Rational Gauss quadrature

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This is dedicated to the memory of Pablo González Vera.

`http://nalag.cs.kuleuven.be/papers/ade/chemnitz13`

Survey

- Prerequisite: Gauss quadrature
  (basics: quadrature, orthogonal polynomials, moment matching, interpolation)
- Generalization: Orthogonal rational functions (ORFs)
  (generalized basics: function spaces, orthogonality, recursion, interpolation, quadrature)
- Special case (Chebyshev weights and rational interpolation), Preassigned nodes, Error bound and convergence
- Application of ORFs (rational Krylov)

Orthogonality and quadrature on $\mathbb{R}, \mathbb{R}^+, [-1,1]$ (Gauss)
[and briefly on $\mathbb{T}$ (Szegő)]

Numerical quadrature

Problem is to compute the integral

$$\mathcal{I}_\mu\{f\} = \int f(z)\mathrm{d}\mu(z)$$

- μ finite positive measure
- usually probability measure ($\int \mathrm{d}\mu(z) = 1$)
- supported on (part of) $\hat{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$
  [or $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$]
- $f \in \mathcal{L} \subseteq L_1^\mu$

Numerical quadrature

Problem is to compute integral $\mathcal{I}_\mu\{f\} = \int f(z)\mathrm{d}\mu(z)$.

Technique:

consider nested subspaces ($\mathcal{L}_{-1} = \varnothing$, $\mathcal{L}_0 = \mathbb{C}$, $\dim(\mathcal{L}_n) = n+1$)

$$\mathcal{L}_0 \subset \mathcal{L}_1 \subset \cdots \subset \mathcal{L}_n \subset \cdots \subset \mathcal{L}_\infty = \bigcup_{k=0}^{\infty} \mathcal{L}_k \subset \mathcal{L} = \mathrm{cl}(\mathcal{L}_\infty).$$

Example $\mathcal{L}_n = \mathcal{P}_n$ (= space of polynomials of degree $\le n$)

Interpolate f **by** $p_{n-1} \in \mathcal{L}_{n-1}$ **and** ***integrate*****:**

$p_{n-1}(z) = \sum_{j=1}^n f(x_{nj})\ell_{nj}(z) \in \mathcal{L}_{n-1}$, $\ell_{nj}(x_{ni}) = \delta_{ij}$, $i,j = 1,\ldots,n$

$$\Rightarrow \boxed{\mathcal{I}_\mu\{f\} \approx \mathcal{I}_\mu\{p_{n-1}\} = \mathcal{I}_{\mu_n}\{f\} = \mathcal{I}_n\{f\}}$$

$$\mathcal{I}_{\mu_n}\{f\} = \sum_{j=1}^n w_{nj} f(x_{nj}), \quad w_{nj} = \mathcal{I}_\mu\{\ell_{nj}\}, \quad \mu_n = \sum_{j=1}^n w_{nj}\delta_{x_{nj}}.$$

Degree of Exactness

$p_{n-1} \in \mathcal{L}_{n-1}$ uniquely defined by interpolation in $\{x_{nj}\}_{j=1}^n$.

Interpolatory qf

$I_\mu\{f\} = \mathcal{I}_{\mu_n}\{f\}$, $\forall f \in \mathcal{L}_k$. Generically $k = n-1$. How about $k \ge n$?
$\max k$ = degree of exactness (DoE).
$\mathcal{L}_k$ is a domain of exactness.

In general DoE can be slightly larger than $n-1$.
E.g. n-point Newton-Cotes qf ($\mathcal{L}_k = \mathcal{P}_k$, $\{x_{nj}\} \subset I \subset \mathbb{R}$ equidistant):

$$\mathrm{DoE} = \begin{cases} n-1, & n \text{ even} \\ n, & n \text{ odd} \end{cases}.$$

Choose nodes x_{nj} to maximize the DoE (in $\{\mathcal{L}_k\}$)

This requires an orthogonal basis, inner product, Hilbert spaces,...

Some facts on $\mathbb{R}$

We need an inner product $\langle f, g\rangle_\mu = \int \overline{f(z)}g(z)\mathrm{d}\mu(z)$.
If $\mathrm{supp}\,\mu \subseteq \hat{\mathbb{R}}$ then $z \in \hat{\mathbb{R}}$ and thus $\overline{f(z)} = \overline{f(\overline{z})}$.

Notation

We set $f_*(z) = \overline{f(\overline{z})}$ for $\mathrm{supp}\,\mu \subseteq \hat{\mathbb{R}}$ i.e. $\langle f, g\rangle_\mu = \mathcal{I}_\mu\{f_* g\}$

On $\mathrm{supp}\,\mu$, both coincide with just taking the complex conjugate, but the definition holds for any $z \in \hat{\mathbb{C}}$.
on $\mathbb{R}$: $\langle z^l, z^k\rangle_\mu = \mathcal{I}_\mu\{z^{k+l}\}$: $z^{k+l} \in \mathcal{P}_* \cdot \mathcal{P} = \mathcal{P}$.
i.e. the Gram matrix $[\langle z^l, z^k\rangle_\mu]_{k,l}$ has a Hankel structure.

Gauss quadrature (on $\mathbb{R}$)

$\mathcal{L}_n = \mathcal{P}_n = \mathrm{span}\{1, z, z^2, \ldots, z^n\} \to$ orthogonalize $\to$ OPs $\{\phi_k\}_{k=0,1,\ldots}$
Zeros $\{x_{nk}\}_{k=1}^n$ of ϕ_n are simple and in $\mathrm{supp}\,\mu$.

Theorem

An n-point interpolatory qf (IQF) with nodes $\{x_{nj}\}_{j=1}^n$ will be exact in $\mathcal{P}_m$ with $m \ge n-1$ if and only if the node polynomial
$N(z) = (z - x_{n1})\cdots(z - x_{nn})$ *is orthogonal to $\mathcal{P}_{m-n}$.*

Thus if $\{x_{nj}\}_{j=1}^n$ are the zeros of an orthogonal polynomial $\phi_n \in \mathcal{P}_n \setminus \mathcal{P}_{n-1}$ (simple and in the support of μ), then we will get a maximal DoE that is $m = 2n-1$ and the quadrature weights are positive.
These are Gauss qf with DoE $2n-1$
note $\dim(\mathcal{P}_{2n-1}) = 2n$.

