) are required), avoids explicit interpolation, requires only evaluation of \( f \) for small matrix \( H_m \) (actually, only \( f(H_m)e_1 \) is needed).

**Disadvantage:** requires basis \( V_m \) (extensive storage), even in the Hermitian case, where the columns of \( V_m \) can be computed via a three-term recurrence relation. Common cure: Two sweeps through Lanczos-process—first to compute \( H_m \) (and \( f(H_m)e_1 \)), and second to form linear combination \( V_m f(H_m)e_1 \). Does not work for non-Hermitian \( A \).
Restarting the Arnoldi Approximation (FOM) to $A^{-1}b$

- Familiar from Krylov methods for $Ax = b$ in non-Hermitian case.
- First, construct Arnoldi approximation to $A^{-1}b$ from $\mathcal{K}_m(A, b)$:
  \[ x_m^{(1)} = \beta_1 V_1 H_1^{-1} e_1. \]
- Write $A^{-1}b = x_m^{(1)} + A^{-1}r_m$ with $r_m := b - Ax_m^{(1)}$.
- Secondly, construct Arnoldi approximation to $A^{-1}r_m$ from $\mathcal{K}_m(A, r_m) = \mathcal{K}_m(A, v_{m+1})$:
  \[ x_m^{(2)} = \beta_2 V_2 H_2^{-1} e_1. \]
- Correct $x_m^{(1)}$ by $x_m^{(2)}$:
  \[ A^{-1}b \approx x_m^{(1)} + x_m^{(2)} = \beta_1 V_1 H_1^{-1} e_1 + \beta_2 V_2 H_2^{-1} e_1 \in \mathcal{K}_2m(A, b). \]
- General $f$ (e.g., $f = \exp$): no residual available.
**First approach:** Restart function.

\[ f(\lambda) = q_{m-1}(\lambda) + \frac{f(\lambda) - q_{m-1}(\lambda)}{p_m(\lambda)} p_m(\lambda) = q_{m-1}(\lambda) + \Delta_m f(\lambda) p_m(\lambda) \]

(block Newton form of interpolation process). Inserting \( A \) and multiplying by \( b \),

\[ f(A)b = f_m + \Delta_m f(A) p_m(A)b = f_m + \beta \Delta_m f(A) v_{m+1} \]

[E., Ernst, 2006], [Ilíc et al., 2007], [Tal-Ezer, 2007].

**Second approach:** Cauchy integral. Solve linear systems in

\[ f(A)b = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda)(\lambda I - A)^{-1}b \, d\lambda \]

by restarted FOM

\[ f(A)b \approx \frac{1}{2\pi i} \int_{\Gamma} f(\lambda) \left[ \beta_1 V_1(\lambda I - H_1)^{-1}e_1 + \beta_2 V_2(\lambda I - H_2)^{-1}e_1 \right] d\lambda \]

[Niehoff, 2006].
**Third approach:** Block orthogonal basis. Two Arnoldi cycles

\[ AV_1 = V_1 H_1 + \eta_1 v_{m+1} e_m^T, \quad V_1 e_1 = \beta b, \]
\[ AV_2 = V_2 H_2 + \eta_2 v_{2m+1} e_m^T, \quad V_2 e_1 = v_{m+1}, \]

glued together,

\[ A\hat{V}_2 = \hat{V}_2 \hat{H}_2 + \eta_2 v_{2m+1} e_{2m}^T, \text{ with } \hat{V}_2 := [V_1 \ V_2], \quad \hat{H}_2 := \begin{bmatrix} H_1 & O \\ \eta_1 e_1 e_m^T & H_2 \end{bmatrix}, \]

lead to \( f(A)b \approx \beta\hat{V}_2 f(\hat{H}_2)e_1 \) [E., Ernst, 2006].

**Theorem 3** All three approaches are equivalent. After \( k \) sweeps of length \( m \) they generate

\[ \hat{f}_k = q_{km-1}(A)b, \]

where \( q_{km-1} \in \mathcal{P}_{km-1} \) interpolates \( f \) at the eigenvalues of \( H_1, H_2, \ldots, H_k \).
Thick restarts

- Well known for eigenproblems [Wu, Simon, 2000], [Stewart, 2001] and linear systems [Morgan, 2002]. For matrix functions first considered by [Niehoff, 2006].

