Rational Lanczos and short term recurrence relations based on orthogonal rational functions

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Outline

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1. Preliminaries
2. Short term recurrence
3. Conclusion and future work

Outline

Krylov sequences and OPs

- $\mathbf{A} \in \mathbb{C}^{N \times N}$ hermitian,
- $\mathbf{b} \in \mathbb{C}^{N}$.
- For $n \leqslant N$,

$$\begin{aligned} \mathcal{K}_n(\mathbf{A}, \mathbf{b}) &= \operatorname{span}\{\mathbf{b}, \mathbf{Ab}, \mathbf{A}^2\mathbf{b}, \ldots, \mathbf{A}^{n-1}\mathbf{b}\} \\ &= \operatorname{span}\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}, \end{aligned}$$

where

$$\mathbf{v}_\ell^* \mathbf{v}_k = \begin{cases} 0, & k \neq \ell \\ \|\mathbf{v}_k\|^2 = 1, & k = \ell. \end{cases}$$

Krylov sequences and OPs

- $\mathbf{v}_{k+1} = P_k(\mathbf{A})\mathbf{b}$, $P_k \in \mathcal{P}_k \setminus \mathcal{P}_{k-1}$.
- There exists a positive measure m on a subset of $\mathbb{R}$ such that

$$\langle P_k , P_\ell \rangle_m = \begin{cases} 0, & k \neq \ell \\ \|P_k\|_m^2 = 1, & k = \ell. \end{cases}$$

Theorem 1

The orthonormal polynomials (OPs) P_k, $k \geqslant 0$, satisfy a 3-term recurrence relation of the form

$$xP_k(x) = \alpha_{k+1}P_{k+1}(x) + \beta_{k+1}P_k(x) + \alpha_k P_{k-1}(x), \quad \alpha_{k+1} \neq 0,$$

with initial conditions $P_{-1}(x) \equiv 0$ and $P_0(x) \equiv \|1\|_m^{-1}$.

- $\mathbf{A}\mathbf{v}_k = \alpha_k \mathbf{v}_{k+1} + \beta_k \mathbf{v}_k + \alpha_{k-1}\mathbf{v}_{k-1}$,
  with $\mathbf{v}_0 = 0$ and $\mathbf{v}_1 = \mathbf{b}/\|\mathbf{b}\|$.

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Rational Krylov sequences and ORFs

- $\mathbf{A} \in \mathbb{C}^{N \times N}$ hermitian,
- $\mathbf{b} \in \mathbb{C}^{N}$,
- sequence of poles $\mu = \{\mu_1, \mu_2, \ldots\} \subset \overline{\mathbb{C}} \setminus (\Lambda(\mathbf{A}) \cup \{\mu_\emptyset\})$, $\overline{\mathbb{C}} := \mathbb{C} \cup \{\infty\}$.
- For $n \leqslant N$,

$$\mathcal{K}_n^r(\mathbf{A}, \mathbf{b}, \mu) = \mathrm{span}\{B_0(\mathbf{A})\mathbf{b}, B_1(\mathbf{A})\mathbf{b}, B_2(\mathbf{A})\mathbf{b}, \ldots, B_{n-1}(\mathbf{A})\mathbf{b}\}$$

where

$$B_0(x) \equiv 1, \quad \text{and} \quad B_k(x) = \left[\frac{x - \mu_\emptyset}{1 - \frac{x - \mu_\emptyset}{\mu_k - \mu_\emptyset}} \right] B_{k-1}(x).$$

Rational Krylov sequences and ORFs

Remarks

- The nested subspaces of rational functions: $\mathcal{L}_{-1} = \{0\}$, $\mathcal{L}_0 = \mathbb{C}$, and

$$\begin{aligned}\mathcal{L}_k &:= \mathcal{L}_k\{\mu_1, \ldots, \mu_k\} \\ &= \mathrm{span}\{B_0(x), B_1(x), B_2(x), \ldots, B_k(x)\}, \quad k > 0.\end{aligned}$$

- For simplicity, we assume that $\mu_\emptyset = 0$; and hence, $B_0(x) \equiv 1$, and

$$\begin{aligned}B_k(x) &= \left[\frac{x}{1 - x/\mu_k}\right] B_{k-1}(x) \\ &= \frac{x^k}{\prod_{j=1}^{k} (1 - x/\mu_j)}.\end{aligned}$$

Rational Krylov sequences and ORFs

Remarks (cont.)

