Rational Krylov sequences and orthogonal rational functions

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Outline

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Problem formulation

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- Consider:

$$\frac{d}{dt}u(t) + Au(t) = h(t), \quad t \in [t_0, t_1], \quad u(t_0) = u_0.$$

- Suppose:
  - $A \in \mathbb{R}^{N \times N}$ is symmetric positive-definite,
  - solution: $u(t) = g(A, t)q(t)$, with $q(t) \in \mathbb{R}^N$,
  - $t = T \in [t_0, t_1]$ is fixed $\Rightarrow f(a) = g(a, T)$ and $q = q(T)$.
- We search for numerical approximations to

$$u = u(T) = f(A)q.$$

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Preliminaries

Krylov subspaces

- searching for polynomial approximations $u^{(m)}$ to u belonging to the Krylov subspaces

$$K_{m+1}(A, q) = \text{span}\{q, Aq, A^2q, \ldots, A^mq\}, \quad m \ll N.$$

- orthogonalize:

$$K_{m+1}(A, q) = \text{span}\{q_0, q_1, q_2, \ldots, q_m\},$$

with

$$q_j^T q_k = \begin{cases} 0, & j \neq k \\ 1, & j = k \end{cases}.$$

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Orthogonal polynomials (OPs)

- $q_k = \phi_k(A)q$,
  where $\phi_k(a) =$ orthonormal polynomial of strict degree k.
- three-term recurrence:

$$Aq_{k-1} = \beta_{k-2}q_{k-2} + \alpha_{k-1}q_{k-1} + \beta_{k-1}q_k, \quad k = 1, \ldots, m$$

with $q_{-1} = 0$ and $q_0 = q/\|q\|$.

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$Q_m^T A Q_m = J_m$, where $Q_m = [q_0, \ldots, q_{m-1}]$, and

$$J_m = \begin{bmatrix} \alpha_0 & \beta_0 & 0 & \cdots & 0 \\ \beta_0 & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \beta_{m-2} \\ 0 & \cdots & 0 & \beta_{m-2} & \alpha_{m-1} \end{bmatrix}.$$

Polynomial approximation

Eigenvalues λ_k, $k = 1, \ldots, m$ of J_m are

- zeros of $\phi_m(a)$,
- approximations for eigenvalues of A.

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$$\begin{aligned} \Rightarrow u^{(m)} &= Q_m f(J_m) Q_m^T q \\ &= Q_m f(J_m) \|q\| e_1^{(N)}. \end{aligned}$$

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$\Rightarrow$ searching for rational approximations to u belonging to rational Krylov subspaces.

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Rational Krylov subspaces

Rational Krylov subspaces (RKS)

- Suppose $\mathcal{M} = \{\mu_0 = \mu_1, \mu_2, \ldots, \mu_m\} \subset \mathbb{R}^+$.
- Define the factors

$$\begin{aligned} Z_k(A) &= (I + \mu_k A)^{-1} A = A(I + \mu_k A)^{-1} \\ &= \frac{A}{I + \mu_k A}, \quad k = 1, 2, \ldots, m, \end{aligned}$$

and products

$$\begin{aligned} b_0(A) &\equiv I, \\ b_k(A) &= Z_k(A) b_{k-1}(A) = b_{k-1}(A) Z_k(A), \\ & \qquad k = 1, 2, \ldots, m. \end{aligned}$$

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- $q_k = \varphi_k(A)q$,
  where $\varphi_k(a) = \frac{p_k(a)}{(1+\mu_1 a)\cdot\ldots\cdot(1+\mu_k a)}$ = orthonormal rational function.
- under *certain conditions on the poles* $\longrightarrow$ three-term recurrence:

$$\begin{aligned} Aq_{k-1} = \beta_{k-2}\left(I + \mu_{k-2}A\right)q_{k-2} \\ + \alpha_{k-1}\left(I + \mu_{k-1}A\right)q_{k-1} + \beta_{k-1}\left(I + \mu_k A\right)q_k, \end{aligned}$$

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Conditions on the poles:

- $\mathcal{M} \cap \sigma(-A^{-1}) = \emptyset$
  $\rightarrow$ OK because $\mathcal{M} \subset \mathbb{R}^+$,
- $\forall k > 0 : q_{k-1}^T Z_k(A) q_{k-1} \neq (\mu_k - \mu_{k-1})^{-1}$
  $\rightarrow$ OK if $\mu_{k-1} \geq \mu_k$,
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$Q_m^T A Q_m = J_m(I_m - D_m J_m)^{-1} + R_m$, where

$$D_m = \begin{bmatrix} \mu_0 & 0 & \cdots & 0 \\ 0 & \mu_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \mu_{m-1} \end{bmatrix}$$

and

$$R_m = \beta_{m-1}\mu_m g_m h_m^T,$$

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Note that

- $B_m \triangleq J_m(I_m - D_m J_m)^{-1} = (I_m - J_m D_m)^{-1} J_m$ is symmetric,
- eigenvalues $\tilde{\lambda}_k$, $k = 1, \ldots, m$ of B_m are zeros of $\varphi_m(a)$,
- if $\mu_k = \mu$ for $k = 0, \ldots, m$
  $\Rightarrow$ eigenvalues of J_m are approximations for eigenvalues of $\frac{A}{I+\mu A}$
  $\Rightarrow$ eigenvalues of $B_m = \frac{J_m}{I_m - \mu J_m}$ are approximations for eigenvalues of A.

Therefore:

- omit R_m: $Q_m^T A Q_m \approx J_m(I_m - D_m J_m)^{-1}$,
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- if $\mu_k = \mu$ for $k = 0, \ldots, m$
  $\Rightarrow$ eigenvalues of J_m are approximations for eigenvalues of $\frac{A}{I+\mu A}$
  $\Rightarrow$ eigenvalues of $B_m = \frac{J_m}{I_m - \mu J_m}$ are approximations for eigenvalues of A.

Therefore:

- omit R_m: $Q_m^T A Q_m \approx J_m(I_m - D_m J_m)^{-1}$,
- $\tilde{\lambda}_k$, $k = 1, \ldots, m$ are approximations for eigenvalues of A.

Rational approximation

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- $u^{(m)} = r_m(A)q$ with $r_m(\tilde{\lambda}_k) = f(\tilde{\lambda}_k)$, $k = 1, \ldots, m$
  where $r_m(a) = \frac{p_m(a)}{(1+\mu_1 a)\cdot\ldots\cdot(1+\mu_m a)}$.
  $\Rightarrow u^{(m)} = Q_m f(B_m) Q_m^T q = Q_m f(B_m) \|q\| e_1^{(N)}$.
- generalized eigenvalue problem:

$$(I_m + J_m D_m)\tilde{\lambda}_k v_k = J_m v_k \Rightarrow B_m = V_m \Lambda_m V_m^T,$$

with $V_m = [v_1, \ldots, v_m]$ and $\Lambda_m = \mathrm{diag}(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_m)$

$$\Rightarrow u^{(m)} = Q_m V_m f(\Lambda_m) V_m^T \|q\| e_1^{(N)}.$$

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Outline

Computing Q_m and J_m

Computing Q_m and J_m

Let

$$\begin{aligned} x_{k-1} &= Z_k(A)\left\{\beta_{k-2}\left(\mu_k - \mu_{k-2}\right) q_{k-2} + q_{k-1}\right\} - \beta_{k-2} q_{k-2} \\ y_{k-1} &= \left[I + \left(\mu_{k-1} - \mu_k\right) Z_k(A)\right] q_{k-1}. \end{aligned}$$

Then,

$$\begin{aligned} \alpha_{k-1} &= \frac{q_l^T x_{k-1}}{q_l^T y_{k-1}}, \quad l \in \{0, \ldots, k-1\} \\ \beta_{k-1} &= \|x^{k-1} - \alpha_{k-1} y_{k-1}\| \\ q_k &= \beta_{k-1}^{-1}\left(x_{k-1} - \alpha_{k-1} y_{k-1}\right). \end{aligned}$$

For $k = 1$: $x_0 = Z_1(A) q_0$ and $y_0 = q_0$.

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Computing Q_m and J_m

Computational effort

If $\mu_k \neq 0$, we need to solve per iteration

- 1 system of equations whenever $\mu_k = \mu_{k-1}$ and/or $\mu_k = \mu_{k-2}$,
- 2 systems of equations whenever $\mu_k \neq \mu_{k-1}$ and $\mu_k \neq \mu_{k-2}$.

Therefore,

- use a limited number of different values in $\mathcal{M}$,
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Outline

Numerical example

Time-periodic problem

$$\frac{d}{dt}u(t) + (A + 0.6I)u(t) = \exp(-0.4t)q, \quad t \in [0, T],$$
$$u(0) = u(T), \quad T = 0.01,$$

where

- $A = 2500 \times 2500$ matrix obtained by discretization of

$$L = -0.1\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right), \quad (x, y) \in [0, 1] \times [0, 1],$$

  with Dirichlet boundary conditions, on a uniform meshgrid, using central differences,
- $q =$ discretization of $q(x, y) = x(1 - x)y(1 - y)$.