- Starting point

\[ AV_1 = V_1 H_1 + \eta_1 v_{m+1} e_m^T. \]

- Extract \( \ell \) wanted eigenvalues of \( H_1 \)

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

We may assume that \( U_1 \in \mathbb{C}^{\ell \times \ell} \) is upper triangular and that \( X_1 \in \mathbb{C}^{m \times \ell} \) has orthonormal columns. Set \( Y_1 := V_1 X_1 \). Then

\[ AY_1 = Y_1 U_1 + \eta_1 v_{m+1} u_1^T, \] where \( u_1 \in \mathbb{C}^{\ell} \) (dense!).
• Extend by $m$ Arnoldi steps

$$A [Y_1 \ V_2] = [Y_1 \ V_2] \begin{bmatrix} U_1 & G_2 \\ \eta_1 e_1 u_1^T & H_2 \end{bmatrix} + \eta_2 v_{2m+1} e_{2m+\ell}^T,$$

where $[Y_1 \ V_2]$ has orthonormal columns, $V_2 e_1 = v_{m+1}$, $H_2 \in \mathbb{C}^{m \times m}$ is upper Hessenberg.

• Known [Morgan, 2002]:

$$\text{span}[Y_1 \ V_2] = \mathcal{K}_{m+\ell}(A, s(A) b),$$

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

(implicitly restarted Arnoldi).

• Next sweep: Extract $\ell$ wanted eigenvalues:

$$\begin{bmatrix} U_1 & G_2 \\ \eta_1 e_1 u_1^T & H_2 \end{bmatrix} [X_2 \ *] = [X_2 \ *] \begin{bmatrix} U_2 & * \\ O & * \end{bmatrix}.$$
After $k$ sweeps:

$$A\hat{V}_k = \hat{V}_k \hat{H}_k + \eta_k v_{k+1} e_k^T,$$

where

$$\hat{V}_k = [V_1|Y_1|V_2|\cdots|Y_{k-1}|V_k] \in \mathbb{C}^{n \times \hat{k}},$$

$$\hat{H}_k = \begin{bmatrix}
  H_1 & & & & \\
  & U_1 & G_2 & & \\
  & E_2 & F_2 & H_2 & \\
  & & \ddots & \ddots & \\
  & & & \ddots & \\
  & & & & E_k
\end{bmatrix} \in \mathbb{C}^{\hat{k} \times \hat{k}}.$$ 

Here, $\hat{k} = m + (k - 1)(m + \ell)$.

$V_j \in \mathbb{C}^{n \times m}$, $Y_j \in \mathbb{C}^{n \times \ell}$, $V_j^H V_j = I_m$, $Y_j^H Y_j = I_\ell$, $Y_{j-1}^H V_j = O$.

$H_j \in \mathbb{C}^{m \times m}$ upper Hessenberg [tridiagonal],

$U_j \in \mathbb{C}^{\ell \times \ell}$ upper triangular [diagonal],

$E_j = \eta_{j-1} e_1 e_m^T \in \mathbb{C}^{m \times m}$, $F_j = e_{j-1} u_{j-1}^T \in \mathbb{C}^{m \times \ell}$, $G_j \in \mathbb{C}^{\ell \times m}$ [\(= F_j^H\)].
Theorem 4  Given the thick-restart-decomposition \( A\hat{V}_k = \hat{V}_k \hat{H}_k + \eta_k v_{k+1} e_k^T \) (\( k \)-th sweep, i.e., after \( k - 1 \) restarts, \( \ell \) Ritz vectors per restart, \( m \) mvm per sweep). Then

\[ \hat{y}_k = \beta \hat{V}_k f(\hat{H}_k) e_1 = q_{km-1}(A) b = \frac{1}{2\pi i} \int_{\Gamma} f(\lambda) \hat{z}_{k,m,\ell}(\lambda) d\lambda, \]

where \( q_{km-1} \in \mathcal{P}_{km-1} \) interpolates \( f \) in \( \Lambda(\hat{H}_k) \setminus (\bigcup_{j=1}^{k-1} \Lambda(U_j)) \), and where \( z_{k,m,\ell} \) is the approximate solution of \( (\lambda I - A)x = b \) which is generated by \( k \) sweeps of \( FOM(m, \ell) \).
\[ \exp(\text{diag}(-20 : 1 : 0))[1, 1, \ldots, 1]^T. \]
4 Implementation

For general $f$, no stable implementation of the restarted Arnoldi method to evaluate $f(A)b$ is known, besides [E., Ernst, 2006]

Algorithm 1.

