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On the Steepest Descent Method for the Evaluation of Matrix Functions

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Freiberg, April 2007

Problem

Given

- a matrix $A \in \mathbb{C}^{N \times N}$ (large and sparse),
- a vector $\boldsymbol{b} \in \mathbb{C}^N$, $\|\boldsymbol{b}\|_2 = 1$,
- a scalar function $f : \mathbb{C} \supseteq D \to \mathbb{C}$ which is analytic in $D \supset \Lambda(A)$.

Task: Compute $f(A)\boldsymbol{b}$ in an efficient way considering

- memory requirements,
- convergence speed.

Typical applications

- Solve the linear system of equations $A\boldsymbol{x} = \boldsymbol{b}$.
  The solution is $\boldsymbol{x} = f(A)\boldsymbol{b}$, where $f(z) = 1/z$.
- Solve an ordinary initial value problem $\boldsymbol{y}'(\tau) = A\boldsymbol{y}(\tau), \boldsymbol{y}(0) = \boldsymbol{y}_0$.
  The solution is $\boldsymbol{y}(\tau) = f(A)\boldsymbol{y}_0$, where $f(z) = f_\tau(z) = \exp(\tau z)$.
- The solution of the identification problem in stochastic semigroups requires the evaluation of $f(A)\boldsymbol{b}$ with $f(z) = \log(z)$. [Singer/Spilermann, 1976]
- To simulate Brownian motion of molecules one needs to determine $f(A)\boldsymbol{b}$ with $f(z) = \sqrt{z}$. [Ericsson, 1990]
- The solution of the algebraic Riccati equation (but also simulations in lattice quantum chromodynamics) requires $f(A)\boldsymbol{b}$ where $f(z) = \mathrm{sign}(z)$.

1 Matrix functions

Let

$$\psi_A(z) = \prod_{\lambda \in \Lambda(A)} (z - \lambda)^{d_\lambda}$$

denote the minimal polynomial of A, $\deg(\psi_A) = d$.

Let $p_A \in \mathscr{P}_{d-1}$ satisfy the d Hermite interpolation conditions

$$p_A^{(\nu)}(\lambda) = f^{(\nu)}(\lambda), \qquad \nu = 0, 1, \ldots, d_\lambda - 1$$

for all $\lambda \in \Lambda(A)$.

Then we define

$$f(A) := p_A(A).$$

[Gantmacher, 1959], [Rinehart, 1955]

2 Krylov approximations

The vector $f(A)\boldsymbol{b} = p_A(A)\boldsymbol{b}$ that we seek lies in some Krylov space

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

The polynomial $p_{A,\boldsymbol{b}}$ such that $f(A)\boldsymbol{b} = p_{A,\boldsymbol{b}}(A)\boldsymbol{b}$ is determined by at most d Hermite interpolation conditions at the eigenvalues of A (those relevant for $\boldsymbol{b}$).

Therefore it makes sense to look for approximations (Krylov approximations)

$$f(A)\boldsymbol{b} \approx p_{m-1}(A)\boldsymbol{b} \in \mathscr{K}_m(A, \boldsymbol{b})$$

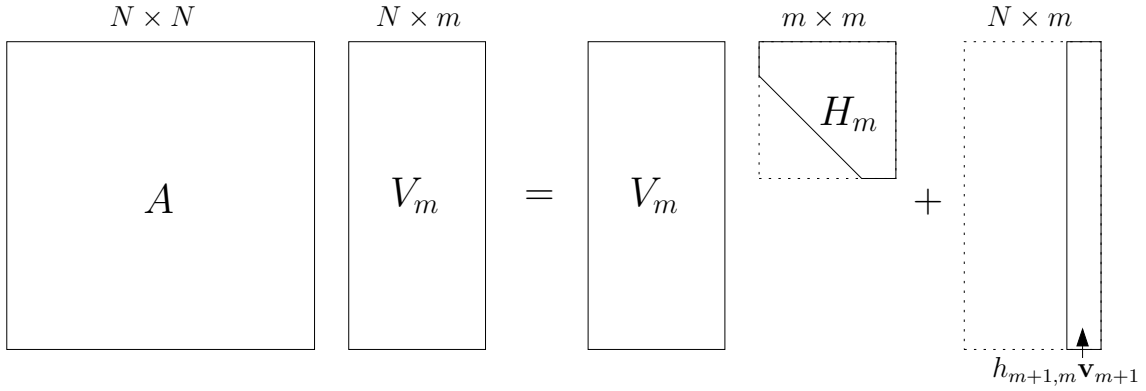
with p_{m-1} determined by interpolation conditions.

