Christoffel-Darboux-type Formulae for Orthonormal Rational Functions

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Outline

1. Orthonormal rational functions
2. Christoffel-Darboux formulae
3. Applications

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Orthonormal rational functions

$$f_n(x) = \frac{c_n x^n + c_{n-1} x^{n-1} + \ldots + c_0}{(1 - x/\alpha_1)(1 - x/\alpha_2) \cdot \ldots \cdot (1 - x/\alpha_n)}, \quad n = 1, 2, \ldots$$

Poles

- $\alpha_1, \alpha_2, \alpha_3, \ldots$
- Arbitrary complex or infinite, but different from $\alpha_\emptyset = 0$
- Fixed in advance

Function spaces

- $\mathcal{L}_{-1} = \{0\}$, $\mathcal{L}_0 = \mathbb{C}$,
- $n > 0$: $\mathcal{L}_n = \mathcal{L}\{\alpha_1, \ldots, \alpha_n\}$ = space of rational functions with poles among $\{\alpha_1, \ldots, \alpha_n\}$
- $\mathcal{L}$ = closure of $\bigcup_{n=0}^{\infty} \mathcal{L}_n$
- $\mathcal{L}_{-1} \subset \mathcal{L}_0 \subset \mathcal{L}_1 \subset \ldots \subset \mathcal{L}_n \subset \ldots \subset \mathcal{L}$

Orthonormal rational functions

Rational basis

$$b_k(x) = \prod_{j=1}^{k} \frac{x}{1 - x/\alpha_j}, \quad k > 0, \ \alpha_j \in \overline{\mathbb{C}}_0$$

$$\mathcal{L}_n = \mathrm{span}\{1, b_1(x), \ldots, b_n(x)\}$$

Polynomials

$$(\forall j : \alpha_j = \infty) \Rightarrow b_k(x) \equiv x^k$$

$$\mathcal{L}_n \equiv \mathcal{P}_n = \mathrm{span}\{1, x, \ldots, x^n\}$$

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Orthonormal rational functions

Orthonormal rational functions (ORFs)

Consider an inner product $\langle f, g\rangle = \mathcal{F}\{fg^c\}$, $f, g \in \mathcal{L}$, where $g^c(x) = \overline{g(\overline{x})}$ and $\mathcal{F}$ is an hermitian positive-definite linear functional:

$$\forall f, g \in \mathcal{L} \; : \; \mathcal{F}\{fg^c\} = \overline{\mathcal{F}\{f^c g\}} \quad \textit{and} \quad \forall f \in \mathcal{L}\backslash\{0\} \; : \; \mathcal{F}\{ff^c\} > 0$$

→ ORFs: $\varphi_k(x)$

$\varphi_k \in \mathcal{L}_k \setminus \mathcal{L}_{k-1}$, $\varphi_k \perp \mathcal{L}_{k-1}$, and $\|\varphi_k\| = \sqrt{\langle \varphi_k, \varphi_k\rangle} = 1$.

Quasi-orthogonal rational functions (qORFs)

$Q_n \in \mathcal{L}_n$ is called a qORF if $Q_n \perp \mathcal{L}_{n-1}(\overline{\alpha}_n)$ where

$$\mathcal{L}_k(\alpha) := \left\{ \frac{p_k}{\pi_k} \in \mathcal{L}_k \; : \; p_k(\alpha) = 0 \right\}.$$

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Orthonormal rational functions

Definitions

Let $f_k = \frac{p_k}{\pi_k} \in \mathcal{L}_k \setminus \mathcal{L}_{k-1}$ with $p_k \in \mathcal{P}_k$. Then f_k is

- exceptional iff $p_k(\alpha_{k-1}) = 0$
- degenerate iff $p_k(\overline{\alpha}_{k-1}) = 0$
- regular iff not exceptional and not degenerate

By convention $p_k(\infty) = 0 \Leftrightarrow p_k \in \mathcal{P}_{k-1}$.