Given $A$, $b$, $\|b\| = 1$, $f$

$v_1 := b$, $\hat{f}_0 := 0$

For $k = 1, 2, \ldots$

Compute Arnoldi decomposition $AV_k = V_k H_k + \eta_{k+1} v_{km+1} e_T$

of $K_m(A, v_{(k-1)m+1})$

If $k = 1$

$\hat{H}_k := H_1$

Else $\hat{H}_k := \begin{bmatrix} \hat{H}_{k-1} & O \\ E_k & H_k \end{bmatrix}$ with $E_k := \eta_k e_1 e_T^{(k-1)m}$

Update the approximation $\hat{f}_k := \hat{f}_{k-1} + V_k [f(\hat{H}_k) e_1]_{(k-1)m+1:km}$. 
Disadvantages:

- Must evaluate $f$ for the matrix $\hat{H}_k$ of size $mk$ in sweep $k$.
- $\hat{H}_k$ is highly non-normal, even if $A$ (and all $H_j$) are Hermitian.

Special Case:

$f$ is a rational function of the form

$$f(\lambda) = r(\lambda) = p(\lambda) + \sum_{\ell=1}^{N} \frac{\alpha_\ell}{\omega_\ell - \lambda}$$

(already considered by [Gallopoulos, Saad, 1992]).
Algorithm 2. [Afanasjew et al., 2007]

Given \( A, b, \| b \| = 1, (\alpha_\ell, \omega_\ell)_{\ell=1}^N \)

\( v_1 := b, \hat{f}_0 := \alpha_0 b \)

For \( k = 1, 2, \ldots \)

Compute Arnoldi decomposition \( AV_k = V_k H_k + \eta_{k+1} v_{km+1} e_m^T \)

of \( \mathcal{K}_m(A, v_{(k-1)m+1}) \)

If \( k = 1 \)

For \( \ell = 1, 2, \ldots, N \)

Solve \( (\omega_\ell I - H_k) r_{\ell,1} = e_1 \)

Else

For \( \ell = 1, 2, \ldots, N \)

Solve \( (\omega_\ell I - H_k) r_{\ell,k} = E_k r_{\ell,k-1} \)

\( h_k := \sum_{\ell=1}^N \alpha_\ell r_{\ell,k} \)

\( \hat{f}_k := \hat{f}_{k-1} + V_k h_k \).
Two (essentially) equivalent approaches:

- Find rational approximation \( r(\lambda) = \sum_{\ell=1}^{N} \alpha_{\ell}/(\omega_{\ell} - \lambda) \) for \( f \) and apply Algorithm 2.

- Solve \( \ell \) large systems \( (\omega_{\ell} I - A)^{-1} x = b \) by FOM\((m)\) and consider linear combination \( \sum_{\ell=1}^{N} \alpha_{\ell} x_{\ell} \).


Note that this approach has the advantage that known technology for linear systems can be applied to matrix functions. Good example: A-posteriori error estimates for \( r(A)b \) of [Frommer, Simoncini, 2007] from CG-estimate of [Strakoš, Tichý, 2005].

Note further that this approach goes far beyond Krylov methods.

- **Problems:** How to find \( r \)? (Faber-Carathédory-Fejér?)
  Is every \( f \) ‘rational’?
**Model problem:** \( f = \exp, \ r_2 = \) best rational approximation to \( f \) on \((-\infty, 0]\) of type \([16, 16]\) [Cody, Meinardus & Varga, 1969],

\[
A = \text{diag}(-100, -99, \ldots, 0) \in \mathbb{R}^{101 \times 101}, \ b = [1, 1, \ldots, 1]^T / \sqrt{101} \in \mathbb{R}^{101}.
\]
Observation: Convergence history of Algorithm 2 shows two phases.
Algorithm 1: Approximates $\exp(\hat{H}_k)$ by $r_1(\hat{H}_k) = r(\hat{H}_k/2^s)^{2^s}$, where $r$ is a Padé-fraction (expm, [Higham, 2005]), $r_1$ depends on the argument and is not a rational function: if the argument is a scalar $\lambda$ then $r_1(\lambda)$ is an accurate approximation to $\exp(\lambda)$ regardless of where in the complex plane $\lambda$ is located; in particular, $r_1$ has no finite poles.

