Rational quasi-Radau quadrature rules on the interval with positive weights

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Outline

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1. Preliminaries
   - Orthonormal rational functions
   - Rational interpolatory quadrature rules
2. Quasi-Radau quadrature rules
   - Existence
   - Construction
3. Conclusion and References

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 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 $\bigcup_{n=0}^{\infty} \mathcal{L}_n$
- $\mathcal{L}_{-1} \subset \mathcal{L}_0 \subset \mathcal{L}_1 \subset \ldots \subset \mathcal{L}_n \subset \ldots \subset \mathcal{L}$

Orthonormal rational functions

Notation

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

Rational basis

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

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

Polynomials

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

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

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

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 $\varphi_{-1}(x) \equiv 0$, $\varphi_0(x) \equiv \eta_0 \|1\|_\mu^{-1}$, $|\eta_0| = 1$, $\alpha_{-1} \in \overline{\mathbb{R}}_I$, 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

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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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Rational interpolatory quadrature rules (RIQs)

RIQs

Given a set of n distinct nodes $\{x_{nk}\}_{k=1}^{n} \subset I$, there exists a unique set of weights $\{\lambda_{nk}\}_{k=1}^{n} \subset \mathbb{C}$ so that

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

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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Rational interpolatory quadrature rules (RIQs)

Positive RIQs

- The weights $\{\lambda_{nk}\}_{k=1}^{n} \subset \mathbb{R}$ iff $\tilde{\mathcal{L}}_m \equiv \tilde{\mathcal{L}}_m^c$;
- Positive RIQ = RIQ with weights $\{\lambda_{nk}\}_{k=1}^{n} \subset \mathbb{R}_0^+$.

Rational Gauss-type quadrature rules

Rational Gauss-type quadrature rule = positive RIQ with j fixed nodes in I, where $0 \leqslant j < n$, and the remaining $n - j$ nodes are such that the domain of validity is of dimension $2n - j$ (at least).

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Rational Gauss-type quadrature rules

- Gaussian: $(j = 0)$
  $\tilde{\mathcal{L}}_m = \mathcal{L}_n \cdot \mathcal{L}^c_{n-1} \Rightarrow$ exists iff $\alpha_n \in \overline{\mathbb{R}}_I$
- quasi-Gaussian (qGauss): one node fixed in I $(j = 1)$
  - $\tilde{\mathcal{L}}_m = \mathcal{L}_n \cdot \mathcal{L}^c_{n-2} \Rightarrow$ can only exist if $\{\alpha_{n-1}, \alpha_n\} = \{\overline{\alpha}_{n-1}, \overline{\alpha}_n\}$
  - $\tilde{\mathcal{L}}_m = \mathcal{L}_{n-1} \cdot \mathcal{L}^c_{n-1}$

  Gauss-Radau = qGauss with fixed node in $+1$ or in -1.
- quasi-quasi-Gaussian (qqGauss): two nodes fixed in I $(j = 2)$
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Characterization

[K. Deckers and A. Bultheel, Appl. Math. Comput., 2012]

qqGauss

The nodes in a qqGauss with domain of validity $\mathcal{L}_{n-1} \cdot \mathcal{L}_{n-2}^{c}$ are the zeros of a quasi-quasi-orthogonal rational function (qqORF) $Q_{n,a,b} \in \mathcal{L}_n \setminus \mathcal{L}_{n-1}$ satisfying
$Q_{n,a,b} \perp_\mu \mathcal{L}_{n-2}(\overline{\alpha}_n) := \{\frac{p_{n-2}}{\pi_{n-2}} \in \mathcal{L}_{n-2} : p_{n-2}(\overline{\alpha}_n) = 0\}$.
i.e., $Q_{n,a,b}$ is a of the form

$$Q_{n,a,b}(x) = \varphi_n(x) + a \cdot \left(\frac{1 - x/\overline{\alpha}_{n-1}}{1 - x/\alpha_n}\right)\varphi_{n-1}(x) + b \cdot \left(\frac{1 - x/\overline{\alpha}_{n-2}}{1 - x/\alpha_n}\right)\varphi_{n-2}(x). \quad (2)$$

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Existence

Property

Suppose the qqORF (2) has all real zeros. Then it has at least $n-2$ zeros inside I.

Consider the qqORF $Q_{n,a,b}(x)$ with fixed zeros in x_{n1} and x_{n2}.