Extra bonus

On our wish list:

- Nodes preferably inside $\mathrm{supp}\,\mu$
- Quadrature weights should be positive (stability and convergence)
- DoE as large as possible

Glory days!

Gauss qf have all these.

QF = moment matching = interpolation

$p, q \in \mathcal{L}_n$: $\langle p, q\rangle_\mu = \sum_{k=0}^{n}\sum_{l=0}^{n} \overline{p}_k m_{k+l} q_l$, $m_{k+l} = \langle x^k, x^l\rangle = \mathcal{I}_\mu\{x^{k+l}\}$

QF = moment matching

$\mathcal{I}_\mu\{p_\ast q\} = \mathcal{I}_n\{p_\ast q\}\ \forall p, q \in \mathcal{P}_n$, i.e., $\mathcal{I}_\mu\{f\} = \mathcal{I}_n\{f\}$, $\forall f \in \mathcal{P}_{2n}$
iff $m_k = \mathcal{I}_\mu\{x^k\} = \mathcal{I}_n\{x^k\}$, $k = 0, 1, \ldots, 2n$

Define $\Omega_\mu(z) = \int \frac{\mathrm{d}\mu(x)}{x-z} = -\sum_{k=0}^{\infty} m_k z^{-k-1}$ and

$\Omega_n(z) = \int \frac{\mathrm{d}\mu_n(x)}{x-z} = -\sum_{k=0}^{\infty} m_{n,k} z^{-k-1}$

moment matching = interpolation at ∞

$m_k = m_{n,k}$, $k = 0, \ldots, 2n$ iff $\Omega_\mu(z) - \Omega_n(z) = O(z^{-(2n+1)})$

Extend to the rationals

Polynomials are rationals with poles at ∞
From 1 point ∞ to multiple points $\{\alpha_k\}$

On $\hat{\mathbb{R}}$: (QF = moment matching)

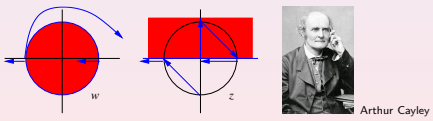
$\infty \in \hat{\mathbb{R}} \Rightarrow$ many possibilities
- $\mathrm{supp}\,(\mu) = \hat{\mathbb{R}}$ all poles on $\hat{\mathbb{R}}$ or all in $\hat{\mathbb{C}} \setminus \mathbb{R}$ — Hamburger
- $\mathrm{supp}\,(\mu) = [0, +\infty]$ all poles on $[-\infty, 0]$ or in $\hat{\mathbb{C}} \setminus [0, +\infty)$ — Stieltjes
- $\mathrm{supp}\,(\mu) = [-1, 1]$ all poles on $\mathbb{R} \setminus [-1, 1]$ or in $\hat{\mathbb{C}} \setminus [-1, 1]$ — Hausdorff

$\mathcal{L}_n = \{\frac{p_n(z)}{\pi_n(z)} : p_n \in \mathcal{P}_n, \pi_n(z) = \prod_{k=1}^{n}(1 - z/\alpha_k)\}$
$\mathcal{L}_n = \mathcal{P}_n$ if all $\alpha_k = \infty$.

ORF on $\mathbb{R}$

Definitions and notation

- $\hat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$, $\hat{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$
  $\mathbb{U} = \{z \in \mathbb{C} : \mathrm{Im}\,(z) > 0\}$
- $f_\ast(z) = \overline{f(\overline{z})}$
- Cayley transform: (note factor $\mathbf{i}$)
  $z = \mathrm{ic}(w) = \mathbf{i}\frac{1-w}{1+w} \leftrightarrow w = \mathrm{ic}^{inv} = \frac{\mathbf{i}-z}{\mathbf{i}+z}$, $w \in \begin{cases}\mathbb{D}\\ \mathbb{T}\end{cases} \leftrightarrow z \in \begin{cases}\mathbb{U}\\ \hat{\mathbb{R}}\end{cases}$



Arthur Cayley

- $\mathbb{T} : \mathrm{d}\lambda(t) \overset{t=e^{i\theta}}{=} \frac{\mathrm{d}\theta}{2\pi} \Leftrightarrow \mathbb{R} : \mathrm{d}\mathring{\lambda}(x) = \frac{\mathrm{d}x}{\pi(1+x^2)}$ (Lebesgue).
  Therefore set $\mathrm{d}\mathring{\mu}(x) = \frac{\mathrm{d}\mu(x)}{1+x^2}$

Definitions and notation

relation

$\mathcal{M} \leftrightarrow \mathcal{C}$

- Nevanlinna kernel: $D(x, z) = \frac{1}{\mathbf{i}}\frac{1+xz}{x-z}$
- Nevanlinna transform: $\Omega_{\mathring{\mu}}(z) = \mathbf{i}c + \int D(x, z)\mathrm{d}\mathring{\mu}(x)$
- If no mass at ∞, then Cauchy transform: $\Omega_\mu(z) = \frac{1}{\mathbf{i}}\int \frac{\mathrm{d}\mu(x)}{x-z}$
- Carathéodory class $\mathcal{C} = \{f \in H(\mathbb{U}) : \mathrm{Re}\, f(\mathbb{U}) \geq 0\}$
  $\Omega_{\mathring{\mu}}$ is *positive real* in $\mathbb{U}$: $\mathrm{Re}\,\Omega_{\mathring{\mu}}(z) \geq 0$ for $z \in \mathbb{U}$
- $\lim_{y \downarrow 0} \mathrm{Re}\,\Omega_{\mathring{\mu}}(x + \mathbf{i}y) = \mu'(x)$
- Remove factor $\mathbf{i}$ in the Nevanlinna and Cauchy kernel results in Ω in
  Pick/Nevanlinna class $= \{f \in H(\mathbb{U}) : f(\mathbb{U}) \subseteq \mathbb{U} \cup \mathbb{R}\}$