Auxiliary rational functions

$$\begin{aligned} \phi_n(x) &= (1 - x/\alpha_n)\varphi_n(x) \\ \psi_n(x) &= (1 - x/\overline{\alpha}_n)\varphi_n(x) \end{aligned}$$

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Orthonormal rational functions

Theorem (Three-term Recurrence)

Whenever φ_n is not exceptional, φ_{n-1} is regular, and φ_{n-2} is not degenerate, they satisfy a three-term recurrence relation:

$$x\varphi_{n-1}(x) = \gamma_n \phi_n(x) + \rho_n \phi_{n-1}(x) + \xi_{n-1}\psi_{n-2}(x),$$

with initial conditions

$$\varphi_{-1}(x) \equiv 0 \text{ and } \varphi_0(x) \equiv \eta_0 \left\|1\right\|^{-1}, \ |\eta_0| = 1,$$

$$\alpha_{-1} \in \overline{\mathbb{R}}_0 \text{ and } \alpha_0 \in \overline{\mathbb{C}}_0,$$

and ξ_{n-1} depends on γ_{n-1}, ρ_n and α_{n-1}.

Reproducing kernels

Reproducing kernels

$$k_n(x,y) = \sum_{k=0}^{n-1} \varphi_k(x)\overline{\varphi_k(y)}.$$

which has the property that

$$\forall f \in \mathcal{L}_{n-1},\ \forall y \in \overline{\mathbb{C}} \ :\ \langle f(\cdot)\,,k_n(\cdot,y)\rangle = f(y).$$

Christoffel-Darboux formula (polynomial case)

$$k_n(x,y) = \gamma_n \left(\frac{\varphi_n(x)\overline{\varphi_{n-1}(y)} - \overline{\varphi_n(y)}\varphi_{n-1}(x)}{x - \overline{y}} \right)$$

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Christoffel-Darboux formulae

Theorem

$$c_n k_n(x,y) = \frac{b_{n-1}^c(\overline{y})}{b_{n-1}(\overline{y})}\left(\frac{\phi_n(x)\psi_{n-1}(\overline{y}) - \phi_n(\overline{y})\psi_{n-1}(x)}{x-\overline{y}}\right)$$

$$\overline{c}_n k_n(x,y) = \frac{b_{n-1}(x)}{b_{n-1}^c(x)}\left(\frac{\phi_n^c(x)\psi_{n-1}^c(\overline{y}) - \phi_n^c(\overline{y})\psi_{n-1}^c(x)}{x-\overline{y}}\right)$$

where

$$c_n = \overline{\kappa}_{n-1}^{-1} \lim_{z\to\overline{\alpha}_{n-1}} \frac{\varphi_n(z)}{b_n(z)} \quad \textit{and} \quad \kappa_{n-1} = \lim_{z\to\alpha_{n-1}} \frac{\varphi_{n-1}(z)}{b_{n-1}(z)}.$$

In the special case in which $\alpha_n \in \overline{\mathbb{R}}_0$ *or* $\alpha_{n-1} \in \overline{\mathbb{R}}_0$, *it holds that* $|c_n| = |\gamma_n^{-1}|$.

Christoffel-Darboux formulae

Outline of the proof:

- The second equality follows from $\overline{k_n(y,x)} = k_n(x,y)$
- For the first equality we will use the connection with qORFs

Lemma

Let

$$\Phi_n(x,y) := \frac{x-y}{(1-x/\alpha_n)(1-y/\overline{\alpha}_n)} k_n(x,\overline{y}).$$

Then for fixed y, $\Phi_n(\cdot,y)$ is a qORF in $\mathcal{L}_n$.

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Christoffel-Darboux formulae

Outline of the proof (cont.):

Lemma

Let $Q_n \in \mathcal{L}_n$ be such that

$$(1 - x/\alpha_n)Q_n(x) = a_n\phi_n(x) + b_n\psi_{n-1}(x), \tag{1}$$

with $a_n, b_n \in \mathbb{C}$. Then Q_n is a qORF.

Conversely, suppose φ_n is not degenerate and let $Q_n \in \mathcal{L}_n$ be a qORF. Then there exist constants $a_n, b_n \in \mathbb{C}$ such that (1) holds true.