Algorithm 2: Approximates $\exp(\hat{H}_k)$ by $r_2(\hat{H}_k)$, where $r_2$ is a fixed rational function, namely the CMV approximation of type [16/16]. $r_2$ approximates $\exp$ well only on $(-\infty, 0]$ and has finite poles.

Main distinction: The restarted Arnoldi method converges superlinearly to an entire function (Algorithm 1) and converges/diverges linearly since $r_2$ has finite singularities (Algorithm 2).
**Restart length** $m = 1$:

- $\hat{f}_k = p_{k-1}(A)b$, where $p_{k-1}$ interpolates $f = \exp$ or $f = r_2$ at the eigenvalues of $\hat{H}_k$,
- $\hat{H}_k$ is bidiagonal, all diagonal entries are equal to $\vartheta = -50$,
- the interpolating polynomials are therefore truncated Taylor series,
- the Taylor series for $\exp$ (Algorithm 1) converges everywhere, whereas the Taylor series for $r_2$ (Algorithm 2) converges only for
  
  $|\lambda + 50| < \min_{\omega = \text{pole of } r_2} |\omega + 50| \approx 44 < 50 = \max_{\lambda \in \Lambda(A)} |\lambda + 50|,$

- Algorithm 2 therefore ultimately diverges like
  
  $\left[ \max_{\lambda \in \Lambda(A)} |\lambda + 50|/44 \right]^k = (50/44)^k \approx 1.14^k.$
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Restart length \( m \geq 1 \):

\[ m = 3 \]

\[ m = 10 \]
To summarize: Algorithm 2 converges as follows

- initially, behavior like polynomial interpolation to $\exp$ (no error reduction in the startup phase and then superlinear convergence) as long as 
  
  \[ \frac{d^{km} r_2}{d\lambda^{km}} \approx \frac{d^{km} \exp}{d\lambda^{km}} , \]

- there is a point from where on the poles of $r_2$ become visible, fairly independent of the restart length,

- after this point of transition, behavior like polynomial interpolation to $r_2$ (slower linear convergence or even linear divergence).

The aim is to choose the restart length large enough such that at the point of transition the desired accuracy is reached.
5 Convergence

Example: Let

\[ A = \begin{bmatrix} 0 & 0 & 0 & * \\ 1 & 0 & 0 & * \\ 0 & 1 & 0 & * \\ 0 & 0 & 1 & * \end{bmatrix} \in \mathbb{C}^{4 \times 4} \]

and \( f \) be such that \( f(A) \) is defined.

Arnoldi-approximation to \( f(A)e_1 \):

\[ f_m = \begin{bmatrix} f(0) & \frac{f'(0)}{1!} & \cdots & \frac{f^{(m-1)}(0)}{(m-1)!} & 0 & \cdots & 0 \end{bmatrix}^T \]

for every \( m < n \).
On the other hand,

\[ \| f(A) b - f_m \|_2 \leq C \max_{\lambda \in W(A)} |f(\lambda) - q_{m-1}(\lambda)| \]

where \( W(A) = \{ x^H A x : x \in \mathbb{C}^n, x^H x = 1 \} \) and \( C \leq 12 \) [Crouzeix, 2007].

Practical error estimates only available for normal \( A \), i.e., if there exists an ON basis \( \{ x_1, \ldots, x_n \} \) of \( \mathbb{C}^n \) with \( A x_j = \lambda_j x_j \). Let \( b = \sum_{j=1}^{n} \beta_j x_j \), where \( \beta_j \neq 0 \) and \( \sum_{j=1}^{n} |\beta_j|^2 = 1 \).

