Orthogonal Rational Functions and Rational Gauss-type Quadrature Rules

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Outline

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Notation

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

Poles

- $\alpha_1, \alpha_2, \alpha_3, \ldots$
- Arbitrary complex or infinite, but outside $[-1, 1]$
- 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 $\bigcup_{n=0}^{\infty} \mathcal{L}_n$
- $\mathcal{L}_{-1} \subset \mathcal{L}_0 \subset \mathcal{L}_1 \subset \ldots \subset \mathcal{L}_n \subset \ldots \subset \mathcal{L}$

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$I = [-1, 1], \quad X \subseteq \mathbb{C}: \ \overline{X} = X \cup \{\infty\}$ and $X_I = \{x \in X : x \notin I\}$

Rational basis

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

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

Polynomials

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

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

Orthonormal rational functions (ORFs)

Given a positive measure μ on I and inner product

$$\langle f, g \rangle_\mu = \int_I f(x) g^c(x) d\mu(x) \quad g^c(x) = \overline{g(\overline{x})}$$

$\rightarrow$ ORFs: $\varphi_k(x)$

$$\varphi_k \in \mathcal{L}_k \setminus \mathcal{L}_{k-1}, \ \varphi_k \perp_\mu \mathcal{L}_{k-1}, \text{ and } \|\varphi_k\|_\mu = \sqrt{\langle \varphi_k, \varphi_k \rangle_\mu} = 1.$$

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Orthonormal rational functions (ORFs)

Theorem (Three-term Recurrence)

The ORFs φ_k, $k > 0$, satisfy a three-term recurrence relation:

$$\varphi_k(x) = E_k \cdot F(\varphi_{k-2}(x), \varphi_{k-1}(x), \alpha_{k-2}, \alpha_{k-1}, \alpha_k, D_k)$$

with initial conditions $\varphi_{-1}(x) \equiv 0$, $\varphi_0(x) \equiv \eta_0 \|1\|_\mu^{-1}$, $|\eta_0| = 1$, and $\alpha_{-1} \in \overline{\mathbb{R}}_I$ and $\alpha_0 = \overline{\mathbb{C}}_I$.

[K. Deckers and A. Bultheel, IMA J. Numer. Anal., 2009]

Corollary (Generalized eigenvalue problem (GEP))

The zeros $\{x_{nk}\}_{k=1}^n$ of the ORF $\varphi_n(x)$ are eigenvalues of a GEP of the form $\mathbf{J}_n \underline{v}_{nk} = x_{nk} \mathbf{B}_n \underline{v}_{nk}$, where $\mathbf{J}_n$ and $\mathbf{B}_n$ are tridiagonal matrices, and $\underline{v}_{nk}$ is the corresponding normalized eigenvector.

[J. Van Deun, Numer. Algorithms, 2007]

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Theorem

The ORF φ_n has n real distinct zeros in I iff $\alpha_n \in \overline{\mathbb{R}}_I$.
[K. Deckers et al., Numer. Math., 2011]

Theorem (Favard Theorem)

Suppose the sequence of rational functions $\{\hat{\varphi}_k\}_{k=0}^{\infty}$, with $\hat{\varphi}_k \in \hat{\mathcal{L}}_k \setminus \hat{\mathcal{L}}_{k-1}$ and $\hat{\mathcal{L}}_k = \mathcal{L}\{\hat{\alpha}_1, \ldots, \hat{\alpha}_k\}$, are generated by the three-term recurrence relation

$$\hat{\varphi}_k(x) = \hat{E}_k \cdot F(\hat{\varphi}_{k-2}(x), \hat{\varphi}_{k-1}(x), \hat{\alpha}_{k-2}, \hat{\alpha}_{k-1}, \hat{\alpha}_k, \hat{D}_k).$$

Then - under certain conditions on $\hat{E}_k$ and $\hat{D}_k$ - the $\hat{\varphi}_k$ form an orthonormal system w.r.t. a positive measure $\hat{\mu}$ on $\hat{S} \subsetneq \mathbb{R}$ and inner product $\langle f, g \rangle_{\hat{\mu}} = \int_{\hat{S}} f(x) g^c(x) d\hat{\mu}(x)$.
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Outline

Rational interpolatory quadrature rules (RIQs)

RIQs

Given a (possible complex) measure σ on I and a set of n distinct nodes $\{x_{nk}\}_{k=1}^{n} \subset I$. Then there exists a unique set of weights $\{\lambda_{nk}\}_{k=1}^{n} \subset \mathbb{C}$ so that

$$J_\sigma(f) := \int_I f(x)d\sigma(x) \approx \sum_{k=1}^{n} \lambda_{nk} f(x_{nk}) =: J_n(f) \tag{1}$$

is exact for (at least) every $f \in \mathcal{L}_{n-1}$.