The Arnoldi process applied to A with initial vector $\boldsymbol{b}$ yields the Arnoldi decomposition

$$AV_m = V_m H_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^T$$

where

$$V_m = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_m] \in \mathbb{C}^{N\times m}, \quad \{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m\} \text{ ON basis of } \mathscr{K}_m(A, \boldsymbol{b}),$$
$$\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{m+1}\} \text{ ON basis of } \mathscr{K}_{m+1}(A, \boldsymbol{b}),$$
$$\boldsymbol{v}_1 = \boldsymbol{b},$$
$$H_m = [h_{i,j}] \in \mathbb{C}^{m\times m} \quad \text{unreduced upper Hessenberg matrix,}$$
$$\boldsymbol{e}_m = [0, \ldots, 0, 1]^T \in \mathbb{R}^m.$$



m-th Arnoldi approximation of $f(A)\boldsymbol{b}$:

$$f(A)\boldsymbol{b} \approx \boldsymbol{f}_m := V_m f(H_m)\boldsymbol{e}_1$$

[Druskin & Knizhnerman, 1989],
[Gallopoulos & Saad, 1992],
[Hochbruck & Lubich, 1995]

Interpretation: By definition there exists a polynomial $p_{m-1} \in \mathscr{P}_{m-1}$ such that

$$f(H_m) = p_{m-1}(H_m).$$

One can show

$$V_m p_{m-1}(H_m)\boldsymbol{e}_1 = p_{m-1}(A)\boldsymbol{b}.$$

Therefore, instead of evaluating $p_A(A)\boldsymbol{b}$ (interpolation at the eigenvalues of A) we compute $\boldsymbol{f}_m = p_{m-1}(A)\boldsymbol{b}$ (interpolation at the eigenvalues of H_m).

Advantage: avoids A (only $\boldsymbol{v} \to A\boldsymbol{v}$), avoids explicit interpolation, requires only evaluation of $f(H_m)$ for (small) matrix H_m.

Drawback: requires basis V_m (extensive storage), even in Hermitian case, high computational costs for Arnoldi decomposition (in the nonsymm. case).

3 Restarting the Arnoldi approximation

- Familiar from Krylov methods for $A\boldsymbol{x} = \boldsymbol{b}$ in non-Hermitian case.
- Idea: construct Arnoldi approximation to $A^{-1}\boldsymbol{b}$ from $\mathscr{K}_k(A, \boldsymbol{b})$:

$$\boldsymbol{x}_k = V_k H_k^{-1} \boldsymbol{e}_1 .$$

- Correction $\boldsymbol{c}$ to $\boldsymbol{x}_k$ obtained by solving the residual equation:

$$A^{-1}\boldsymbol{b} = \boldsymbol{x}_k + \boldsymbol{c}, \qquad A\boldsymbol{c} = \boldsymbol{b} - A\boldsymbol{x}_k =: \boldsymbol{r}_k .$$

- (Approximate) solution of residual equation in new Krylov space $\mathscr{K}_k(A, \boldsymbol{r}_k)$, hence storage requirements are fixed.
- General f (e.g., $f = \exp$): no residual available.

Consider two cycles of restarted Arnoldi for $A, \boldsymbol{b}$:

$$AV_k^{(1)} = V_k^{(1)} H_k^{(1)} + h_{k+1,k}^{(1)} \boldsymbol{v}_{k+1}^{(1)} \boldsymbol{e}_k^T, \qquad \boldsymbol{v}_1^{(1)} = \boldsymbol{b},$$
$$AV_k^{(2)} = V_k^{(2)} H_k^{(2)} + h_{k+1,k}^{(2)} \boldsymbol{v}_{k+1}^{(2)} \boldsymbol{e}_k^T, \qquad \boldsymbol{v}_1^{(2)} = \boldsymbol{v}_{k+1}^{(1)}.$$

Since columns of $W_{2k} := [V_k^{(1)}, V_k^{(2)}]$ form (nonorthogonal) basis of $\mathscr{K}_{2k}(A, \boldsymbol{b})$, we can combine to Arnoldi-like decomposition

$$AW_{2k} = W_{2k} H_{2k} + h_{k+1,k}^{(2)} \boldsymbol{v}_{k+1}^{(2)} \boldsymbol{e}_{2k}^T,$$

$$H_{2k} := \begin{bmatrix} H_k^{(1)} & O \\ h_{k+1,k}^{(1)} \boldsymbol{e}_1 \boldsymbol{e}_k^T & H_k^{(2)} \end{bmatrix}.$$

Arnoldi-like approximation: $\boldsymbol{f}_{2k} = W_{2k} f(H_{2k}) \boldsymbol{e}_1$.

Interpretation: $\boldsymbol{f}_{2k} = p_{2k-1}(A)\boldsymbol{b}$, where p_{2k-1} interpolates f at $\Lambda(H_{2k}) = \Lambda(H_k^{(1)}) \cup \Lambda(H_k^{(2)})$.