- 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

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

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

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Existence

Lemma

Suppose $c_n := b\frac{\overline{E}_{n-1}}{E_n} \in (-\infty, 1)$*, and let* $k_n^{-2} = 1 - c_n$*. Then there exist poles* $\alpha \in \overline{\mathbb{C}}_I$ *(not unique), and constants* $\hat{E}_n \neq 0$ *and*

$$\hat{D}_n = D_n + d_n |E_n|^{-2}, \quad d_n := a\overline{E}_n,$$

satisfying conditions Favard theorem, so that

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

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

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

Existence

Corollary

- *the zeros of a qqORF $Q_{n,a,b}$, for which $c_n \in (-\infty, 1)$, are all distinct;*
- *if $c_n = 1$, then $Q_{n,a,b}(x) = \left(\frac{Ax+B}{1-x/\alpha_n}\right) \varphi_{n-1}(x)$;*
- *a quadrature rule based on the zeros of a qqORF $Q_{n,a,b}$, for which $c_n \notin (-\infty, 1)$, can never be a qqGauss;*
- *the zeros of a qqORF $Q_{n,a,b}$, for which $c_n \in (-\infty, 1)$, are all real iff $\Im\{d_n\} = \Im\{1/\alpha_n\} - c_n \left|\frac{E_n}{E_{n-1}}\right|^2 \Im\{1/\alpha_{n-2}\}$;*
- *the weights in a quadrature rule based on the zeros of a qqORF $Q_{n,a,b}$, for which $c_n \in (-\infty, 1)$ and $\Im\{d_n\} = \Im\{1/\alpha_n\} - c_n \left|\frac{E_n}{E_{n-1}}\right|^2 \Im\{1/\alpha_{n-2}\}$, are all non-negative real.*

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- *a quadrature rule based on the zeros of a qqORF* $Q_{n,a,b}$, *for which* $c_n \notin (-\infty, 1)$, *can never be a qqGauss;*
- *the zeros of a qqORF* $Q_{n,a,b}$, *for which* $c_n \in (-\infty, 1)$, *are all real iff* $\Im\{d_n\} = \Im\{1/\alpha_n\} - c_n \left|\frac{E_n}{E_{n-1}}\right|^2 \Im\{1/\alpha_{n-2}\}$;
- *the weights in a quadrature rule based on the zeros of a qqORF* $Q_{n,a,b}$, *for which* $c_n \in (-\infty, 1)$ *and* $\Im\{d_n\} = \Im\{1/\alpha_n\} - c_n \left|\frac{E_n}{E_{n-1}}\right|^2 \Im\{1/\alpha_{n-2}\}$, *are all non-negative real.*

Existence

Lemma

Suppose that $\Im\{d_n\} = \Im\{1/\alpha_n\} - c_n \left|\frac{E_n}{E_{n-1}}\right|^2 \Im\{1/\alpha_{n-2}\}$, *and let* $\xi \in \{\pm 1\}$.

(**quasi-Radau**)
For every $c_n \in (-\infty, 1]$ *there exists a unique constant* $d_n^{qR(\xi)} \in \mathbb{R}$ *such that the qqORF* $Q_{n,a,b}$ *corresponding to* c_n *and* $d_n = d_n^{qR(\xi)} + \mathbf{i}\Im\{d_n\}$ *has a zero at* ξ, *while at least* $(n-2)$ *of the remaining* $(n-1)$ *zeros are in* I.

(**Gauss-Lobatto**)
Moreover, there exists a constant c_n^{GL} *such that* $d_n^{qR(\xi)} = d_n^{qR(-\xi)} = d_n^{GL}$.

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Existence

Lemma

There exists a qqGauss with fixed nodes in x_{n1} and x_{n2} iff the constants a and b corresponding to the qqORF $Q_{n,a,b}(x)$ with fixed zeros in x_{n1} and x_{n2} satisfy the following conditions:

1. $b\frac{\overline{E}_{n-1}}{E_n} = c_n \in [c_n^{GL}, 1)$;
2. $a\overline{E}_n = d_n$, *with*

$$\Im\{d_n\} = \Im\{1/\alpha_n\} - c_n \left|\frac{E_n}{E_{n-1}}\right|^2 \Im\{1/\alpha_{n-2}\}$$

and

$$\Re\{d_n\} \in \left[\min_{\xi\in\{\pm 1\}} d_n^{qR(\xi)}, \max_{\xi\in\{\pm 1\}} d_n^{qR(\xi)}\right].$$

Existence

Corollary

Let

- $X_n^{GL} := \{x_{n,k}^{GL}\}_{k=1}^{n}$ *denote the nth rational Gauss-Lobatto nodes such that* $-1 = x_{n,1}^{GL} < \ldots < x_{n,k}^{GL} < \ldots < x_{n,n}^{GL} = 1$;
- $X_{n-1}^{G} := \{x_{n-1,k}^{G}\}_{k=1}^{n-1}$ *denote the* $(n-1)$*th rational Gaussian nodes such that* $x_{n-1,1}^{G} < \ldots < x_{n-1,k}^{G} < \ldots < x_{n-1,n-1}^{G}$.