Domain of validity

Assume that (1) is exact for every $f \in \tilde{\mathcal{L}}_m$, where $\mathcal{L}_{n-1} \subseteq \tilde{\mathcal{L}}_m \subset \mathcal{L}\{\alpha_1, \ldots, \alpha_n, \overline{\alpha}_1, \ldots, \overline{\alpha}_n\} =: \mathcal{L}_n \cdot \mathcal{L}_n^c$, and suppose there is no larger space of rational functions for which (1) is exact. Then $\tilde{\mathcal{L}}_m$ is called the domain of validity.

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Characterization

In the remainder we only consider positive measures $\sigma = \mu$ (for complex measures, see [K. Deckers and A. Bultheel, Report TW 574, 2010])

RIQs can be characterized by means of quasi-orthogonal rational functions (qORFs)
$\rightarrow$ two kinds of RIQs / qORFs:

- RIQs of the first kind: $\tilde{\mathcal{L}}_m = \mathcal{L}_n \cdot \mathcal{L}_{k-1}^c$ with $1 \leqslant k \leqslant n$;
- RIQs of the second kind: $\tilde{\mathcal{L}}_m = \mathcal{L}_{n-1} \cdot \mathcal{L}_k^c$ with $0 \leqslant k \leqslant n-1$.

[K. Deckers and A. Bultheel, Report TW 573, 2010]

Characterization

RIQs of the first kind

The nodes in a RIQ with domain of validity $\mathcal{L}_n \cdot \mathcal{L}_{k-1}^c$, where $1 \leqslant k \leqslant n$, are the zeros of a $P_{n,n-k} \in \mathcal{L}_n \setminus \mathcal{L}_{n-1}$ satisfying $P_{n,n-k} \perp_\mu \mathcal{L}_{k-1}$.

i.e., $P_{n,n-k}$ is a qORF of the form

$$P_{n,n-k}(x) = \varphi_n(x) + \sum_{j=1}^{n-k} a_j \varphi_{n-j}(x), \quad a_{n-k} \neq 0. \tag{2}$$

Property

Suppose the qORF (2) has all real zeros. Then it has at least k zeros inside I.

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RIQs of the second kind

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i.e., $Q_{n,n-k}$ is a qORF of the form

$$Q_{n,n-k}(x) = \varphi_n(x) + \sum_{j=1}^{n-k} a_j \cdot \left(\frac{1 - x/\overline{\alpha}_{n-j}}{1 - x/\alpha_n}\right) \varphi_{n-j}(x), \quad a_{n-k} \neq 0. \tag{3}$$

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Suppose the qORF (3) has all real zeros. Then it has at least k zeros inside I.

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Suppose the qORF (3) has all real zeros. Then it has at least k zeros inside I.

Positive RIQs

Positive rational interpolatory quadrature rules

- Positive rational interpolatory quadrature = RIQ with weights $\{\lambda_{nk}\}_{k=1}^{n} \subset \mathbb{R}_0^+$.
- Domain of validity satisfies $\tilde{\mathcal{L}}_m \equiv \tilde{\mathcal{L}}_m^c$;

Rational Gauss-type quadrature rules

- Rational Gauss-type quadrature = positive RIQ with j fixed nodes in I, where $0 \leqslant j \leqslant 2$, and the remaining $n-j$ nodes are such that the domain of validity has dimension $2n-j$ (or larger).
- Existence not only depends on the fixed node(s), but also on the sequence of poles

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Rational Gauss-type quadrature rules

- Rational Gaussian quadrature: $j = 0$ and $\tilde{\mathcal{L}}_m = \mathcal{L}_n \cdot \mathcal{L}_{n-1}^c$
- Rational Gauss-Radau quadrature: $j = 1$ and
  - $\tilde{\mathcal{L}}_m \supseteqq \mathcal{L}_n \cdot \mathcal{L}_{n-2}^c$ (first kind), or
  - $\tilde{\mathcal{L}}_m \supseteqq \mathcal{L}_{n-1} \cdot \mathcal{L}_{n-1}^c$ (second kind)
- Rational Gauss-Lobatto quadrature: $j = 2$ and
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In what follows: existence and construction of these rational Gauss-type quadrature rules.