[Eiermann & Ernst, 2006]

4 Convergence

The simplest example: $k = 1$

Smallest possible restart length ($k = 1$) leads to

$$AV_m = V_m B_m + \beta_{m+1} \boldsymbol{v}_{m+1} \boldsymbol{e}_m^T$$

with

$$B_m = \begin{bmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & \beta_m & \alpha_m \end{bmatrix}$$

where the columns $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m$ of V_m are a basis of $\mathscr{K}_m(A, \boldsymbol{b})$ such that $\|\boldsymbol{v}_j\| = 1$, $\boldsymbol{v}_j \perp \boldsymbol{v}_{j+1}$ $(j = 1, 2, \ldots)$.

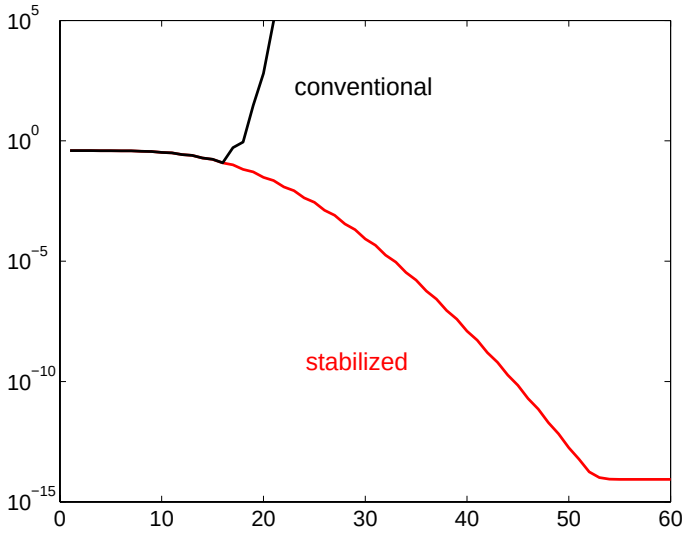
Now, with $\beta_1 = \|\boldsymbol{b}\| = 1$,

$$\boldsymbol{f}_{m+1} = \beta_1 [V_m \ \boldsymbol{v}_{m+1}] f\left(\begin{bmatrix} B_m & \boldsymbol{0} \\ \beta_{m+1}\boldsymbol{e}_m^T & \alpha_{m+1} \end{bmatrix} \right) \boldsymbol{e}_1 = \boldsymbol{f}_m + \beta_1 \left(\boldsymbol{e}_{m+1}^T f(B_{m+1}) \boldsymbol{e}_1 \right) \boldsymbol{v}_{m+1}$$

$$= \boldsymbol{f}_m + \left(\prod_{j=1}^{m+1} \beta_j \right) \ \Delta_f^m(\alpha(1:m+1)) \, \boldsymbol{v}_{m+1}$$

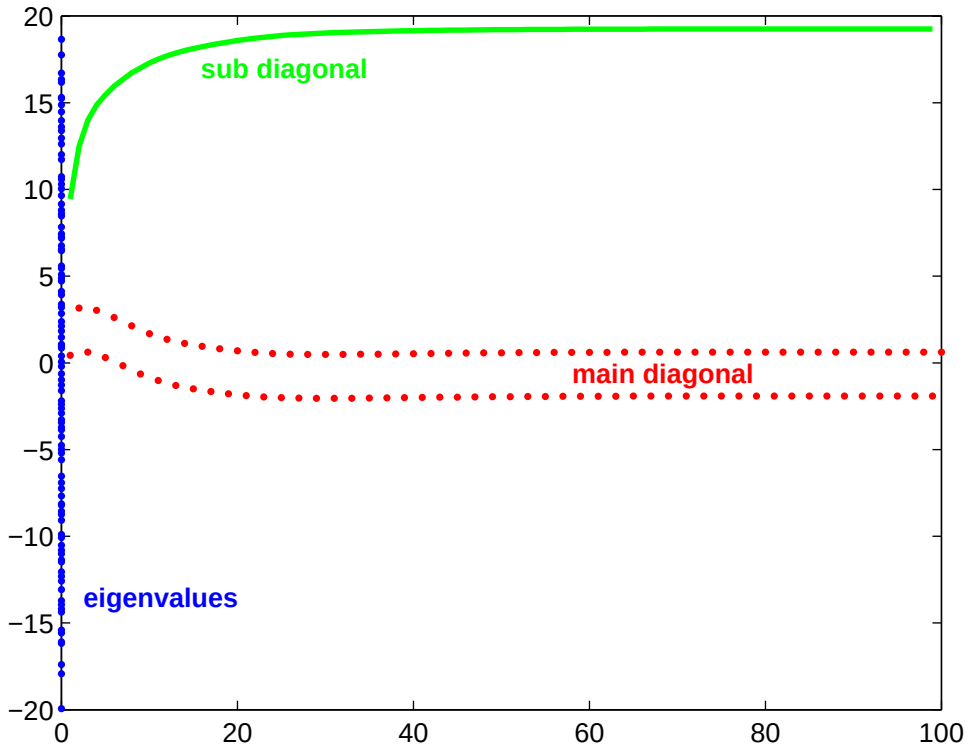
by a Theorem of [Opitz, 1964]. One can show: For $f(z) = 1/z$ and A spd this method coincides with the Steepest Descent Method.