The spaces $\mathcal{L}_n$

We start with poles $\{\alpha_k\}_{k\geq 1} \in \hat{\mathbb{R}} \setminus \{0\}$ and $\mathrm{supp}\,(\mu) = \hat{\mathbb{R}}$, $\alpha_0 = \infty$

- set $b_0 = 1$, $b_n(z) = Z_n(z)b_{n-1}(z)$, $Z_n(z) = \frac{z}{1-z/\alpha_n}$, $n \geq 1$,
- $\mathcal{L}_n = \mathrm{span}\{b_0, b_1, \ldots, b_n\}$
  $\mathcal{L}_n = \left\{\frac{p_n}{\pi_n} : p_n \in \mathcal{P}_n; \pi_n(z) = \prod_{k=1}^{n}(1 - z/\alpha_k)\right\}$
- if all $\alpha_k = \infty$ then $Z_n(z) = z$, $b_n(z) = z^n$, and $\mathcal{L}_n = \mathcal{P}_n$
- $p \in \mathcal{P}_n$ has a zero at ∞ of order m means that its degree is $n - m$.

Inner product in $\mathcal{L}_n$

- $\langle\cdot,\cdot\rangle_{\mathring{\mu}}$ defined by Gram matrix $G_n = [\langle b_k, b_l\rangle_{\mathring{\mu}}]_{k,l=0}^{n} = [m_{k,l}]_{k,l=0}^{n}$.
- Moments $m_{k,l} = \int b_{k\ast}(x)b_l(x)\mathrm{d}\mathring{\mu}(x)$
- $\mathcal{A}_n^{\mathbf{i}} = \{\mathbf{i}, \alpha_1, \ldots, \alpha_n\}$ and $\alpha^\#$ is the multiplicity of $\alpha \in \mathcal{A}_n^{\mathbf{i}}$
- Recall $\Omega_{\mathring{\mu}}(z) = \int D(x, z)\mathrm{d}\mathring{\mu}(x) = \frac{1}{\mathbf{i}}\int \frac{1+xz}{x-z}\mathrm{d}\mathring{\mu}(x)$ then
  G_n defined by $\Omega_{\mathring{\mu}}^{(s)}(\alpha)$ for $\alpha \in \mathcal{A}_n^{\mathbf{i}}$ and $s = 0, \ldots 2\alpha^\# - 1$
  partial fractions: $m_{k,l} = \sum_{\alpha,s}\int D^{(s)}(x, \alpha)\mathrm{d}\mathring{\mu}(x)$
- $\langle f, g\rangle_{\mathring{\mu}} = \langle f, g\rangle_{\mathring{\nu}}$, $\forall f, g \in \mathcal{L}_n$ iff $\Omega_{\mathring{\mu}}$ is an Hermite interpolant for $\Omega_{\mathring{\nu}}$
  for the points $\{\mathbf{i}, -\mathbf{i}, \alpha_1, \alpha_1, \alpha_2, \alpha_2, \ldots, \alpha_n, \alpha_n\}$
- The $\mathbf{i}$ appears because $D(t, \mathbf{i}) = 1$ and
  $1 = \int \mathrm{d}\mathring{\mu}(t) = \int \frac{\mathrm{d}\mu(x)}{1+x^2} = \int D(x, \mathbf{i})\mathrm{d}\mathring{\mu}(x) = \Omega_{\mathring{\mu}}(\mathbf{i}) = \overline{\Omega_{\mathring{\mu}}(-\mathbf{i})}$

- (QF =) moment matching = interpolation

The ORF ϕ_n

- ORF $\mathcal{L}_{n-1} \perp_\mu \phi_n \in \mathcal{L}_n$
- $\phi_n(z) = a_{nn}b_n(z) + a_{n,n-1}b_{n-1}(z) + \cdots + a_{n0}b_0$,
  $a_{nn} = \kappa_n > 0$, $a_{n,n-1} = \kappa_n'$
- We may assume all functions are real ☺ + ☹ = ☺
- Note that $\mathcal{L}_{n\ast} = \mathcal{L}_n$ if the α_k are real (recall $f_\ast(z) = \overline{f(\overline{z})}$)
- $\phi_n = \frac{p_n}{\pi_n}$ then ϕ_n is singular if $p_n(\alpha_{n-1}) = 0$, and regular otherwise.
- Singularity does not occur in the polynomial case ☹
- Set $\mathcal{L}_\infty = \bigcup_{k=0}^{\infty}\mathcal{L}_k$, then $\mathcal{L}_\infty \cdot \mathcal{L}_\infty \neq \mathcal{L}_\infty$ (doubles poles)
  unless a finite number of poles with infinite multiplicity ☺

Recurrence for ORF ϕ_n

- Define $\phi_{-1} = 0$, $\phi_0 = 1$ (assuming $\int \mathrm{d}\hat{\mu} = 1$), $\alpha_{-1} = \alpha_0 = \infty$, so that $Z_{-1}(z) = Z_0(z) = z$, then clearly $\exists E_1, B_1$ such that

$$(1 - \frac{z}{\alpha_1})\phi_1(z) = E_1 z + B_1 = (E_1 z + B_1)\phi_0.$$

Theorem

$\exists E_1, B_1 \in \mathbb{R}$, $E_1 \neq 0$ *s.t.*

$$\frac{\phi_1(z)}{Z_1(z)} = (E_1 Z_0(z) + B_1)\frac{\phi_0(z)}{Z_0(z)} + C_1\frac{\phi_{-1}(z)}{Z_{-1}(z)}$$

- This is the first step of the 3-term recurrence relation (TTRR)

Recurrence for ORF ϕ_n

Theorem

If ϕ_n and ϕ_{n-1} are regular then for $n \geq 2$

$$\begin{aligned}\frac{\phi_n(z)}{Z_n(z)} &= \left(A_n + \frac{B_n}{Z_{n-2}(z)}\right)\phi_{n-1}(z) + C_n\frac{\phi_{n-2}(z)}{Z_{n-2}(z)}\\ \tilde{\phi}_n(z) &= (E_n Z_{n-1}(z) + B_n)\tilde{\phi}_{n-1}(z) + C_n\tilde{\phi}_{n-2}(z)\end{aligned}$$

with $C_n = -\frac{E_n}{E_{n-1}} \neq 0$ *and* $E_n = A_n + \frac{B_n}{Z_{n-2}(\alpha_{n-1})} = A_n - \frac{B_n}{Z_{n-1}(\alpha_{n-2})} \neq 0$.