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Outline

Rational Gaussian quadrature

- has maximal domain of validity; i.e., $\tilde{\mathcal{L}}_m = \mathcal{L}_n \cdot \mathcal{L}_{n-1}^c$
- exists iff $\alpha_n \in \overline{\mathbb{R}}_I$
- the nodes $\{x_{nk}^{(\mu,\alpha_n)}\}_{k=1}^n$ are zeros of the ORF $\varphi_n \in \mathcal{L}_n$; hence, can be computed by means of the GEP
- the corresponding weights $\{\lambda_{nk}^{(\mu,\alpha_n)}\}_{k=1}^n$ can be computed by means of the GEP too:

$$\lambda_{nk}^{(\mu,\alpha_n)} = |v_{nk}|^2 \, \|1\|_\mu^2 \,,$$

where v_{nk} represents the first component of the eigenvector $\underline{v}_{nk}$.

Outline

Rational Gauss-Radau quadrature: Second kind

Consider the qORF $Q_{n,1}(x)$ with fixed zero in x_{n1}:

$$Q_{n,1}(x) = \varphi_n(x) + a_{n1}\left(\frac{1 - x/\overline{\alpha}_{n-1}}{1 - x/\alpha_n}\right)\varphi_{n-1}(x),$$

$$a_{n1} = -\frac{(1 - x_{n1}/\alpha_n)\varphi_n(x_{n1})}{(1 - x_{n1}/\overline{\alpha}_{n-1})\varphi_{n-1}(x_{n1})} \in \mathbb{C}.$$

Questions:

- are the zeros $\{x_{nk}\}_{k=1}^n$ all real distinct and in I?
- are the weights $\{\lambda_{nk}\}_{k=1}^n$ in the corresponding RIQ

$$\int_I f(x)d\mu(x) = \sum_{k=1}^n \lambda_{nk} f(x_{nk}), \quad \forall f \in \mathcal{L}_{n-1} \cdot \mathcal{L}_{n-1}^c$$

all in $\mathbb{R}_0^+$?

Rational Gauss-Radau quadrature: Second kind

[K. Deckers et al., Numer. Math., 2011]

Theorem

Suppose $c_n := \frac{a_{n1}}{E_n}\left(\frac{1}{\alpha_{n-1}} - \frac{1}{\overline{\alpha}_{n-1}}\right) \neq -1$. *Then there exist poles* $\alpha \in \overline{\mathbb{C}}_I$ *(not unique), and constants* $\hat{E}_n \neq 0$ *and*

$$\hat{D}_n = \frac{D_n + a_{n1}/E_n}{1 + c_n} \rightarrow \textit{satisfying condition Favard theorem},$$

so that

$$\left(\frac{1 - x/\alpha_n}{1 - x/\alpha}\right) Q_{n,1}(x) = \hat{E}_n \cdot F(\varphi_{n-2}(x), \varphi_{n-1}(x), \alpha_{n-2}, \alpha_{n-1}, \alpha, \hat{D}_n);$$

hence, $\left(\frac{1-\cdot/\alpha_n}{1-\cdot/\alpha}\right) Q_{n,1}(\cdot) \perp_{\hat{\mu}} \mathcal{L}_{n-1}$, *where* $\hat{\mu}$ *is a (not unique) positive measure on* $\hat{S} \subsetneq \mathbb{R}$.

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Rational Gauss-Radau quadrature: Second kind

If $c_n = -1$, then numerator polynomial of $Q_{n,1}(x)$ has zero in $x = \alpha_{n-1}$.