The standard evaluation of the finite differences leads to dramatic cancellation:



Assume that

- A is Hermitian with eigenvalues $\lambda_1 < \lambda_2 < \cdots < \lambda_N$ and eigenvectors $\boldsymbol{x}_j$, $\|\boldsymbol{x}_j\| = 1$.
- $\boldsymbol{b} = \sum_j \gamma_j \boldsymbol{x}_j$, $\|\boldsymbol{b}\|^2 = \sum_j |\gamma_j|^2 = 1$, $\gamma_j \neq 0$.



Theorem 1 *There are $c, s \in \mathbb{R} \setminus \{0\}$, $c^2 + s^2 = 1$, depending on λ_j, $|\gamma_j|^2$ such that*

$$\lim_{m\to\infty} \alpha_{2m} = \zeta_1 := c^2\lambda_1 + s^2\lambda_N,$$
$$\lim_{m\to\infty} \alpha_{2m+1} = \zeta_2 := s^2\lambda_1 + c^2\lambda_N.$$

Thus, if f has finite singularities,

$$\limsup_{m\to\infty} \|f(A)\boldsymbol{b} - \boldsymbol{f}_m\|^{1/m} = \limsup_{m\to\infty} \left[\max_{1\le j\le N} |f(\lambda_j) - q_{m-1}(\lambda_j)|\right]^{1/m} = \frac{\kappa_A}{\kappa_f},$$

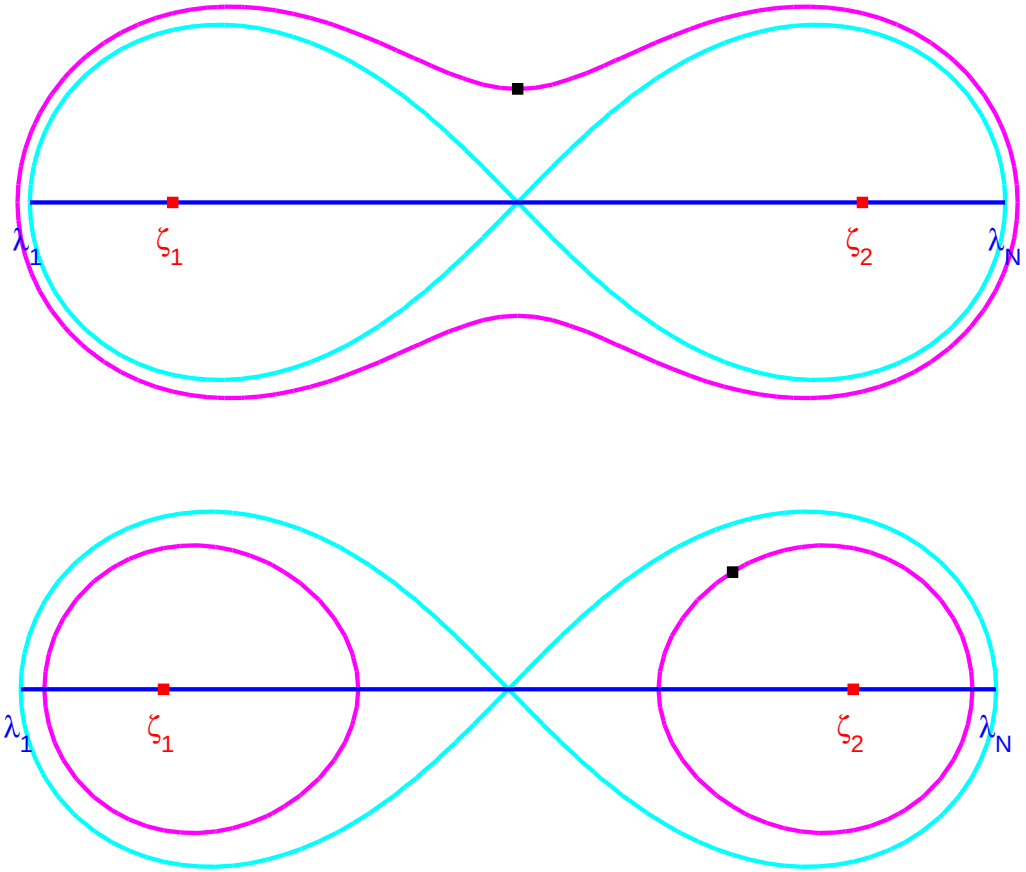
where $q_{m-1} \in \mathscr{P}_{m-1}$ interpolates f in ζ_1 (with multiplicity $\lfloor m/2+1 \rfloor$) and in ζ_2 (with multiplicity $\lfloor m/2 \rfloor$).

$$\Gamma_\rho := \{z \in \mathbb{C} : |z-\zeta_1||z-\zeta_2| = \rho^2\}$$

(lemniscate with foci ζ_1, ζ_2)