- The B_k's are of increasing 'degree'; this is not the case when considering the rational basis

$$\frac{1}{\prod_{j=1}^{n-1}(1-x/\mu_j)}, \frac{x}{\prod_{j=1}^{n-1}(1-x/\mu_j)}, \ldots, \frac{x^{n-1}}{\prod_{j=1}^{n-1}(1-x/\mu_j)}.$$

- The classical (polynomial) case is recovered by assuming that for every $k > 0$, $\mu_k = \infty$; this is not the case when considering the rational basis

$$1, \frac{1}{x-\mu_1}, \frac{1}{x-\mu_2}, \ldots, \frac{1}{x-\mu_{n-1}}.$$

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- $$\mathcal{K}_n^r(\mathbf{A}, \mathbf{b}, \mu) = \text{span}\{\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n\},$$
  where
  $$\mathbf{q}_\ell^* \mathbf{q}_k = \begin{cases} 0, & k \neq \ell \\ \|\mathbf{q}_k\|^2 = 1, & k = \ell. \end{cases}$$
- $\mathbf{q}_{k+1} = \varphi_k(\mathbf{A})\mathbf{b}$, $\varphi_k \in \mathcal{L}_k \setminus \mathcal{L}_{k-1}$.
- There exists a positive measure m on a subset of $\mathbb{R}$ such that
  $$\langle \varphi_k, \varphi_\ell \rangle_m = \begin{cases} 0, & k \neq \ell \\ \|\varphi_k\|_m^2 = 1, & k = \ell. \end{cases}$$

Rational Krylov sequences and ORFs

Theorem 2

Suppose $\varphi_k = \frac{r_k}{\pi_k}$, $r_k, \pi_k \in \mathcal{P}_k$. The orthonormal rational functions (ORFs) φ_k, $k \geqslant 0$, satisfy a 3-term recurrence relation of the form

$$x\varphi_k(x) = \alpha_{k+1}(1 - x/\mu_{k+1})\varphi_{k+1}(x) + \beta_{k+1}(1 - x/\mu_k)\varphi_k(x) + \gamma_{k+1}(1 - x/\overline{\mu}_{k-1})\varphi_{k-1}(x), \qquad \alpha_{k+1}, \gamma_{k+1} \neq 0,$$

with initial conditions $\varphi_{-1}(x) \equiv 0$ and $\varphi_0(x) \equiv \|1\|_m^{-1}$ iff $r_{k+1}(\mu_k) \neq 0$ and $r_k(\overline{\mu}_{k-1}) \neq 0$. Whenever $r_k(\mu_{k-1}) \neq 0$ and $r_{k-1}(\overline{\mu}_{k-2}) \neq 0$ too, it holds that $\gamma_{k+1} = \overline{\alpha}_k \left[1 + \beta_{k+1}(\overline{\mu}_k^{-1} - \mu_k^{-1})\right]$.

Aim is to derive a short term recurrence relation for the orthonormal vectors $\mathbf{q}_k$, $k > 0$, based on their relation with the ORFs φ_k, $k \geqslant 0$.

Rational Krylov sequences and ORFs

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Aim is to derive a short term recurrence relation for the orthonormal vectors $\mathbf{q}_k$, $k > 0$, based on their relation with the ORFs φ_k, $k \geqslant 0$.

Short term recurrence

Polynomial case

- Multiply $P_{k-1}(x)$ with x;
- expand $xP_{k-1}(x)$ in the orthormal basis $\{P_j(x)\}_{j=0}^{k}$;
- note that $\langle xP_{k-1}(x), P_j(x)\rangle_m = \langle P_{k-1}(x), xP_j(x)\rangle_m$, where $xP_j(x) \in \mathcal{P}_{j+1} \subseteq \mathcal{P}_{k-2}$ for every $j < k-2$;
- $xP_{k-1}(x) \perp \mathcal{P}_{k-3}$.