$E_n = 0$ iff ϕ_n is singular and
$E_n = \frac{1}{\kappa_{n-1}}\left[\kappa_n + \frac{\kappa'_n}{Z_n(\alpha_{n-1})}\right]$, $n \geq 2$.
$\tilde{\phi}_k(z) = \frac{z\phi_k(z)}{Z_k(z)} = (1 - \frac{z}{\alpha_k})\phi_k(z)$

Recurrence

$p_n(\alpha_{n-1})p_{n-1}(\alpha_{n-2}) \neq 0$

Theorem

$$\tilde{\phi}_n(z) = (E_n Z_{n-1}(z) + B_n)\tilde{\phi}_{n-1}(z) + C_n\tilde{\phi}_{n-2}(z).$$

2 parameter sequences: $\{E_n\}$ and $\{B_n\}$ ($C_n = -\frac{E_n}{E_{n-1}}$)
Define $a_n = \frac{1}{E_n}$ and $b_n = -\frac{B_n}{E_n}$ then

$$a_n\tilde{\phi}_n(z) = (Z_{n-1}(z) - b_n)\tilde{\phi}_{n-1}(z) - a_{n-1}\tilde{\phi}_{n-2}(z).$$

or, since $Z_{n-1}(z)\tilde{\phi}_{n-1}(z) = z\phi_{n-1}(z)$

Theorem

$$a_n\tilde{\phi}_n(z) + b_n\tilde{\phi}_{n-1}(z) + a_{n-1}\tilde{\phi}_{n-2}(z) = z\phi_{n-1}(z).$$

Proof of recurrence

Skip proof

- There is an A_n such that (use regularity of ϕ_{n-1}) $W_n(z) = \frac{Z_{n-2}(z)}{Z_n(z)}\phi_n(z) - A_n Z_{n-2}(z)\phi_{n-1}(z) \in \mathcal{L}_{n-1}$
- Check that $W_n \perp_\mu \mathcal{L}_{n-3}$, so that $W_n(z) = B_n\phi_{n-1}(z) + C_n\phi_{n-2}(z)$ proves first form
- Second form: note $D_n = \frac{1}{Z_{n-2}(z)} - \frac{1}{Z_{n-1}(z)}$ does not depend on z
- $E_n \neq 0$: take numerator of recurrence for $z = \alpha_{n-1}$ + regularity ϕ_n
- $C_n \neq 0$ follows by writing out $\frac{b_{n-1}}{Z_n} \in \mathcal{L}_{n-1} \perp \phi_n$ + recurrence
- the 'only if' part is simple QED
- To prove that $E_n = -C_n E_{n-1}$ requires more work...

Functions of the second kind

- Define $\psi_n(z) = \int D(x,z)[\phi_n(x) - \phi_n(z)]\mathrm{d}\hat{\mu}(x)$, $n \geq 1$ with appropriate initial conditions ($\psi_0(z) = \mathbf{i}z$, $\psi_{-1}(z) = \mathbf{i}(1+z^2)$, $\alpha_{-1} = \infty$, $E_0 = 1$)

Theorem

The ψ_n are independent solutions of the same recurrence as for the ϕ_n

- Note because $D(x,z) = \frac{1}{\mathbf{i}}\frac{1+xz}{x-z}$, the coefs of ψ_n are in $\mathbf{i}\mathbb{R}$
- Note $\psi_k \in \mathcal{L}_k$ for $k \geq 1$. Starting with $\sigma_0 = 0, \sigma_{-1} = \mathbf{i}$ recurrence generates $\sigma_n \in \mathcal{L}_n(\infty)$, i.e., with numerator of degree $n-1$
- Note with $F_n = E_n Z_{n-1} + B_n$, the recurrence for $\tilde{\phi}_n(z) = \frac{z\phi_n(z)}{Z_n(z)} = (1 - \frac{z}{\alpha_n})\phi_n(z)$, $\tilde{\psi}_n(z) = (1 - \frac{z}{\alpha_n})\psi_n(z)$, i.e., pole $\alpha_n \to \infty$

$$\begin{bmatrix}\tilde{\phi}_n(z) & \tilde{\psi}_n(z)\\ \tilde{\phi}_{n-1}(z) & \tilde{\psi}_{n-1}(z)\end{bmatrix} = \begin{bmatrix}F_n(z) & C_n\\ 1 & 0\end{bmatrix}\begin{bmatrix}\tilde{\phi}_{n-1}(z) & \tilde{\psi}_{n-1}(z)\\ \tilde{\phi}_{n-2}(z) & \tilde{\psi}_{n-2}(z)\end{bmatrix}$$

Christoffel-Darboux relation

Theorem (CD relation)

For $x \neq y$ and $xy \neq 0$

$$\frac{\tilde{\phi}_n(y)\tilde{\phi}_{n-1}(x) - \tilde{\phi}_n(x)\tilde{\phi}_{n-1}(y)}{y - x} = E_n k_{n-1}(x,y) = E_n\sum_{k=0}^{n-1}\phi_k(x)\phi_k(y)$$

If $x \to y$

$$\tilde{\phi}'_n(x)\tilde{\phi}_{n-1}(x) - \tilde{\phi}_n(x)\tilde{\phi}'_{n-1}(x) = E_n k_{n-1}(x,x)$$

Follows from recurrence, but can also be proved independent of regularity.

Rational qf

- An n-point interpolatory qf (IQF) for $\mathcal{L}_{n-1}$ with nodes $\{\xi_{nk}\}_{k=1}^n$ none in $\mathcal{A}_n^0 = \{\alpha_0, \ldots, \alpha_{n-1}\}$ will give qf exact in $\mathcal{L}_{n-1}$: $\mathcal{I}_\mu\{f\} \approx \mathcal{I}_\mu\{f_n\}$, $f_n(z) = \sum_{k=1}^n f(\xi_{nk})L_{nk}(z) \in \mathcal{L}_{n-1}$.
- Choose ξ_{nk} such that qf exact in $\mathcal{L}_{n-1,n-1}$ or larger if possible.