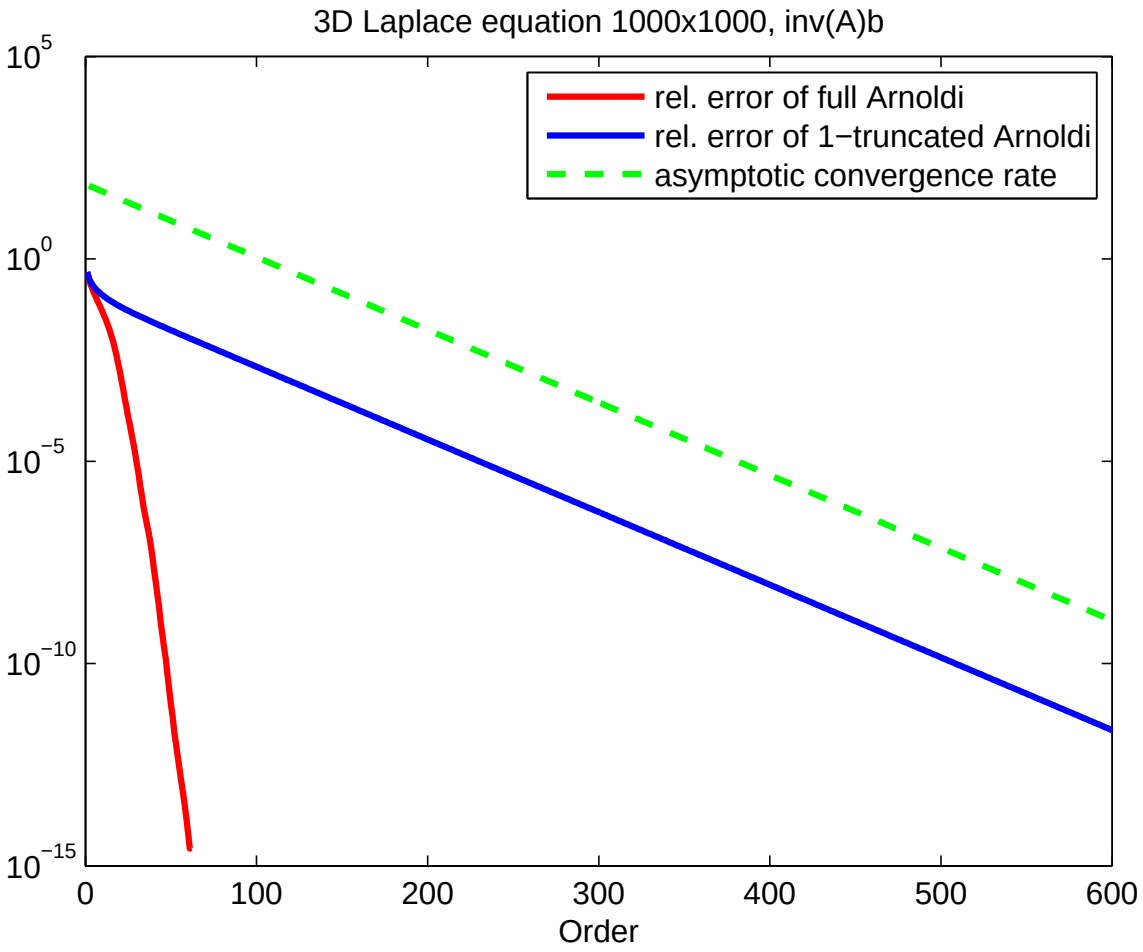
$$\kappa_A := \min\{\rho > 0 : \Lambda(A) \subset \operatorname{int}\Gamma_\rho \cup \Gamma_\rho\},$$

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



Summary. For $k = 1$, the restarted Arnoldi method is asymptotically equivalent to cyclic interpolation at two nodes which are both convex combinations of λ_1 and λ_N.

If f is an analytic (but not an entire) function then the restarted Arnoldi method converges (diverges) asymptotically like θ^m, where θ is determined by the singularities of f and the spectrum of A.


3D Laplace equation 1000x1000, inv(A)b
rel. error of full Arnoldi
rel. error of 1−truncated Arnoldi
asymptotic convergence rate
10^5
10^0
10^−5
10^−10
10^−15
0
100
200
300
400
500
600
Order