Rational case

$$\left\langle \frac{x}{1-x/\mu_k}\varphi_{k-1}(x), \varphi_j(x)\right\rangle_m = \left\langle \varphi_{k-1}(x), \frac{x}{1-x/\overline{\mu}_k}\varphi_j(x)\right\rangle_m,$$

but $\frac{x}{1-x/\overline{\mu}_k}\varphi_j(x)$ is not necessarily in $\mathcal{L}_{k-2}$ for (every) $j < k-2$ unless $\overline{\mu}_k = \mu_{k-2}$.

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Short term recurrence

Theorem 3

For every $k > 2$, there exists $\phi_{k-1} \in \mathcal{L}_{k-1} \setminus \{0\}$ such that

- $\phi_{k-1} \perp \mathcal{L}_{k-3}$;
- $\left(\frac{x}{1-x/\mu_k}\right) \phi_{k-1}(x) \perp \mathcal{L}_{k-3}$.

Or, equivalently, there exist constants a_k, b_k, c_k, d_k, and e_k, such that

$$\frac{x}{1-x/\mu_k} \{a_k \varphi_{k-2}(x) + b_k \varphi_{k-1}(x)\} = c_k \varphi_{k-2}(x) + d_k \varphi_{k-1}(x) + e_k \varphi_k(x). \quad (1)$$

Short term recurrence

Outline of proof:

For every $p_{k-3} \in \mathcal{P}_{k-3}$ it holds that

$$\left\langle \frac{x}{1-x/\mu_k} \cdot \phi_{k-1}(x)\,, \frac{1-x/\overline{\mu}_k}{x} \cdot \frac{p_{k-3}(x)}{\prod_{j=1}^{k-3}(1-x/\mu_j)} \right\rangle_m = 0.$$

Suppose that $p_{k-3}(x) = xp_{k-4}(x)$, then

$$\left\langle \frac{x}{1-x/\mu_k} \cdot \phi_{k-1}(x)\,, \frac{(1-x/\overline{\mu}_k)p_{k-4}(x)}{\prod_{j=1}^{k-3}(1-x/\mu_j)} \right\rangle_m = 0.$$

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Short term recurrence

Outline of proof (cont.):

Note that $\mathcal{L}_{k-3} = \left\{ \frac{(1-x/\overline{\mu}_k)p_{k-4}(x)}{\prod_{j=1}^{k-3}(1-x/\mu_j)} \right\} \oplus \{\psi_{k-3}(x)\}$, where

- $\psi_{k-3}(x) = \varphi_0(x)$ if $\overline{\mu}_k \notin \{\mu_1, \ldots, \mu_{k-3}\}$;
- $\psi_{k-3}(x) = \varphi_\ell(x)$ if $\overline{\mu}_k = \mu_\ell$ and $\overline{\mu}_k \notin \{\mu_{\ell+1}, \ldots, \mu_{k-3}\}$.

Hence, it follows that $\frac{x}{1-x/\mu_k}\phi_{k-1}(x) \perp \mathcal{L}_{k-3}$ iff

$$a_k \left\langle \frac{x}{1-x/\mu_k}\varphi_{k-2}(x), \psi_{k-3}(x) \right\rangle_m + b_k \left\langle \frac{x}{1-x/\mu_k}\varphi_{k-1}(x), \psi_{k-3}(x) \right\rangle_m = 0. \quad (2)$$

Short term recurrence

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Short term recurrence

Remarks

- Eq (2) always has a non-trivial solution for ϕ_{k-1};
- ϕ_{k-1} is (up to a nonzero multiplicative factor) unique unless

$$\left\langle \frac{x}{1-x/\mu_k}\varphi_{k-2}(x)\,,\psi_{k-3}(x)\right\rangle_m = \left\langle \frac{x}{1-x/\mu_k}\varphi_{k-1}(x)\,,\psi_{k-3}(x)\right\rangle_m = 0;$$