Weighted (eigenvalue) counting measure \( \mu = \mu_{A,b} = \sum_{j=1}^{n} |\beta_j|^2 \delta_{\lambda_j} : \)

\[ \mu(M) = \sum_{j, \lambda_j \in M} |\beta_j|^2 \quad (M \subseteq \mathbb{C}) \]

Associated function space \( \mathcal{L}_2(\mu) = \mathcal{P}_{n-1} \) with norm

\[ \| f \|_{\mu} = \left( \int_{\mathbb{C}} |f(\zeta)|^2 d\mu(\zeta) \right)^{1/2} = \left[ \sum_{j=1}^{n} |\beta_j|^2 |f(\lambda_j)|^2 \right]^{1/2}. \]
\[(\mathcal{K}_m(A, b); \| \cdot \|_2) \ni q_{m-1}(A)b \leftrightarrow q_{m-1} \in (\mathcal{P}_{m-1}; \| \cdot \|_\mu) \]

\[\cap \quad \downarrow \quad \downarrow \quad \cap \]

\[(\mathbb{C}^n; \| \cdot \|_2) \ni f(A)b \leftrightarrow f \in L_2(\mu)\]

are isometric isomorphisms.

The problem of approximating \(f(A)b\) by \(q_{m-1}(A)b \in \mathcal{K}_m(A, b)\) turns out to be a classical interpolation problem:

**Approximate** \(f \in L_2(\mu)\) **by some interpolating polynomial** \(q_{m-1} = Pf \in \mathcal{P}_{m-1}\).

\(P\) is a projection onto \(\mathcal{P}_{m-1}\), i.e.,

\[\|f(A)b - q_{m-1}(A)b\|_2 = \|f - Pf\|_\mu = \|f - Pf + Pq - q\|_\mu\]

\[= \|(I - P)(f - q)\|_\mu \leq \|I - P\|_\mu \|f - q\|_\mu\]

for every \(q \in \mathcal{P}_{m-1}\).

For the Arnoldi approximation: \(\|I - P\|_\mu \leq 2\) and therefore,

\[\|f(A)b - f_m\|_2 \leq 2 \min_{q \in \mathcal{P}_{m-1}} \max_{\lambda \in W(A)} |f(\lambda) - q(\lambda)|\]

[Stewart, Leyk, 1996].
Convergence Analysis for Restarted Arnoldi

Recall

\[ \hat{f}_k = q_{mk-1}(A) b, \]

where \( q_{mk-1} \) interpolates \( f \) at the eigenvalues of \( \hat{H}_k \) (i.e., at the eigenvalues of \( H_j, j = 1, 2, \ldots, k \)).

1. Where in the complex plane is \( \Lambda(\hat{H}_k) \), the spectrum of \( \hat{H}_k \), located?

2. For which \( \lambda \in \mathbb{C} \) do the interpolation polynomials of \( f \) (with nodal set \( \Lambda(\hat{H}_k) \)) tend to \( f(\lambda) \)?

In the sequel, we assume that

\( A \) is Hermitian with eigenvalues \( \lambda_{\text{min}} = \lambda_1 < \cdots < \lambda_n = \lambda_{\text{max}} \)

and \( m = 1 \) (unit restart length).
Drawing on results of [Akaike, 1959]:

**Theorem 5 ([Afanasjew et al., 2007])** Let $\rho_1, \rho_2, \ldots, \rho_k$ denote the eigenvalues of $\hat{H}_k$ ($k = 1, 2, \ldots$). Then there holds

$$\lim_{k \to \infty} \rho_{2k-1} = \zeta_1 \text{ and } \lim_{k \to \infty} \rho_{2k} = \zeta_2.$$ 

These limits are contained in $(\lambda_{\min}, \lambda_{\max})$ and lie symmetric to $\frac{1}{2}(\lambda_{\min} + \lambda_{\max})$. The restarted Arnoldi method is asymptotically equivalent to cyclic interpolation at two nodes, $\zeta_1$ and $\zeta_2$.

