Rational Krylov sequences and orthogonal rational functions

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## Outline

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   - Problem formulation
   - Preliminaries

2. Rational Krylov subspaces
   - RKS
   - Rational approximation

3. Computational aspects
   - Computing $Q_m$ and $J_m$

4. Numerical example
   - Time-periodic problem
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Problem formulation

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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Krylov subspaces

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

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

- orthogonalize:

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

with

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

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Orthogonal polynomials (OPs)

- \( q_k = \phi_k(A)q \),
  where \( \phi_k(a) = \text{orthonormal polynomial} \) 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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Preliminaries

**OPs**

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

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

**Polynomial approximation**

Eigenvalues \( \lambda_k, k = 1, \ldots, m \) of \( J_m \) are

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

\[ u^{(m)} = p_m(A)q \text{ with } p_m(\lambda_k) = f(\lambda_k), \ k = 1, \ldots, m \]

\[ \Rightarrow u^{(m)} = Q_m f(J_m) Q_m^T q = Q_m f(J_m) \|q\| e_1^{(N)}. \]

Problem

Polynomial approximations may converge very slowly
\[ \Rightarrow \] searching for rational approximations to \( u \) belonging to rational Krylov subspaces.
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Rational Krylov subspaces

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

$$Z_k(A) = (I + \mu_k A)^{-1}A = A(I + \mu_k A)^{-1}$$

$$= \frac{A}{I + \mu_k A}, \quad k = 1, 2, \ldots, m,$$

and products

$$b_0(A) \equiv I,$$

$$b_k(A) = Z_k(A)b_{k-1}(A) = b_{k-1}(A)Z_k(A),$$

$$k = 1, 2, \ldots, m.$$
Rational Krylov subspaces (RKS)

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Rational Krylov subspaces

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

$$K_{m+1}(A, q, M) = \text{span}\{b_0(A)q, b_1(A)q, \ldots, b_m(A)q\}, \quad m \ll N.$$ 

- orthogonalize:

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Orthogonal rational functions (ORFs)

- $q_k = \varphi_k(A)q$, where
  
  $$\varphi_k(a) = \frac{p_k(a)}{(1+\mu_1 a)\ldots(1+\mu_k a)} = \text{orthonormal rational function}.$$ 

- under certain conditions on the poles → three-term recurrence:

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

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

Rational Krylov subspaces
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Rational Krylov subspaces

ORFs

Conditions on the poles:

1. $\mathcal{M} \cap \sigma(-A^{-1}) = \emptyset$
   - OK because $\mathcal{M} \subset \mathbb{R}^+$,

2. $\forall k > 0 : q_k^T Z_k(A) q_{k-1} \neq (\mu_k - \mu_{k-1})^{-1}$
   - OK if $\mu_{k-1} \geq \mu_k$,

3. $\forall k > 1 : \varphi_{k-1}(a) = \frac{p_{k-1}(a)}{(1+\mu_1 a) \cdots (1+\mu_{k-1} a)} \Rightarrow p_{k-1}(-\mu_k^{-1}) \neq 0$
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Rational Krylov subspaces

**ORFs**

\[
Q^T_m AQ_m = J_m(I_m - D_m J_m)^{-1} + R_m,
\]

where

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

and

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

\[
g_m = Q^T_m A q_m, \quad h_m = (I_m - J_m D_m)^{-1} e_m^{(m)}
\]

\[\Rightarrow \text{rank}(R_m) \leq 1\]
Rational Krylov subspaces

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Rational approximation

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

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

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- 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 $A$.

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Rational approximation

- $u^{(m)} = r_m(A)q$ with $r_m(\tilde{\lambda}_k) = f(\tilde{\lambda}_k)$, $k = 1, \ldots, m$
  where $r_m(a) = \frac{p_m(a)}{(1+\mu_1a)\cdots(1+\mu_ma)}$.

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

- Generalized eigenvalue problem:

  $\begin{pmatrix} I_m & J_m D_m \end{pmatrix} \tilde{\lambda}_k v_k = J_m v_k \Rightarrow B_m = V_m \Lambda_m V_m^T,$

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

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**generalized eigenvalue problem:**

\[ (I_m + J_mD_m)\tilde{\lambda}_k v_k = J_m v_k \Rightarrow B_m = V_m \Lambda_m V_m^T, \]
with \( V_m = [v_1, \ldots, v_m] \) and \( \Lambda_m = \text{diag}(\tilde{\lambda}_1, \ldots, \tilde{\lambda}_m) \)

\[ \Rightarrow u^{(m)} = Q_m V_m f(\Lambda_m) V_m^T \|q\|_e^{(N)}. \]
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\[ u^{(m)} = r_m(A)q \] with \( r_m(\tilde{\lambda}_k) = f(\tilde{\lambda}_k), \ k = 1, \ldots, m \)

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Outline

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   - Problem formulation
   - Preliminaries

2 Rational Krylov subspaces
   - RKS
   - Rational approximation

3 Computational aspects
   - Computing $Q_m$ and $J_m$

4 Numerical example
   - Time-periodic problem
Computing $Q_m$ and $J_m$

Let

$$
x_{k-1} = Z_k(A) \{ \beta_{k-2} (\mu_k - \mu_{k-2}) q_{k-2} + q_{k-1} \} - \beta_{k-2} q_{k-2},
$$

$$
y_{k-1} = [I + (\mu_{k-1} - \mu_k) Z_k(A)] q_{k-1}.
$$

Then,

$$
\alpha_{k-1} = \frac{q_i^T x_{k-1}}{q_i^T y_{k-1}}, \quad l \in \{0, \ldots, k-1\}
$$

$$
\beta_{k-1} = \| x_{k-1} - \alpha_{k-1} y_{k-1} \|
$$

$$
q_k = \beta_{k-1}^{-1} (x_{k-1} - \alpha_{k-1} y_{k-1}).
$$

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

Let
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\begin{align*}
x_{k-1} &= Z_k(A) \{ \beta_{k-2} (\mu_k - \mu_{k-2}) q_{k-2} + q_{k-1} \} - \beta_{k-2} q_{k-2} \\
y_{k-1} &= [I + (\mu_{k-1} - \mu_k) Z_k(A)] q_{k-1}.
\end{align*}
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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 $\mathcal{M}$,
- use a sorted list of numbers,
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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

\[ u(t) = g(A, t)q, \text{ with} \]

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

For \( t = 0 \) or \( t = T \):

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

\[ \Rightarrow f(a) \text{ has singularity in } a = -3/5 \]

\[ f(\infty) = 0. \]
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Numerical example

One multiple pole

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

Relative error $e = \frac{\|u^{(m)} - u\|}{\|u\|}$ for the case of $\mu = 0$, respectively $\mu = 0.01$. 
Relative error $e = \|u^{(m)} - u\| / \|u\|$ for the case of $\mu = 5/3$, respectively $\mu = 0.01$. 

![Graph showing relative error over iterations for different values of $\mu$.]
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

<table>
<thead>
<tr>
<th>$\mathcal{M}$</th>
<th>$e$</th>
<th>$m$</th>
<th>CF</th>
<th>SOE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mu = 0$</td>
<td>$9.5e-12$</td>
<td>140</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\mu = 0.01$</td>
<td>$8.3e-12$</td>
<td>32</td>
<td>1</td>
<td>32</td>
</tr>
<tr>
<td>${5/3, 5/3, 0.01, \ldots}$</td>
<td>$9.4e-12$</td>
<td>14</td>
<td>2</td>
<td>15</td>
</tr>
</tbody>
</table>

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