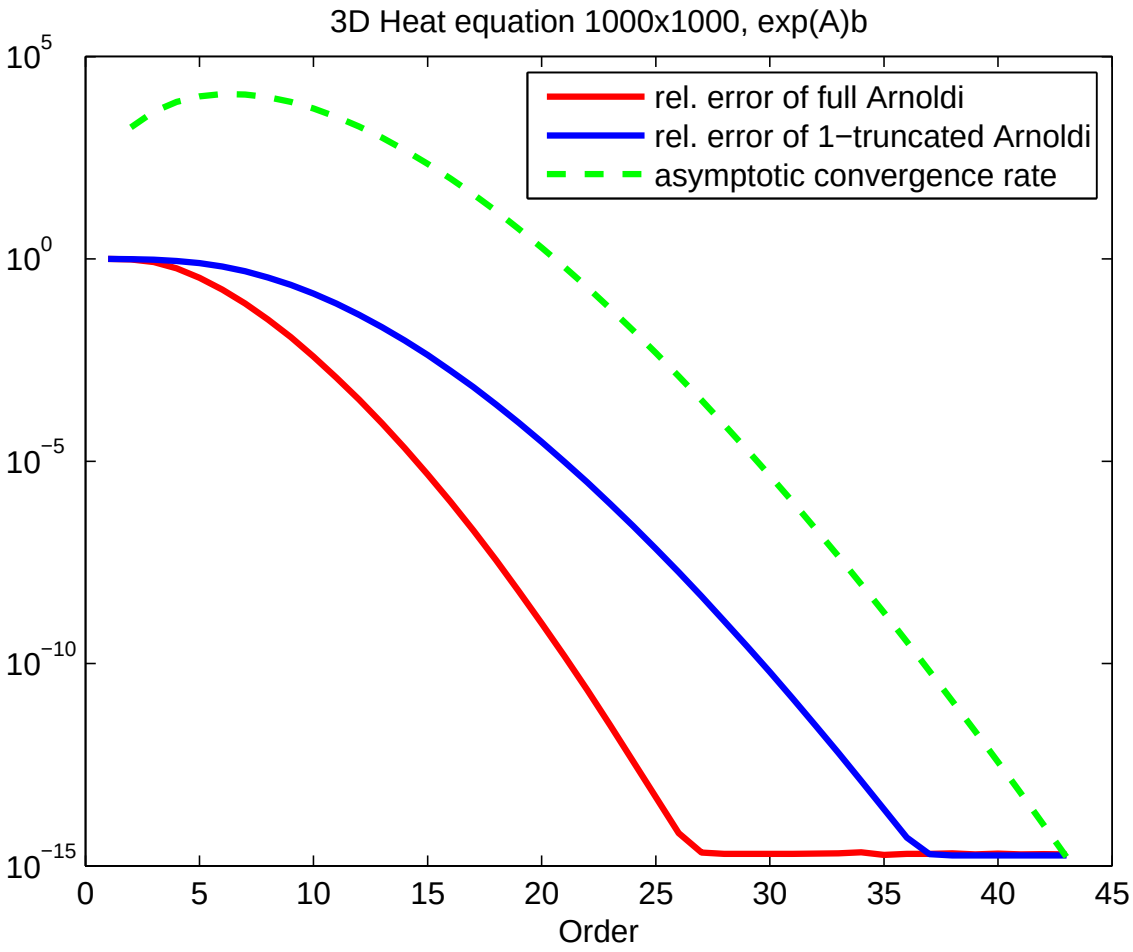
Theorem 2 *If* $f(z) = \exp(\tau z)$, $\tau > 0$, *then*

$$\begin{aligned}\limsup_{m\to\infty} \left[m! \, \|f(A)\boldsymbol{b} - \boldsymbol{f}_m\|\right]^{1/m} &= \limsup_{m\to\infty} \left[m! \left(\max_{1\le j\le N} |f(\lambda_j) - q_{m-1}(\lambda_j)|\right)\right]^{1/m} \\ &= \tau\delta,\end{aligned}$$

where $q_{m-1} \in \mathscr{P}_{m-1}$ *interpolates* f *in* ζ_1 *(with multiplicity* $\lfloor m/2+1 \rfloor$*) and in* ζ_2 *(with multiplicity* $\lfloor m/2 \rfloor$*) and*

$$\delta = \min\left\{\delta \,:\, |\lambda - \zeta_1||\lambda - \zeta_2| \le \delta^2 \quad \forall \lambda \in \Lambda(A)\right\}.$$

Summary. If f is an entire function of order 1 and type τ then the restarted Arnoldi method ($k = 1$) converges (always!) superlinearly like $(\tau\delta/m)^m$.


3D Heat equation 1000x1000, exp(A)b
rel. error of full Arnoldi
rel. error of 1−truncated Arnoldi
asymptotic convergence rate
10^{5}
10^{0}
10^{-5}
10^{-10}
10^{-15}
0
5
10
15
20
25
30
35
40
45
Order

Tools used in proof. Consider the basis vectors

$$\boldsymbol{v}_1 = \frac{\boldsymbol{b}}{\|\boldsymbol{b}\|},\ \boldsymbol{v}_{m+1} = \frac{A\boldsymbol{v}_m - \alpha_m \boldsymbol{v}_m}{\beta_{m+1}} = \frac{A\boldsymbol{v}_m - (\boldsymbol{v}_m^T A\boldsymbol{v}_m)\boldsymbol{v}_m}{\|A\boldsymbol{v}_m - (\boldsymbol{v}_m^T A\boldsymbol{v}_m)\boldsymbol{v}_m\|},\ m = 1, 2, \ldots$$