- the coefficient e_k in the short term recurrence (1) is different from zero iff $\phi_{k-1} \notin \mathcal{L}_{k-1}(\mu_k) := \left\{\frac{p_{k-1}(x)}{\pi_{k-1}(x)} : p_{k-1}(\mu_k) \neq 0\right\}$. $(p_j(\infty) = 0 \Leftrightarrow p_j \in \mathcal{P}_{j-1})$

Short term recurrence

Lemma 1

Suppose $\varphi_{k-1} = \frac{r_{k-1}}{\pi_{k-1}}$, $r_{k-1}, \pi_{k-1} \in \mathcal{P}_{k-1}$. If $r_{k-1}(\overline{\mu}_{k-2}) \neq 0$, then Eq (2) has a (up to a nonzero multiplicative factor) unique solution $\phi_{k-1} \notin \mathcal{L}_{k-1}(\mu_k)$.

Outline of proof (cont.):

- Directly follows from 3-term recurrence relation for ORFs under the assumption that $r_k(\mu_{k-1}) \neq 0$ too;
- if $r_k(\mu_{k-1}) = 0$, there exists a constant $\delta_k \neq 0$ such that

$$\begin{aligned}\varphi_k(x) &= \delta_k \left[\frac{1 - x/\mu_{k-1}}{1 - x/\mu_k}\right] \varphi_{k-1}(x) \\ &= \delta_k \left[1 + (\mu_k^{-1} - \mu_{k-1}^{-1}) \frac{x}{1 - x/\mu_k}\right] \varphi_{k-1}(x).\end{aligned}$$

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Short term recurrence

Remarks

- Suppose $r_{k-1}(x_*) = 0$, then it holds that $\mathrm{sign}(\Im\{\mu_{k-1}\}) = -\mathrm{sign}(\Im\{x_*\})$
  $\Rightarrow$ if μ_{k-2} lies in the upper (resp. lower) complex half plane, the equality $r_{k-1}(\overline{\mu}_{k-2}) = 0$ can easily be avoided by choosing μ_{k-1} in the lower (resp. upper) complex half plane or on the real line;
- if the poles $\{\mu_j\}_{j>0}^{k-1}$ are all outside the convex hull of $\mathrm{supp}(m)$, then $r_{k-1}(\overline{\mu}_{k-2}) \neq 0$
  $\Rightarrow$ the equality $r_{k-1}(\overline{\mu}_{k-2}) = 0$ can be avoided by choosing pairs of complex conjugate poles with real part inside the convex hull of $\mathrm{supp}(m)$, instead of real poles inside the convex hull of $\mathrm{supp}(m)$.

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  $\Rightarrow$ if μ_{k-2} lies in the upper (resp. lower) complex half plane, the equality $r_{k-1}(\overline{\mu}_{k-2}) = 0$ can easily be avoided by choosing μ_{k-1} in the lower (resp. upper) complex half plane or on the real line;
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  $\Rightarrow$ the equality $r_{k-1}(\overline{\mu}_{k-2}) = 0$ can be avoided by choosing pairs of complex conjugate poles with real part inside the convex hull of $\text{supp}(m)$, instead of real poles inside the convex hull of $\text{supp}(m)$.

Short term recurrence

For practical applications it may be better to only consider complex poles, because

- the alternation between μ and $\overline{\mu}$ can be stopped at any time (there is no need to have 'pairs');
- computations simplify in the case of complex poles (2 independent coefficients for the case of real poles versus 1 independent coefficient for the case of complex poles).

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Conclusion

- We obtained a rational generalization of the 3-term recurrence relation;
- the short term recurrence certainly has a non-trivial solution $\phi_{k-1}(x)$ for which the numerator polynomial does not vanish at $x = \mu_k$ when considering complex poles alternating between the upper and lower half plane;
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Future work

- Other rational generalizations of the form

$$\frac{x}{1 - x/\mu_k}\phi_{k-1}(x) = \sum_{j=0}^{k} c_j \varphi_j(x)$$

  leading to a short term recurrence;
- comparison of different methods;
- numerical algorithm.

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Thank you ...