Theorem

The interpolatory qf will be exact in $\mathcal{L}_{n-1,n-m}$, $m \geq 0$ if its nodes are the zeros of q_n where $Q_n = \frac{q_n}{\pi_n} \in \mathcal{L}_n$ is orthogonal to $\mathcal{L}_{n-m}(\alpha_n)$.

- The largest possible space $\mathcal{L}_{n-1,n} = \mathcal{L}_{n,n-1}$ is obtained for $m = 0$ so that $Q_n \perp \mathcal{L}_n(\alpha_n) = \mathcal{L}_{n-1}$, i.e., $Q_n = c\phi_n$.
- The corresponding weights will be positive. Indeed $\lambda_{nk} = \mathcal{I}_\mu\{L_{nk}\} = \mathcal{I}_\mu\{L_{nk}^2\} > 0$. ($L_{nk}(z) = \ell_{nk}(z)\frac{\pi_{n-1}(\xi_{nk})}{\pi_{n-1}(z)}$)
- Problem: Does ϕ_n have simple zeros on $\mathbb{R}$ not in $\mathcal{A}_n^0 = \{\alpha_0, \ldots, \alpha_n\}$?

Quasi orthogonal rational functions (QORF)

- We might introduce a parameter τ at the cost of loosing 1 degree of exactness. Define the QORF $Q_n(z) = Q_n(z;\tau)$ for $\tau \in \hat{\mathbb{R}}$ as

$$Q_n(z) = \phi_n(z) + \tau\frac{Z_n(z)}{Z_{n-1}(z)}\phi_{n-1}(z) \in \mathcal{L}_n$$

- 'Almost' orthogonal: $Q_n \perp \mathcal{L}_{n-1} \cap \mathcal{L}_{n-1}(\alpha_n) = \mathcal{L}_{n-1}(\alpha_n)$

Theorem

If Q_n has n simple zeros in $\hat{\mathbb{R}} \setminus \mathcal{A}_n^0$, $\mathcal{A}_n^0 = \{\alpha_0, \alpha_1, \ldots, \alpha_n\}$ then the IQF is exact in $\mathcal{L}_{n-1,n-1}$ and has positive weights.

Quasi orthogonal rational functions (QORF)

Lemma

If $Q_n = \frac{p_n}{\pi_n}$ then p_n has n simple zeros in $\hat{\mathbb{R}}$

Skip proof

- Let $p_n = c\prod_{i=1}^{l}(x-x_i)^{2m_i+1}\prod_{j=1}^{k}(x-\xi_j)^2, \quad n = 2M+l+2k$
  x_i odd multiplicity $2m_i+1$, $M = \sum_{i=1}^{l} m_i$. Need $M = k = 0$
- Suppose $M+k \geq 1$, set $T(x) = \frac{(x-x_1)\cdots(x-x_l)(1-x/\alpha_n)}{(1-x/\alpha_1)\cdots(1-x/\alpha_{n-1})} \in \mathcal{L}_{n-1}(\alpha_n)$
- $\therefore \langle T, Q_n\rangle_\mu = 0$, but $\langle T, Q_n\rangle_\mu = c\langle W, W\rangle_\mu > 0$ for
  $W(x) = \frac{\prod_{i=1}^{l}(x-x_i)^{m_i+1}\prod_{j=1}^{k}(x-\xi_j)}{\pi_{n-1}(x)} \neq 0$
- Contradiction!

Quasi orthogonal rational functions (QORF)

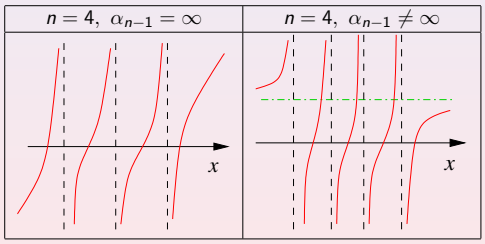
Lemma

If $Q_n = \frac{p_n}{\pi_n}$ then p_n has n simple zeros in $\hat{\mathbb{R}}$

- Problem zeros of p_n can be in $\mathcal{A}_n^0 = \{\alpha_0, \alpha_1, \ldots, \alpha_n\}$
- If ORFs $\{\phi_k\}$ are regular, then ϕ_n and ϕ_{n-1} have no common zeros.
- $\therefore$ except for $n+1$ values of τ, all zeros of p_n are not in $\mathcal{A}_n^0$
- All other values of τ are called *regular* and also Q_n is called regular
- If $\tau = 0$ is a regular value, then $Q_n = \phi_n$ and IQF is exact in $\mathcal{L}_{n,n-1}$

Proof

$$Q_n(x) = \phi_n(x) + \tau\frac{1-\frac{x}{\alpha_{n-1}}}{1-\frac{x}{\alpha_n}}\phi_{n-1}(x) = 0 \Rightarrow \quad \tau = -\frac{p_n(x)}{p_{n-1}(x)(1-\frac{x}{\alpha_{n-1}})}$$



!!! Integrating over a subinterval of $\mathbb{R}$, not all nodes may be in it. !!!

Interpolation

- If ϕ_k are ORFs for $\mathring{\mu}$, Q_k are QORFs, $\mathring{\mu}_n = \sum_k \lambda_{nk}\delta_{\xi_{nk}}$ the IQF in zeros of Q_n, exact in $\mathcal{L}_{n-1,n-1}$
- Thus $\langle f, g\rangle_{\mathring{\mu}} = \langle f, g\rangle_{\mathring{\mu}_n}$, $\forall f, g \in \mathcal{L}_{n-1}$ implies interpolation of corresponding $\mathcal{C}$-functions $\Omega_{\mathring{\mu}}$ and $\Omega_{\mathring{\mu}_n}$ in points
  $\mathcal{A}_{n-1}^{\mathbf{i}} = \{\mathbf{i}, -\mathbf{i}, \alpha_1, \alpha_1, \alpha_2, \alpha_2, \ldots, \alpha_{n-1}, \alpha_{n-1}\}$.
- What is $\Omega_{\mathring{\mu}_n}$?