Write $\boldsymbol{v}_m = \sum_{j=1}^{N} \gamma_{m,j}\boldsymbol{x}_j$, $\sum_j |\gamma_{m,j}|^2 = 1$, and define discrete probability distributions

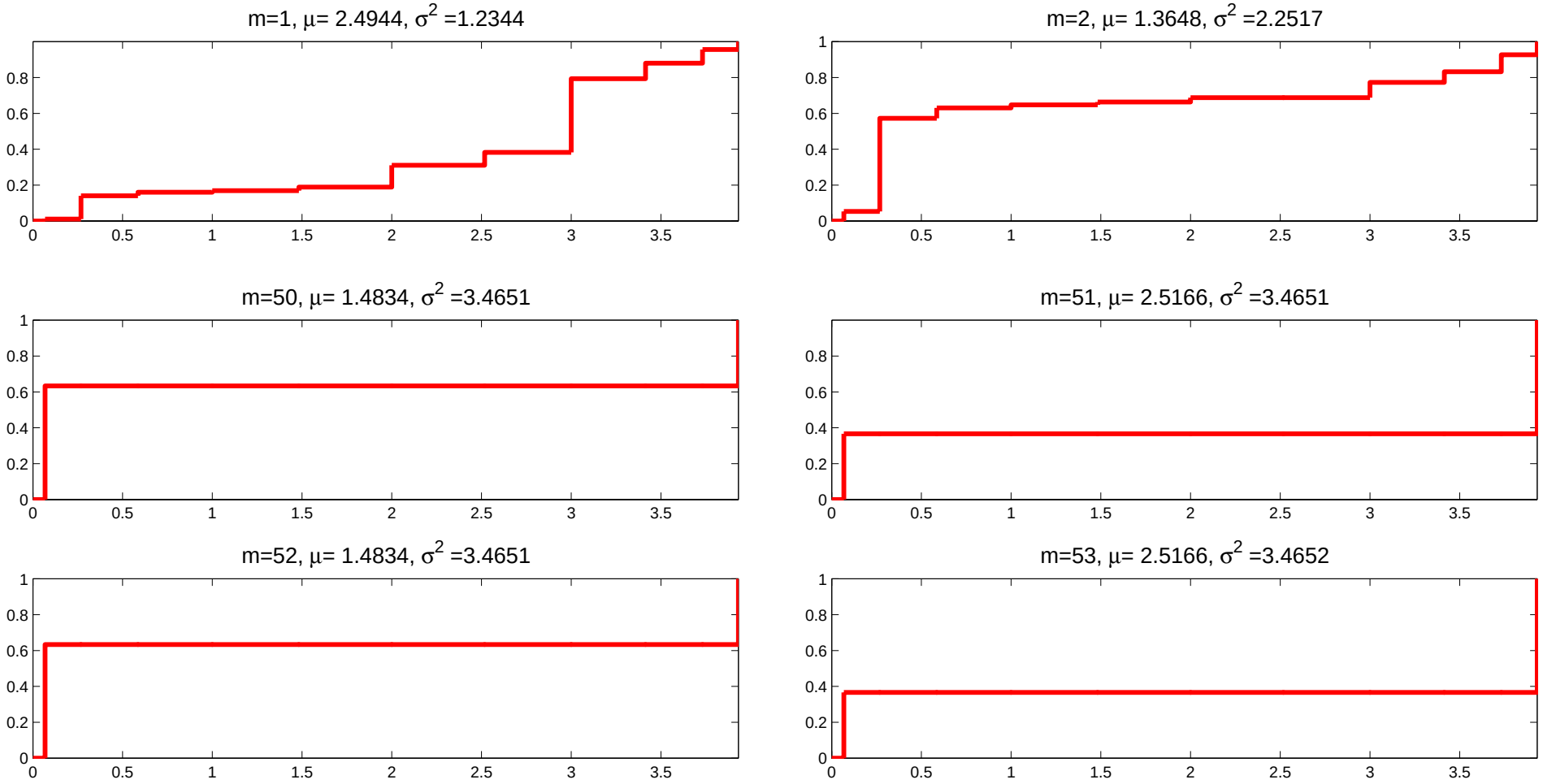
$$w_m(x) := \begin{cases} 0, & x < \lambda_1, \\ \sum_{j=1}^{k} |\gamma_{m,j}|^2, & \lambda_k \le x < \lambda_{k+1}, \\ 1, & \lambda_N \le x \end{cases}$$

with

$$\text{means} \qquad \mu_m = \sum \lambda_j |\gamma_{m,j}|^2 = \boldsymbol{v}_m^T A \boldsymbol{v}_m,$$

$$\text{and variances} \qquad \sigma_m^2 = \sum (\lambda_j - \mu_m)^2 |\gamma_{m,j}|^2 = \|A\boldsymbol{v}_m - (\boldsymbol{v}_m^T A\boldsymbol{v}_m)\boldsymbol{v}_m\|^2.$$

(Note that $\mu_m = \alpha_m$ and $\sigma_m^2 = \beta_{m+1}^2$.)