Christoffel-Darboux formulae

Outline of the proof (cont.):
From the previous two lemmas it follows that, if φ_n is not degenerate, then

$$\frac{x-y}{(1-y/\overline{\alpha}_n)}k_n(x,\overline{y}) = a_n(y)\phi_n(x) + b_n(y)\psi_{n-1}(x),$$

where

- $a_n, b_n \in \mathcal{L}_n^c = \mathcal{L}\{\overline{\alpha}_1, \ldots, \overline{\alpha}_n\}$
- $a_n(y)\phi_n(y) = -b_n(y)\psi_{n-1}(y)$
- ϕ_n and ψ_{n-1} have common zeros iff φ_n is degenerate

hence, the Christoffel-Darboux formula follows.

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Christoffel-Darboux formulae

If $\varphi_n = \frac{p_n}{\pi_n}$ is degenerate, then

- $\frac{\phi_n(x)}{\psi_{n-1}(x)} \equiv$ const, hence $\phi_n(x)\psi_{n-1}(\overline{y}) - \phi_n(\overline{y})\psi_{n-1}(x) \equiv 0$
- $p_n(\overline{\alpha}_{n-1}) = 0$, hence

$$c_n = \overline{\kappa}_{n-1}^{-1} \lim_{z\to\overline{\alpha}_{n-1}} \frac{\varphi_n(z)}{b_n(z)} = 0$$

hence, the Christoffel-Darboux formula remains valid.

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Christoffel-Darboux formulae

Christoffel function $\lambda_n(x) = k_n^{-1}(x,x)$

$$c_n k_n(x,\overline{x}) = \frac{b_{n-1}^c(x)}{b_{n-1}(x)} \left(\phi_n(x)\psi_{n-1}'(x) - \phi_n'(x)\psi_{n-1}(x) \right),$$

where the prime denotes the derivative w.r.t. x; hence, for $x \in \overline{\mathbb{R}}$,

$$\lambda_n(x) = |c_n| \cdot \left| \phi_n(x)\psi_{n-1}'(x) - \phi_n'(x)\psi_{n-1}(x) \right|^{-1}.$$

Applications

- construction of ORFs w.r.t. rational modifications of a measure on a subset of the real line; see e.g. K. Deckers and A. Bultheel (JAT 2009).
- construction of an orthogonal basis for rational wavelets; see e.g. A. Bultheel and P. González-Vera (Numer. Funct. Anal. Optim. 2000).
- asymptotics for $k_n(x, y)$ as $n \to \infty$ based on known asymptotics for ORFs; see e.g. K. Deckers and A. Bultheel (IMA Journal of Numer. Anal. 2009).

Applications

- Rational Krylov methods to find numerical approximations to the matrix function $f(\mathbf{A})$ for the computation of $f(\mathbf{A})\mathbf{v}$ or $\mathbf{v}^H f(\mathbf{A})\mathbf{v}$), where $\mathbf{A}$ is an Hermitian $N \times N$ matrix, $\mathbf{v}$ is a nonzero vector in $\mathbb{C}^N$, and f has singularities at $\alpha_k \notin \Lambda(\mathbf{A})$, $k > 0$; see K. Deckers and A. Bultheel (Report TW 499, 2007) and K. Deckers (IMA Journal of Numerical Analysis 2015).

Rational Krylov methods

Let $\mathbf{q}_n = \varphi_{n-1}(\mathbf{A})\mathbf{v}$ and $\mathbf{p}_n = k_n(\mathbf{A}, 0)\mathbf{v}$, $n > 0$. Then there exist $\rho_{n,j} \in \mathbb{C}$, $j = 1, 2, 3$, s.t.

$$\begin{aligned} \mathbf{q}_{n+1} &= \rho_{n,2}\{\mathbf{q}_n + (\alpha_n^{-1} - \alpha_{n-1}^{-1})\mathbf{x}_n - \rho_{n,1}\mathbf{y}_n\} \\ \mathbf{p}_{n+1} &= \mathbf{p}_n + \rho_{n,3}\mathbf{q}_{n+1}, \end{aligned}$$

where

$$(\mathbf{I} - \alpha_n^{-1}\mathbf{A})\mathbf{x}_n = \mathbf{A}\mathbf{q}_n \qquad \text{and} \qquad (\mathbf{I} - \alpha_n^{-1}\mathbf{A})\mathbf{y}_n = \mathbf{A}\mathbf{p}_n$$

and with initialization $\alpha_0 = \infty$, $\mathbf{q}_1 = \mathbf{v}/\|\mathbf{v}\|$, and $\mathbf{p}_1 = \mathbf{q}_1/\|\mathbf{v}\|$.