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Numerical example

Exact solution

- $u(t) = g(A, t)q$, with

$$g(a,t) = \frac{\exp(-0.4t)}{a+0.2} - \frac{[1-\exp(-0.4T)]\exp(-(a+0.6)t)}{(a+0.2)[1-\exp(-(a+0.6)T)]}.$$

- For $t = 0$ or $t = T$:

$$f(a) = \frac{\exp(-0.4T)[1-\exp(-(a+0.2)T)]}{(a+0.2)[1-\exp(-(a+0.6)T)]}.$$

$\Rightarrow$ $f(a)$ has singularity in $a = -3/5$

$f(\infty) = 0.$

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Numerical example

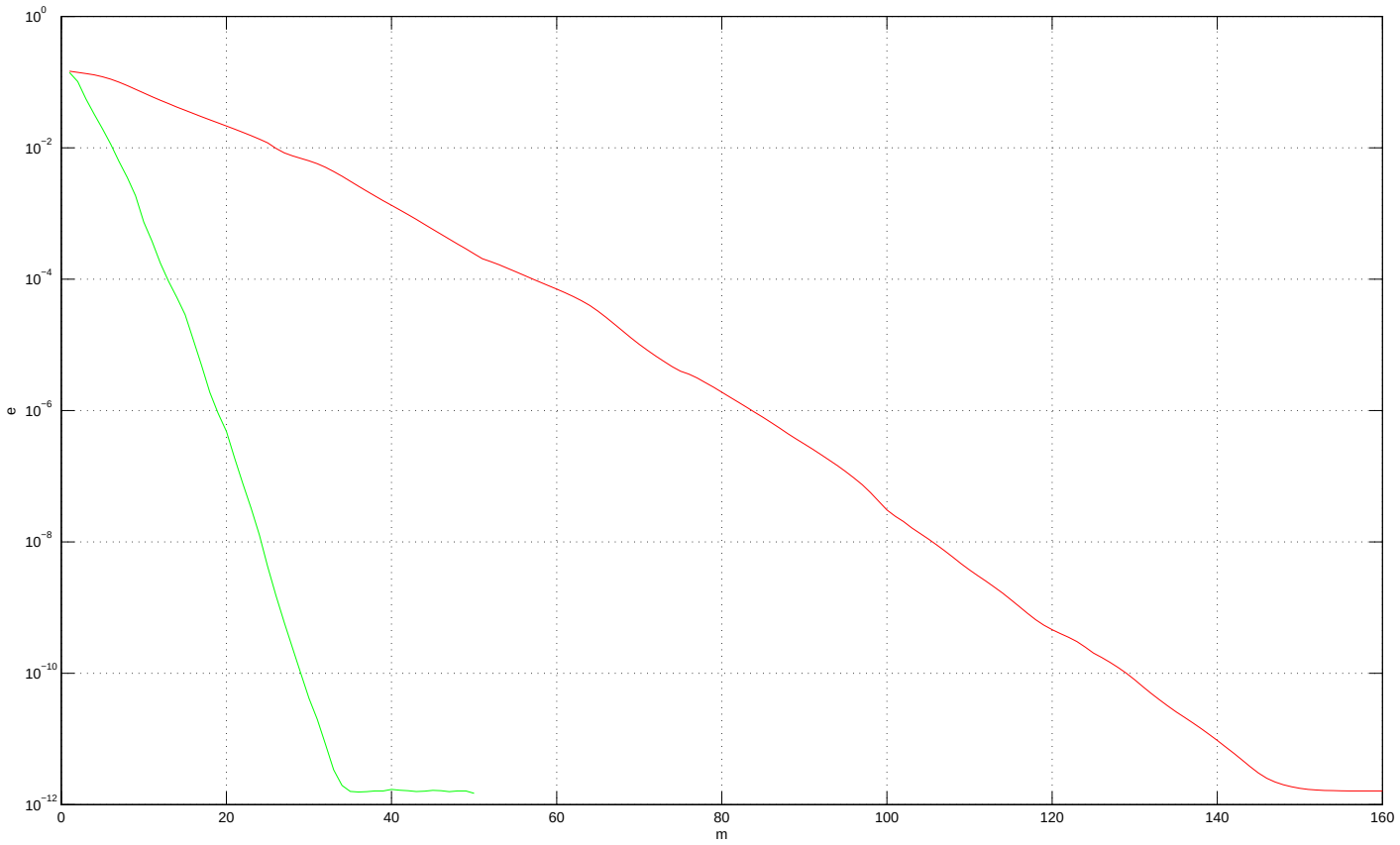
One multiple pole

optimal value: $\mu \approx T$, see:

I. Moret and P. Novati, *"A rational Krylov method for solving time-periodic differential equations"*, Appl. Num. Math., 58:212-222, 2008.