Corollary

The zeros of $Q_{n,1}(x)$ are all real distinct iff

$$\Im\{\hat{D}_n\} = \Im\{1/\alpha_{n-2}\}\,|E_{n-1}|^{-2}, \quad \alpha_{n-1} \in \overline{\mathbb{R}}_I,$$

respectively

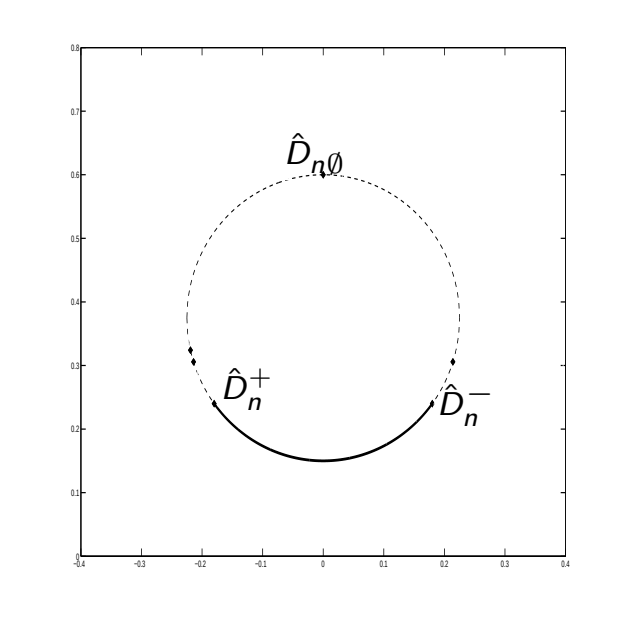
$$\Re\{\hat{D}_n\}^2 + \left\{\Im\{\hat{D}_n\} - \frac{1}{\Im\{1/\overline{\alpha}_{n-1}\}}\right\}^2 = \frac{\left(\frac{1}{\Im\{1/\overline{\alpha}_{n-1}\}}\right)^2}{1 + r_n}, \quad \alpha_{n-1} \notin \overline{\mathbb{R}},$$

where

$$r_n = 4\Im\{1/\overline{\alpha}_{k-1}\} \cdot \Im\{1/\alpha_{k-2}\}\,|E_{n-1}|^{-2} > -1.$$

Rational Gauss-Radau quadrature: Second kind

- Under the same condition on $\hat{D}_n \to n-1$ zeros are in I
- Boundary values $\hat{D}_n^{\pm}$ for $\hat{D}_n$, in order to have that $\{x_{nk}\}_{k=1}^{n} \subset I$, are obtained by setting $a_{n1}^{\pm} := -\frac{(1\mp 1/\alpha_n)\varphi_n(\pm 1)}{(1\mp 1/\overline{\alpha}_{n-1})\varphi_{n-1}(\pm 1)}$
- Forbidden value $\hat{D}_{n\emptyset}$ for $\hat{D}_n$ is obtained by setting $a_{n1\emptyset} := -\lim_{x\to\infty} \frac{(1-x/\alpha_n)\varphi_n(x)}{(1-x/\overline{\alpha}_{n-1})\varphi_{n-1}(x)}$



Rational Gauss-Radau quadrature: Second kind

- the nodes $\{x_{nk}\}_{k=1}^{n}$ are rational Gaussian nodes: $x_{nk} = x_{nk}^{(\hat{\mu},\alpha)}$, $k = 1, \ldots, n$ and $\alpha \in \overline{\mathbb{R}}_I$
- $\{\varphi_0, \ldots, \varphi_{n-1}\}$ forms an orthonormal system for the inner product $\langle \cdot\,, \cdot \rangle_{\hat{\mu}} \Rightarrow$
  $\forall f \in \mathcal{L}_{n-1} \cdot \mathcal{L}_{n-1}^{c} \supset \mathcal{L}_{n-1} : \int_I f(x) d\mu(x) = \int_{\hat{S}} f(x) d\hat{\mu}(x)$;
  hence, the weights $\{\lambda_{nk}\}_{k=1}^{n}$ are rational Gaussian weights:
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and $\underline{\hat{v}}_{nk}$ is the corresponding normalized eigenvector.