Rational Krylov methods

From $\mathbf{q}_k^H \mathbf{q}_\ell = \delta_{k,\ell}$ it follows that

$$\rho_{n,1} = \frac{\delta_{k,n} + (\alpha_n^{-1} - \alpha_{n-1}^{-1})\mathbf{q}_k^H \mathbf{x}_n}{\mathbf{q}_k^H \mathbf{y}_n}, \quad k \leq n,$$

while from the orthogonality of $k_{n+1}(\cdot, 0)$ w.r.t. $\{f \in \mathcal{L}_n \ : \ f(0) = 0\}$ it follows that,

$$\rho_{n,3} = -\frac{\mathbf{y}_n^H \mathbf{p}_n}{\mathbf{y}_n^H \mathbf{q}_{n+1}} = -\frac{\mathbf{x}_n^H \mathbf{p}_n}{\mathbf{x}_n^H \mathbf{q}_{n+1}}.$$

Rational Gaussian quadrature

Consider the case in which

$$\langle f, g\rangle = \int_a^b f(x)g^c(x)d\mu(x), \quad -\infty \leq a < b \leq \infty,$$

where μ is a positive measure with infinite support on $[a, b]$. Suppose $\{x_{n,k}\}_{k=1}^{n} \subset [a, b]$ are the zeros of φ_n if $\alpha_n \in \overline{\mathbb{R}} \setminus [a, b]$ (respectively of an n-th qORF if $\alpha_n \notin \overline{\mathbb{R}}$), and let $\lambda_{n,k} = \lambda_n(x_{n,k})$, $k = 1, \ldots, n$. Then the approximation

$$\int_a^b f(x)d\mu(x) \approx \sum_{k=1}^{n} \lambda_{n,k} f(x_{n,k})$$

is exact for every $f \in \mathcal{L}_n \cdot \mathcal{L}_{n-1}^c$ (respectively $f \in \mathcal{L}_{n-1} \cdot \mathcal{L}_{n-1}^c$).

Rational Gaussian quadrature

K. Deckers, A. Bultheel, and J. Van Deun (Numer. Math. 2011)

Theorem

Suppose $\alpha_n \notin \overline{\mathbb{R}}$. Let $\tilde{\varphi}_n$ denote the n-th ORF in $\tilde{\mathcal{L}}_n = \mathcal{L}\{\alpha_1, \ldots, \alpha_{n-1}, \tilde{\alpha}\}$, with $\tilde{\alpha} \in \overline{\mathbb{R}} \setminus [a, b]$. Then the zeros of $\tilde{\varphi}_n$ coincide with the zeros of an $n - th$ qORF in $\mathcal{L}_n$.

Rational Gaussian quadrature

Theorem (cont.)

Conversely, suppose the zeros of an n-th qORF $Q_n \in \mathcal{L}_n$ are all in $[a, b]$. Then $\exists \tilde{\alpha} \in \overline{\mathbb{R}} \setminus [a, b]$ s.t.

$$\left\{ \varphi_0, \ldots, \varphi_{n-1}, \tilde{\varphi}_n = \left(\frac{1 - \cdot/\alpha_n}{1 - \cdot/\tilde{\alpha}} \right) Q_n \right\}$$

forms an orthonormal system w.r.t. some positive measure $\tilde{\mu}$.

Rational Gaussian quadrature

Consequently,

$$\begin{aligned} \lambda_{n,k}^{-1} &= \left|\tilde{\gamma}_n(1 - x_{n,k}/\tilde{\alpha})\tilde{\varphi}_n'(x_{n,k})\psi_{n-1}(x_{n,k})\right| \\ &= \left|\tilde{\gamma}_n(1 - x_{n,k}/\alpha_n)Q_n'(x_{n,k})\psi_{n-1}(x_{n,k})\right|, \end{aligned}$$

where

$$\tilde{\gamma}_n = \lim_{x \to \alpha_{n-1}} \frac{(1 - x/\tilde{\alpha})\tilde{\varphi}_n(x)}{x\varphi_{n-1}(x)} = \lim_{x \to \alpha_{n-1}} \frac{(1 - x/\alpha_n)Q_n(x)}{x\varphi_{n-1}(x)}$$

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