Interpolation

- QORF: $Q_n(z) = \phi_n(z) + \tau\frac{Z_n(z)}{Z_{n-1}(z)}\phi_{n-1}(z)$
- QORF of the second kind: $P_n(z) = \psi_n(z) + \tau\frac{Z_n(z)}{Z_{n-1}(z)}\psi_{n-1}(z)$
- Then
  $\frac{z-\alpha_n}{z-\alpha_{n-1}}P_n(z) = \int D(x,z)\left[\frac{x-\alpha_n}{x-\alpha_{n-1}}Q_n(x) - \frac{z-\alpha_n}{z-\alpha_{n-1}}Q_n(z)\right]\mathrm{d}\mathring{\mu}(x).$
- integrand$(x)\in \mathcal{L}_{n-1,n-1}$ thus IQF in zeros Q_n exact

$$\therefore \int [*]\mathrm{d}\mathring{\mu} = -\left[\sum_k D(\xi_{nk}, z)\lambda_{nk}\right]\frac{z-\alpha_n}{z-\alpha_{n-1}}Q_n(z) = -\Omega_{\mathring{\mu}_n}(z)\frac{z-\alpha_n}{z-\alpha_{n-1}}Q_n(z).$$

- Thus $\Omega_{\mathring{\mu}_n}(x) = -\frac{P_n(z)}{Q_n(z)}$ (for $\tau = 0$ this is $-\frac{\psi_n(z)}{\phi_n(z)}$, extra in α_n)

Quadrature weights

Theorem

IQF with nodes zeros $\{\xi_{nk}\}$ of QORF Q_n has weights

$$\lambda_{nk} = \lambda_{nk}(\tau) = \frac{\mathbf{i}}{(1+\xi_{nk}^2)}\frac{P_n(\xi_{nk})}{Q_n'(\xi_{nk})} = \frac{1}{k_{n-1}(\xi_{nk},\xi_{nk})} > 0, \quad k = 1, \ldots, n$$

Proof of $\lambda_{nk} = 1/k_{n-1}(\xi_{nk}, \xi_{nk})$

Skip proof

- Set $f_n = \phi_n/Z_n$, then $Q_n(\xi_{nk}) = 0 \Rightarrow \tau = -f_n(\xi_{nk})/f_{n-1}(\xi_{nk})$
- CD gives
  $\frac{f_{n-1}(\xi_{nk})}{Z_n(x)}[-Q_n(x)] = \frac{f_{n-1}(\xi_{nk})}{Z_n(x)}[Q_n(\xi_{nk}) - Q_n(x)] = E_n k_{n-1}(x, \xi_{nk})\frac{\xi_{nk}-x}{x\xi_{nk}}$
- multiply by $Z_n(z)Z_{n-1}(\xi_{nk})/(\xi_{nk}-x)$ and $x \to \xi_{nk}$ gives
  $-\phi_{n-1}(\xi_{nk})Q_n'(\xi_{nk}) = \frac{E_n k_{n-1}(\xi_{nk},\xi_{nk})}{(1-\xi_{nk}/\alpha_n)(1-\xi_{nk}/\alpha_{n-1})}$
- Similarly it holds that
  $\frac{f_{n-1}(\xi_{nk})}{Z_n(x)}P_n(x) = E_n[\sum_{j=0}^{n-1}\psi_j(x)\phi_j(\xi_{nk}) - D(\xi_{nk}, x)]\frac{\xi_{nk}-x}{x\xi_{nk}}$
- multiply by $Z_n(z)Z_{n-1}(\xi_{nk})$ and $x \to \xi_{nk}$ gives
  $\phi_{n-1}(\xi_{nk})P_n(\xi_{nk}) = E_n\frac{1+\xi_{nk}^2}{\mathbf{i}(1-\xi_{nk}/\alpha_n)(1-\xi_{nk}/\alpha_{n-1})}.$
- Division gives the result

Interpolation and kernels

- Define

$$\mathrm{d}\mathring{\mu}_n(x) = \frac{\mathrm{d}\mathring{\lambda}(x)}{|K_n(x,\mathbf{i})|^2}, \quad \mathrm{d}\mathring{\lambda}(x) = \frac{\mathrm{d}\lambda(x)}{|x-\mathbf{i}|^2} = \frac{\mathrm{d}x}{\pi(1+x^2)}$$

$$K_n(x,w) = \frac{k_n(x,w)}{\sqrt{k_n(w,w)}}, \quad k_n(x,w) = \sum_{k=0}^{n}\phi_k(x)\overline{\phi_k(w)}$$

  then the inner product in $\mathcal{L}_n$ with respect to $\mathring{\mu}$ and with respect to $\mathring{\mu}_n$ is the same.
- Hence there must be an interpolation property for $\Omega_{\mathring{\mu}}$ and $\Omega_{\mathring{\mu}_n}$.
- But what is $\Omega_{\mathring{\mu}_n}$ in this case? (ratio of 2 rational functions)

The half-line

- Let $\mathrm{supp}\,(\mu) = [0, +\infty]$, then we may choose poles in $[-\infty, 0]$
- In the polynomial case his corresponds to the Stieltjes moment problem:
  find μ, given $m_k = \int x^k \mathrm{d}\mu(x)$, $k = 0, 1, \ldots \Rightarrow$ orthog. polynomials
- Strong Stieltjes moment problem:
  find μ, given $m_k = \int x^k \mathrm{d}\mu(x)$, $k \in \mathbb{Z} \Rightarrow$ orthog. Laurent polynomials
- polynomials = poles at $\infty \rightarrow$ poles near ∞
  Laurent polynomials = poles at 0 and $\infty \rightarrow$ poles near 0 and near ∞

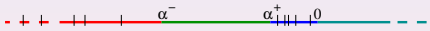
The half-line

- Suppose we work with μ and $D(x, y)$ replaced by $C(x, y) = \frac{1}{x-y}$, i.e. $\Omega_\mu(z) = \int \frac{\mathrm{d}\mu(x)}{x-z}$.
- A solution for the rational case uses ORF ϕ_k satisfying the recurrence with initial values $(\phi_{-1}, \phi_0) = (0, 1)$ and associated functions σ_k, solutions of the same recurrence but with initial values $(\sigma_{-1}, \sigma_0) = (1, 0)$.

$$\begin{bmatrix} \tilde\phi_n & \tilde\sigma_n \\ \tilde\phi_{n-1} & \tilde\sigma_{n-1} \end{bmatrix} = \begin{bmatrix} F_n & C_n \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \tilde\phi_{n-1} & \tilde\sigma_{n-1} \\ \tilde\phi_{n-2} & \tilde\sigma_{n-2} \end{bmatrix},$$

  where $F_n = E_n Z_{n-1} + B_n$.
- Note that singularity is excluded!