Rational Gauss-Radau quadrature: Second kind

- the nodes $\{x_{nk}\}_{k=1}^{n}$ are rational Gaussian nodes: $x_{nk} = x_{nk}^{(\hat{\mu},\alpha)}$, $k = 1, \ldots, n$ and $\alpha \in \overline{\mathbb{R}}_I$
- $\{\varphi_0, \ldots, \varphi_{n-1}\}$ forms an orthonormal system for the inner product $\langle \cdot\,, \cdot \rangle_{\hat{\mu}} \Rightarrow$
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and $\underline{\hat{v}}_{nk}$ is the corresponding normalized eigenvector.

Rational Gauss-Radau quadrature: First kind

Consider the qORF $P_{n,1}(x)$ with fixed zero in x_{n1}:

$$P_{n,1}(x) = \varphi_n(x) + a_{n1}\varphi_{n-1}(x), \quad a_{n1} = -\frac{\varphi_n(x_{n1})}{\varphi_{n-1}(x_{n1})} \in \mathbb{C}.$$

Questions:

- are the zeros $\{x_{nk}\}_{k=1}^n$ all real distinct and in I?
- are the weights $\{\lambda_{nk}\}_{k=1}^n$ in the corresponding RIQ

$$\int_I f(x)d\mu(x) = \sum_{k=1}^n \lambda_{nk} f(x_{nk}), \quad \forall f \in \mathcal{L}_n \cdot \mathcal{L}_{n-2}^c$$

all in $\mathbb{R}_0^+$?

Rational Gauss-Radau quadrature: First kind

Conditions on $\{\alpha_{n-1}, \alpha_n\}$

- If $\alpha_n = \overline{\alpha}_{n-1}$, then First kind = Second kind.
  So, suppose $\alpha_n \neq \overline{\alpha}_{n-1}$.
- If $\alpha_{n-1} \notin \overline{\mathbb{R}}$, then
  - $\alpha_n \notin \overline{\mathbb{R}} \Rightarrow \{\lambda_{nk}\}_{k=1}^n \not\subseteq \mathbb{R}_0^+$
  - $\alpha_n \in \overline{\mathbb{R}}_I \Rightarrow \{\lambda_{nk}\}_{k=1}^n \subset \mathbb{R}_0^+$ iff $a_{n1} = 0$, i.e.,
    Rational Gaussian quadrature: $x_{nk} = x_{nk}^{(\mu,\alpha_n)}$ and
    $\lambda_{nk} = \lambda_{nk}^{(\mu,\alpha_n)}$, exact in $\mathcal{L}_n \cdot \mathcal{L}_{n-1}^c \supset \mathcal{L}_n \cdot \mathcal{L}_{n-2}^c$

  So, suppose $\alpha_{n-1} \in \overline{\mathbb{R}}_I$.

Rational Gauss-Radau quadrature: First kind

[K. Deckers and A. Bultheel, Report TW 573, 2010]

Theorem

Suppose $c_n := \frac{a_{n1}}{E_n}\left(\frac{1}{\alpha_{n-1}} - \frac{1}{\alpha_n}\right) \in (-1, \infty)$. *Then there exist poles* $\alpha \in \overline{\mathbb{C}}_I$ *(not unique), and constants* $\hat{E}_n \neq 0$, $|k_n|^2 = 1 + c_n$, *and*

$$\hat{D}_n = \frac{D_n + a_{n1}/E_n}{1 + c_n} \rightarrow \textit{satisfying condition Favard theorem},$$

so that

$$\left(\frac{1-x/\alpha_n}{1-x/\alpha}\right) P_{n,1}(x) = \hat{E}_n \cdot F(\varphi_{n-2}(x), k_n\varphi_{n-1}(x), \alpha_{n-2}, \alpha_{n-1}, \alpha, \hat{D}_n);$$

hence, $\left(\frac{1-\cdot/\alpha_n}{1-\cdot/\alpha}\right) P_{n,1}(\cdot) \perp_{\hat{\mu}} \mathcal{L}_{n-1}$, *where* $\hat{\mu}$ *is a (not unique) positive measure on* $\hat{S} \subsetneq \mathbb{R}$.