Now the convergence of the restarted Arnoldi method can be analyzed using well known results on the interpolation of analytic functions (see [Walsh, 1969], [Gaier, 1980]) and new results on the interpolation of entire functions.
\[ \Gamma_\rho := \{ z \in \mathbb{C} : |z - \zeta_1||z - \zeta_2| = \rho^2 \} \]

(lemniscate with foci \( \zeta_1, \zeta_2 \)).

\[ \kappa_A := \min\{ \rho > 0 : \Lambda(A) \subset \text{int} \Gamma_\rho \cup \Gamma_\rho \}, \]

\[ \kappa_f := \max\{ \rho > 0 : f \text{ analytic in } \text{int} \Gamma_\rho \}. \]
Theorem 6 (Afanasjew et al., 2007) \[ ] Let \( A \) be Hermitian and let \( f \) denote a function which is analytic in a neighborhood of the spectral interval \([\lambda_{\text{min}}, \lambda_{\text{max}}]\) of \( A \). For the approximants \( f_k \) generated by the Arnoldi method with unit restart length and initial vector \( b \), there holds:

If \( f \) possesses finite singularities then

\[
\limsup_{k \to \infty} \| f(A)b - f_k \|^{1/k} \leq \frac{\kappa_A}{\kappa_f}.
\]

If \( f(\lambda) = \exp(\tau \lambda), \tau \neq 0 \), then

\[
\limsup_{k \to \infty} \left[ k \| f(A)b - f_k \|^{1/k} \right] \leq \kappa_A |\tau| e.
\]

In each case, there exist vectors \( b \) such that equality holds.

The method converges if and only if \( \Gamma_{\kappa_A} \) and its interior contain no singularities of \( f \). The convergence is then at least linear with convergence factor

\[
\theta = \frac{\lambda_{\text{max}} - \lambda_{\text{min}}}{|\eta_0 - \lambda_{\text{min}}| + |\eta_0 - \lambda_{\text{max}}|},
\]

where \( \eta_0 \) is a singularity of \( f \) closest to \([\lambda_{\text{min}}, \lambda_{\text{max}}]\).
Example

\[ A = \text{diag}(-1, 0, 1), \quad b = \begin{bmatrix} \gamma_1, \gamma_2, \gamma_3 \end{bmatrix}^T, \]
\[ \gamma_1^2 + \gamma_2^2 + \gamma_3^2 = 1. \]

We know that the eigenvalues of \( \tilde{H}_k \) ‘tend’ to two limits
\[ \zeta_{1,2} = \pm \rho, \quad \rho \in [0, 1). \]

Is it possible to analytically describe \( \rho = \rho(\gamma_1, \gamma_2, \gamma_3) \)?
Standard restarts ($m = 1$). **Fact:**

\[
\hat{H}_k \rightarrow \begin{bmatrix}
\cdots \\
\rho_1 \\
\sigma & \rho_2 \\
\cdots
\end{bmatrix},
\]

where $\rho_1, \rho_2 \in [\lambda_{\text{min}}, \lambda_{\text{max}}]$ lie symmetric to $\frac{1}{2}(\lambda_{\text{min}} + \lambda_{\text{max}})$.

Thick restarts ($m = 1, \ell = 1$). **Guess:**

\[
\hat{H}_k \rightarrow \begin{bmatrix}
\cdots \\
\tau \\
\sigma & \rho_1 \\
\tau \\
\sigma & \rho_2 \\
\cdots
\end{bmatrix},
\]

where $\tau$ is the target of the restarts, $\rho_1, \rho_2 \in [\lambda^*_{\text{min}}, \lambda^*_{\text{max}}]$ lie symmetric to $\frac{1}{2}(\lambda^*_{\text{min}} + \lambda^*_{\text{max}})$, and $\lambda^*_{\text{min}} = \min\{\lambda \in \Lambda(A), \lambda \neq \tau\}$. 

Summary

- Is there a stable implementation of the restarted Arnoldi approximation for $f(A)b$ with
  - constant work/storage per sweep,
  - which does not compute $f(H_k)$ but $f(H_k)b_k$,
  - is not based on an a-priori choice of a rational approximation for $f$.

- For the solution of semi-discrete convection-diffusion problems $u_t = Au(t) + b(t)$ (for instance):
  Can we find $r(tA) \approx \exp(tA)$ for $t \geq 0$.
  Can we find a fast multigrid method for $(\lambda I - A)x = b$ (complex shifts)?

- Can we generalize the convergence results for restarted Arnoldi from $m = 1$ to arbitrary restart lengths? This would answer a forty-year-old conjecture of Forsythe. (Same question for thick restarts.)