Then it holds that

$$x_{n,1}^{GL} < x_{n-1,1}^{G} < \ldots < x_{n,k}^{GL} < x_{n-1,k}^{G} < \ldots < x_{n,n-1}^{GL} < x_{n-1,n-1}^{G} < x_{n,n}^{GL}.$$

Existence

Theorem (Existence of qRadau)

Suppose $x_* \in I$. Then either

- *there exists an n-point rational qRadau rule with two nodes fixed in x_* and $+1$ (i.e., in the case in which $x^{GL}_{n,k} < x_* < x^{G}_{n-1,k}$);*
- *there exists an n-point rational qRadau rule with two nodes fixed in x_* and -1 (i.e., in the case in which $x^{G}_{n-1,k-1} < x_* < x^{GL}_{n,k}$);*
- *x_* is one of the nodes in the n-point rational Gauss-Lobatto rule; or,*
- *x_* is one of the nodes in the $(n-1)$-point rational Gaussian rule.*

Existence

Theorem (Existence of qqGauss)

Suppose $x_* \subset (-1,1) \setminus \left(X_n^{GL} \cup X_{n-1}^{G}\right)$, *and let* $\{\hat{x}_{n,k}^{G}\}_{k=1}^{n} = X_{n-1}^{G} \cup \{x_*\}$. *Then there exists an n-point rational qqGauss rule with two nodes fixed in* x_* *and* $\hat{x}_*$ *iff either*

- $x_{n,k}^{GL} < x_* < x_{n-1,k}^{G}$ *and* $\hat{x}_{n,\ell}^{G} < \hat{x}_* \leqslant x_{n,\ell}^{qR(x_*,+1)}$; *or,*
- $x_{n-1,k-1}^{G} < x_* < x_{n,k}^{GL}$ *and* $x_{n,\ell}^{qR(x_*,-1)} \leqslant \hat{x}_* < \hat{x}_{n,\ell}^{G}$.

Outline

Construction

Rational Gaussian quadrature

- the nodes $\{x_{nk}^G\}_{k=1}^n$ are zeros of the ORF $\varphi_n \in \mathcal{L}_n$; hence, can be computed by means of the GEP
- the corresponding weights $\{\lambda_{nk}^G\}_{k=1}^n$ can be computed by means of the GEP too:

$$\lambda_{nk}^G = |v_{nk}|^2 \, \|1\|_\mu^2 \, ,$$

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

Construction

- the rational qqGauss nodes are in fact rational Gaussian nodes w.r.t. a modified measure $\hat{\mu}$ and modified nth pole;
- $\{\varphi_0, \ldots, \varphi_{n-2}, k_n\varphi_{n-1}\}$ forms an orthonormal system for the inner product $\langle \cdot, \cdot \rangle_{\hat{\mu}} \Rightarrow$
  $\forall f \in \mathcal{L}_{n-1} \cdot \mathcal{L}_{n-2}^c \supset \mathcal{L}_{n-1} : \int_I f(x) d\mu(x) = \int_{\hat{S}} f(x) d\hat{\mu}(x)$;
  hence, the rational qqGauss weights are rational Gaussian weights w.r.t. the same modified measure $\hat{\mu}$ and the same modified nth pole;
- the rational qqGauss nodes and weights can be computed by means of a modified GEP: $\hat{\mathbf{J}}_n \underline{\hat{v}}_{nk} = x_{nk} \hat{\mathbf{B}}_n \underline{\hat{v}}_{nk}$, where

$$\hat{\mathbf{J}}_n = \left(\begin{array}{c|c} \mathbf{J}_{n-1} & \begin{array}{c} \underline{0}_{n-2} \\ \times \end{array} \\ \hline \underline{0}_{n-2}^T \quad \times & \times \end{array} \right), \quad \hat{\mathbf{B}}_n = \left(\begin{array}{c|c} \mathbf{B}_{n-1} & \begin{array}{c} \underline{0}_{n-2} \\ \times \end{array} \\ \hline \underline{0}_{n-2}^T \quad \times & \times \end{array} \right)$$

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

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Conclusion

- We characterized rational Gauss-type quadrature rules with two nodes fixed in advance and domain of validity $\mathcal{L}_{n-1} \cdot \mathcal{L}_{n-2}^c$;
- we provided conditions on the sequence of poles and the nodes fixed in advance to ensure the existence of these quadrature rules; and
- we discussed the construction of these quadrature rules.
- Still open for further investigation:
  - characterization, existence and construction of rational qqGauss for the case in which the domain of validity is of the form $\mathcal{L}_n \cdot \mathcal{L}_{n-3}^c$;
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Thank you …