Numerical example

Relative error $e = \|u^{(m)} - u\|/\|u\|$ for the case of $\mu = 0$, respectively $\mu = 0.01$.



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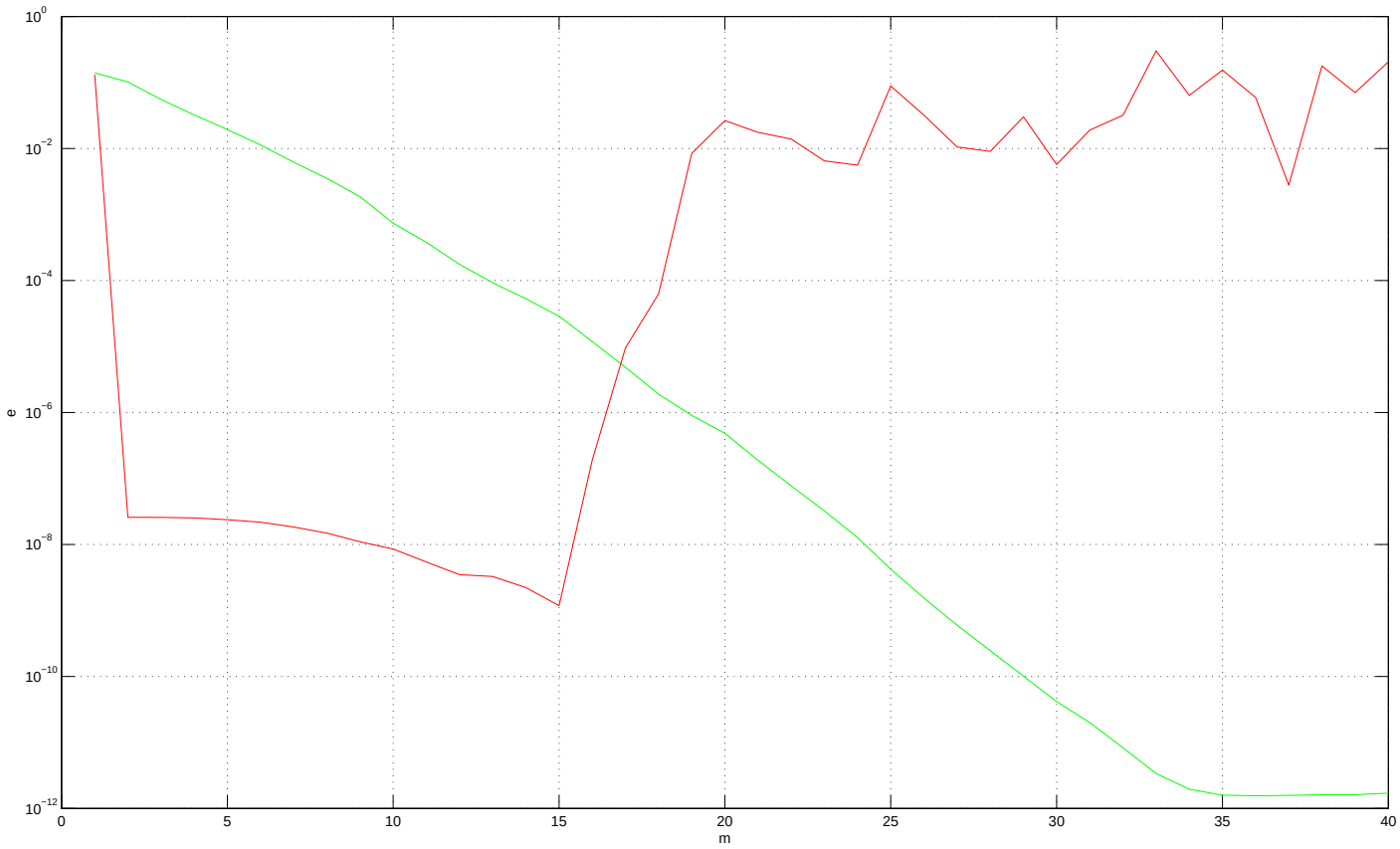
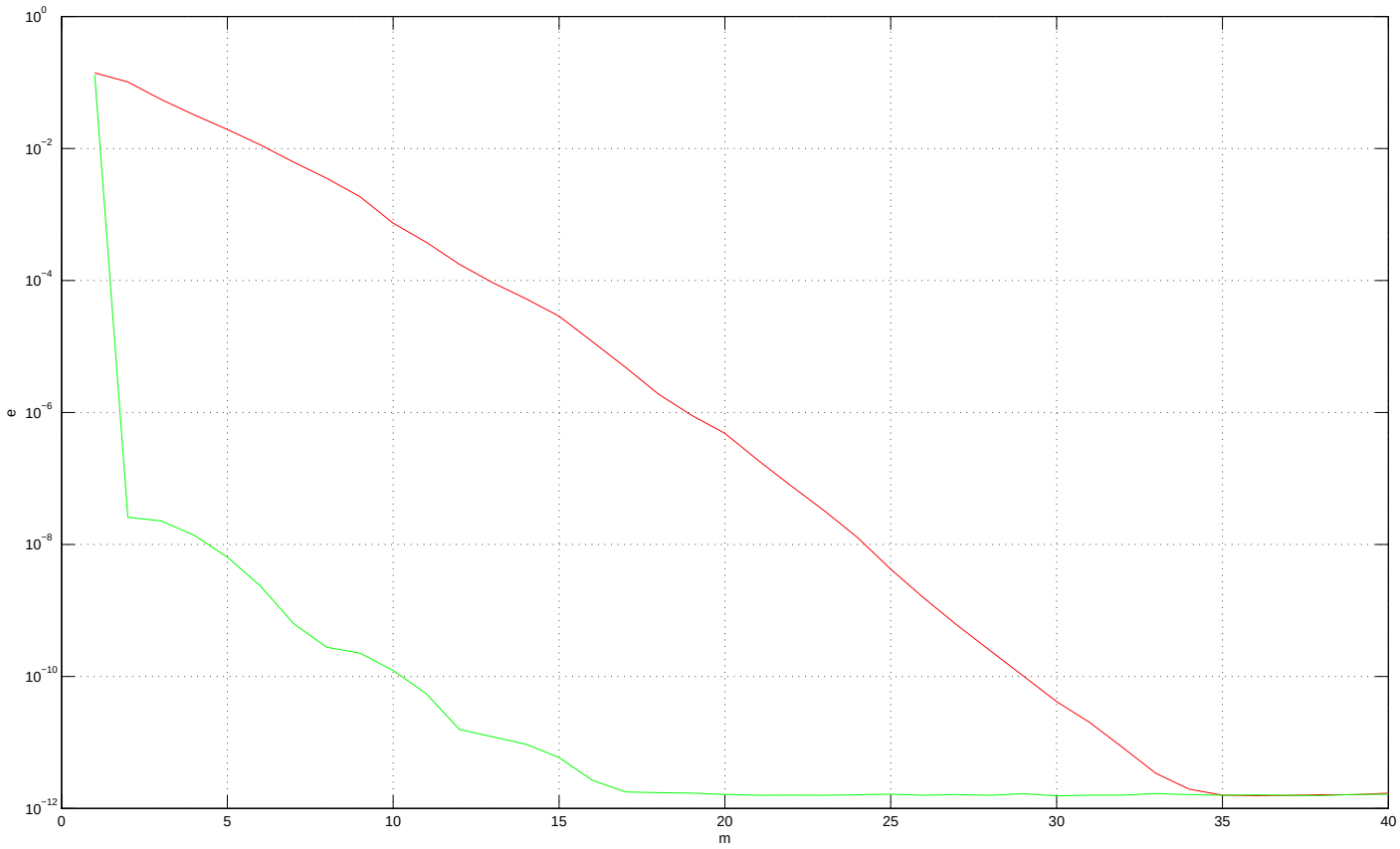
Relative error $e = \|u^{(m)} - u\|/\|u\|$ for the case of $\mu = 5/3$, respectively $\mu = 0.01$.



Numerical example

Relative error $e = \|u^{(m)} - u\|/\|u\|$ for the case of $\mu_0 = \mu_1 = 5/3$ and $\mu_2 = \ldots = \mu_{40} = 0.01$, respectively $\mu = 0.01$.



Numerical example

$\mathcal{M}$	e	m	CF	SOE
$\mu = 0$	$9.5e-12$	140	0	0
$\mu = 0.01$	$8.3e-12$	32	1	32
$\{5/3, 5/3, 0.01, \ldots\}$	$9.4e-12$	14	2	15

CF = total number of Cholesky Factorizations
SOE = total number of Systems Of Equations