The (non-linear) transformation $\boldsymbol{v}_{m+1} = T(\boldsymbol{v}_m)$ translates into a transformation $w_{m+1} = T(w_m)$ of the corresponding distributions.

Hirotuko Akaike [1959] showed:

Theorem 3 *For any discrete probability distribution* w*,*

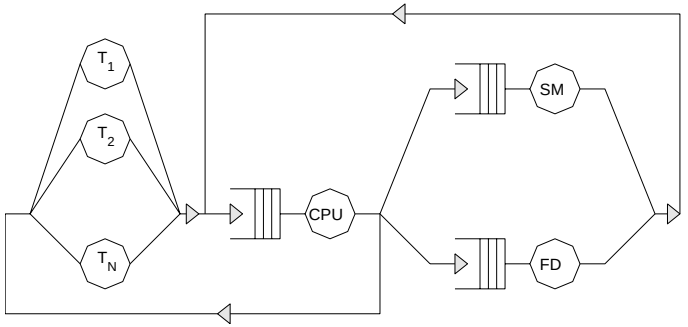
$$\operatorname{Var} T(w) \geq \operatorname{Var} w$$

with equality holding if and only if the support of w *consists of two points.*

The sequence $\{T^m(w)\}$ *ultimately alternates between two probability distributions which are both supported on* λ_1 *and* λ_N*.*

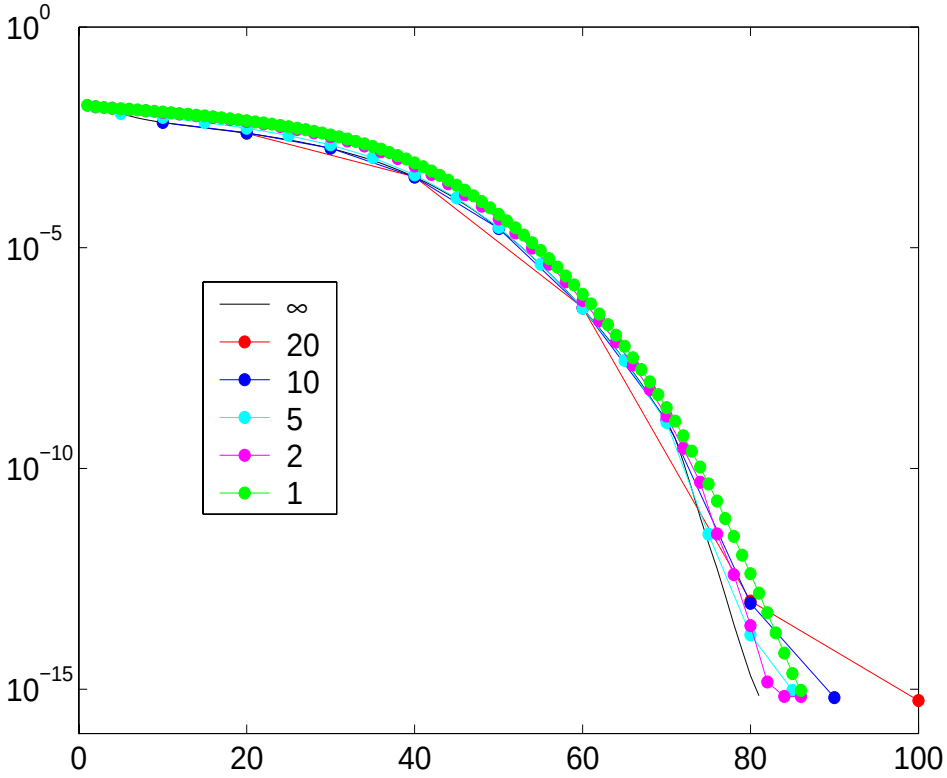
In addition, well known results on the interpolation of analytic functions (see [Walsh, 1969], [Gaier, 1980]) and new results on the interpolation of entire functions are used. □

Summary. For $k = 1$, the restarted Arnoldi method is asymptotically equivalent to interpolation at two nodes which are both convex combinations of λ_1 and λ_N.



Last example: time-continuous Markov chain

[Philippe, Saad & Stewart, 1996]
$N = 62169$, $\rho(A) = 70$.



m	k	time [s]
∞	1	75.4
20	5	11.0
10	9	5.8
5	17	3.7
2	43	3.2
1	86	3.4

Summary

- The presented method requires only minimal storage costs even for very large matrices.
- The asymptotic convergence behavior is (nearly) understood (up to the location of ζ_1, ζ_2).

Interesting questions

- Impact on the convergence analysis of restarted/truncated Arnoldi method for $k > 1$?
- Non-Hermitian, non-normal case?

Vielen Dank für Ihre Aufmerksamkeit...

... und Guten Appetit!