Rational Gauss-Radau quadrature: First kind

Lemma

Suppose $c_n \notin (-1, \infty)$. Then there cannot exist distinct nodes $\{x_{nk}\}_{k=1}^n \subset I$ and weights $\{\lambda_{nk}\}_{k=1}^n \subset \mathbb{R}_0^+$ so that

$$\int_I f(x) d\mu(x) = \sum_{k=1}^n \lambda_{nk} f(x_{nk}), \quad \forall f \in \mathcal{L}_n \cdot \mathcal{L}_{n-2}^c.$$

Corollary

The zeros of $P_{n,1}(x)$ are all real distinct iff

$$\Im\{\hat{D}_n\} = \frac{\Im\{1/\alpha_{n-2}\}}{|k_n|^2 \, |E_{n-1}|^2}; \text{ i.e., iff } \Im\{a_{n1}\overline{E_n}\} - \Im\{1/\alpha_n\} = 0. \quad (4)$$

Rational Gauss-Radau quadrature: First kind

- $\alpha_n \in \overline{\mathbb{R}}_I$: (4) holds true for every a_{n1} for which $c_n \in (-1, \infty)$ Boundary values $c_n^- < 0 < c_n^+$ for c_n, in order to have that $\{x_{nk}\}_{k=1}^n \subset I$, are obtained by setting $a_{n1}^{\pm} := -\frac{\varphi_n(\pm 1)}{\varphi_{n-1}(\pm 1)}$.
- $\alpha_n \notin \overline{\mathbb{R}}$: (4) holds true iff $a_{n1}\overline{E}_{n-1} = \frac{1}{\alpha_{n-1}} - \frac{1}{\overline{\alpha}_n}$ Rational Gaussian quadrature (when changing the order of the last two poles), exact in $\mathcal{L}_n \cdot \mathcal{L}\{\overline{\alpha}_1, \ldots, \overline{\alpha}_{n-2}, \overline{\alpha}_n\} \supset \mathcal{L}_n \cdot \mathcal{L}_{n-2}^c$

Rational Gauss-Radau quadrature: First kind

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Rational Gauss-Radau quadrature: First kind

- the nodes $\{x_{nk}\}_{k=1}^{n}$ are rational Gaussian nodes: $x_{nk} = x_{nk}^{(\hat{\mu},\alpha)}$, $k = 1, \ldots, n$ and $\alpha \in \overline{\mathbb{R}}_I$
- $\{\varphi_0, \ldots, \varphi_{n-2}, k_n\varphi_{n-1}\}$ forms an orthonormal system for the inner product $\langle \cdot\,, \cdot \rangle_{\hat{\mu}} \Rightarrow$
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Rational Gauss-Radau quadrature: First kind

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and $\underline{\hat{v}}_{nk}$ is the corresponding normalized eigenvector.

Rational Gauss-Radau quadrature: First kind

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and $\underline{\hat{v}}_{nk}$ is the corresponding normalized eigenvector.

Outline

Rational Gauss-Lobatto quadrature: Second kind

Consider the qORF $Q_{n,2}(x)$ with fixed zero in x_{n1} and x_{n2}:

$$Q_{n,2}(x) = \varphi_n(x) + a_{n1}\left(\frac{1 - x/\overline{\alpha}_{n-1}}{1 - x/\alpha_n}\right)\varphi_{n-1}(x) + a_{n2}\left(\frac{1 - x/\overline{\alpha}_{n-2}}{1 - x/\alpha_n}\right)\varphi_{n-2}(x)$$

Questions:

- are the zeros $\{x_{nk}\}_{k=1}^n$ all real distinct and in I?
- are the weights $\{\lambda_{nk}\}_{k=1}^n$ in the corresponding RIQ $\int_I f(x)d\mu(x) = \sum_{k=1}^n \lambda_{nk} f(x_{nk})$, $\forall f \in \mathcal{L}_{n-1} \cdot \mathcal{L}_{n-2}^c$, all in $\mathbb{R}_0^+$?

Answer: similar story as rational Gauss-Radau of the First kind, but a little bit more complicated.
[K. Deckers and A. Bultheel, Report TW 573, 2010]

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Answer: similar story as rational Gauss-Radau of the First kind, but a little bit more complicated.

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Conclusion

- We characterized rational Gaussian, Gauss-Radau (two kinds) and Gauss-Lobatto (only Second kind) quadrature rules based on (quasi-)orthogonal rational functions.
- Still open for further investigation:
  - characterization of rational Gauss-Lobatto of the First kind,
  - other quasi-orthogonal rational functions leading to positive rational interpolatory quadrature rules

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Thank you ...