The half-line



- Suppose $-\infty < \alpha_{2m} \le \alpha^- < x < \alpha^+ \le \alpha_{2m+1} < 0$
- The QF in zeros of ϕ_n (nodes and weights positive) exact in $\mathcal{L}_{n,n-1}$
- $\Omega_n = \frac{\sigma_n}{\phi_n}$ then Ω_n interpolates Ω_μ in $\{\alpha_0, \alpha_1, \alpha_1, \alpha_2, \alpha_2, \ldots, \alpha_n\}$
- $\Omega_{2m+1}(x) \nearrow \Omega^-(x) \le \Omega_\mu(x) \le \Omega^+(x) \swarrow \Omega_{2m}(x)$, $\alpha^- < x < \alpha^+$

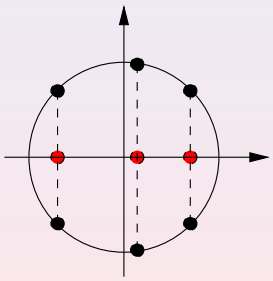
The finite interval $\mathbf{I} = [-1, 1]$

- One may still choose the poles outside $\mathbf{I}$: in $\hat{\mathbb{C}}^{\mathbf{I}} = \hat{\mathbb{C}} \setminus \mathbf{I}$ or in $\hat{\mathbb{R}}^{\mathbf{I}}$
- For complex poles the functions (and the inner product) will no longer be real and the formulas become much more complex.
- The case of complex poles has been worked out usually making use of the Joukowski transform mapping $z \in \mathbb{T}$ onto $x \in \mathbf{I}$:
  $x = \mathrm{j}(z) = \frac{1}{2}(z + 1/z)$
  also expressed as $x = \cos\theta$, $\theta \in [-\pi, \pi]$, $z = e^{\mathrm{i}\theta}$
- $w(x)$, $x = \cos\theta \in \mathbf{I} \Leftrightarrow \hat w(z) = w(\cos\theta)|\sin\theta|$, $z = e^{\mathrm{i}\theta}$
- There are other possibilities e.g. $x \in [0, \infty) \leftrightarrow y = \frac{1-x}{1+x} \in [-1, 1]$

Szegő quadrature on $\mathbb{T}$

- inner product $\langle f, g\rangle_\mu = \int_{\mathbb{T}} \overline{f(z)} g(z) \mathrm{d}\mu(z)$
- $\mathring{\mathcal{L}}_n = \frac{\mathcal{P}_n}{\mathring\pi_n}$, $\mathring\pi_n(z) = \prod_{k=1}^n (1 - \overline\beta_k z)$, $\{\beta_k\} \subset \mathbb{D}$
- $\mathring{\mathcal{L}}_{n-1} \perp \mathring\phi_n \in \mathring{\mathcal{L}}_n$, $\phi_n^*(z) = \frac{p_n^*(z)}{\mathring\pi_n(z)}$, $p_n^*(z) = z^n \overline{p_n(1/\bar z)}$
- $\phi_n(z) = c\left[\frac{z-\beta_{n-1}}{1-\overline\beta_n z}\phi_{n-1}(z) + \upsilon_n \frac{1-\overline\beta_{n-1} z}{1-\overline\beta_n z}\phi_{n-1}^*(z)\right]$
- $\upsilon_n \in \mathbb{D}$ is Schur/Szegő/Verblunsky/reflection/parcor coefficient
- ϕ_n all zeros in $\mathbb{D}$
- PORF: $Q_n(z) = \phi_n(z) + \tau\phi_n^*(z)$, $\tau \in \mathbb{T}$ all zeros simple and on $\mathbb{T}$.
- Its zeros as nodes of IQF $\rightarrow$ all weights positive = Szegő QF.
- $\alpha_k \in \mathbb{R} \setminus [-1, 1] \Rightarrow \beta_k = \mathrm{j}^{inv}(\alpha_k) \in \mathbb{D}$

Symmetric case

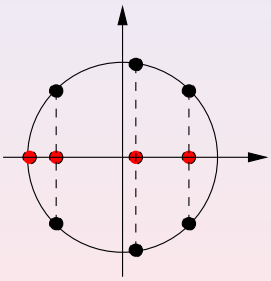


Carl F. Gauss



Szegő qf with PORF
$Q_n(z) = \phi_n(z) + \tau\phi_n^*(z)$ with
n even and $\tau = 1 \rightarrow$
Gauss qf on $\mathbf{I}$

Symmetric case

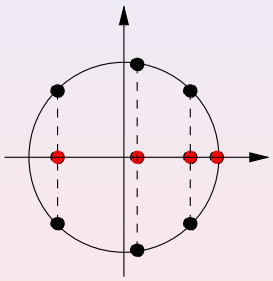


Carl F. Gauss Rodolphe Radau




Szegő qf with PORF
$Q_n(z) = \phi_n(z) + \tau\phi_n^*(z)$ with
n odd and $\tau = 1 \rightarrow$
Gauss-Radau qf on $\mathbf{I}$

Symmetric case

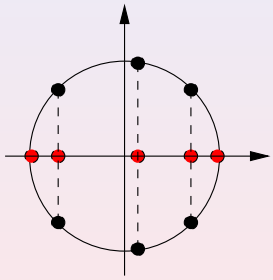


Carl F. Gauss Rodolphe Radau




Szegő qf with PORF
$Q_n(z) = \phi_n(z) + \tau\phi_n^*(z)$ with
n odd and $\tau = -1 \rightarrow$
Gauss-Radau qf on $\mathbf{I}$

Symmetric case



Carl F. Gauss Rehuel Lobatto




Szegő qf with PORF
$Q_n(z) = \phi_n(z) + \tau\phi_n^*(z)$ with
n even and $\tau = -1 \rightarrow$
Gauss-Lobatto qf on $\mathbf{I}$

Computations on $\mathbb{R}$

Polynomials (Golub-Welsch algorithm)

- $x\phi_{n-1}(x) = a_{n-1}\phi_{n-2}(x) + b_n\phi_{n-1}(x) + a_n\phi_n(x), \quad \phi_0 = 1, \phi_{-1} = 0$
- $\Phi_n(x) = [\phi_0, \ldots, \phi_{n-1}(x)]$,
  $J_n = \text{tridiag}\begin{pmatrix} a_1, \ldots, a_{n-1} \\ b_1, b_2, \ldots, b_{n-1}b_n \\ a_1, \ldots, a_{n-1} \end{pmatrix}$ (Jacobi matrix)
  Then
  $$x\Phi_n(x) = \Phi_n(x)J_n + [0, 0, \ldots, 0, a_n\phi_n(x)]$$
  J_∞ representation of the 'shift' in $\mathcal{L}_\infty$ w.r.t. $\{\phi_0, \phi_1, \ldots\}$
- If ξ is a zero of ϕ_n then $\xi\Phi_n(\xi) = \Phi_n(\xi)J_n$, i.e., ξ is an eigenvalue of J_n and $\Phi_n(\xi)$ is the corresponding eigenvector.
- ξ is node of qf and weight is $1/\sum_{j=0}^{n-1}|\phi_j(\xi)|^2 = 1/\|\Phi_n(\xi)\|^2$
- Normalization!! If $\int \mathrm{d}\mu = 1$, then $\phi_0 = 1$. Thus take any eigenvector Φ, normalize it ($\|\Phi\| = 1$) then the weight for ξ is the square of the first component.

Computations on $\mathbb{R}$

ORFs One way to write the TTRR

- $x\phi_{n-1}(x) = \frac{1}{E_n}\tilde{\phi}_n(x) - \frac{B_{n-1}}{E_n}\tilde{\phi}_{n-1}(x) + \frac{1}{E_{n-1}}\tilde{\phi}_{n-2}(x)$
- $\Phi_n(x) = [\phi_0, \ldots, \phi_{n-1}(x)]$, $\Delta_n(x) = \text{diag}(1 - \frac{x}{\alpha_0}, \ldots, 1 - \frac{x}{\alpha_{n-1}})$
  $J_n = \text{tridiag}\begin{pmatrix} a_1, \ldots, a_{n-1} \\ b_1, b_2, \ldots, b_{n-1}b_n \\ a_1, \ldots, a_{n-1} \end{pmatrix}$, $\begin{matrix} a_k = 1/E_k \\ b_k = -B_k/E_k. \end{matrix}$ Then
  $$x\Phi_n(x) = \tilde{\Phi}_n(x)J_n + [0, 0, \ldots, 0, a_n\tilde{\phi}_n(x)]$$
  $\tilde{\phi}_n(x) = \phi_n(x)(1 - x\alpha_n^{-1}) = \phi_n(x) - x\phi_n(x)\alpha_n^{-1}$
- If ξ is a zero of ϕ_n then $\xi\Phi_n(\xi)[I_n + D_n^{-1}J_n] = \Phi_n(\xi)J_n$, $D_n = \text{diag}(\alpha_0, \ldots, \alpha_{n-1})$. I.e. ξ is a generalized eigenvalue of the pencil $(J_n, I_n + D_n^{-1}J_n)$ and $\Phi_n(\xi)$ is the corresponding eigenvector.

Computations on $\mathbb{R}$

ORFs

- $$\xi\Phi_n(\xi)[I_n + D_n^{-1}J_n] = \Phi_n(\xi)J_n, \quad D_n = \text{diag}(\alpha_0, \ldots, \alpha_{n-1}).$$
- Basis $\{1, x, x^2, \ldots\}$ replaced by products of the form $\tilde{x} = x(1 - \alpha^{-1}x)^{-1}$ with inverse $x = \tilde{x}(1 + \alpha^{-1}\tilde{x})^{-1}$.
  Therefore representation of shift in $\mathcal{L}_\infty$ w.r.t. the new ORF basis is $J_\infty(I_\infty + D_\infty^{-1}J_\infty)^{-1}$.
- Still needs a_k and b_k recurrence for the ORFs (not for the OPs!). Only known in some special cases.
- Needs recursion!! Hence regularity condition required!

Practical Problem

- Implementation very efficient (using special structure) and stable (unitary transformations)
- Problem: need recurrence coefficients explicitly.
- Only known in few of the rational cases.
- Also explicit expressions for the ϕ_n only known is few cases.
- Example ORF for $\mathrm{d}\lambda$ on $\mathbb{T}$:
  $$\phi_n(z) = \frac{\sqrt{1 - |\alpha_n|^2}}{1 - \overline{\alpha}_n z} z \prod_{j=1}^{n-1} \frac{z - \alpha_j}{1 - \overline{\alpha}_j z}$$
  Takenaka-Malmquist basis.

Rational Gauss-Chebyshev qf

- Recall $\mathbf{I} = [-1, 1]$, $\mathcal{A} = \{\alpha_1, \alpha_2, \ldots\} \subset \hat{\mathbb{C}}^{\mathbf{I}} = \hat{\mathbb{C}} \setminus \mathbf{I}$
- $b_0 = 1$, $b_k = \prod_{j=1}^k Z_j$, $Z_j(x) = \frac{x}{1 - x/\alpha_j}$
- Joukowski tf: $x = \mathrm{j}(z) = \frac{1}{2}(z + \frac{1}{z}) \in \mathbf{I}$, $z = \mathrm{j}^{inv}(x) \in \mathbb{T}$

on $\mathbb{T} \leftrightarrow$ on $[-\pi, \pi]$	on $[-1, 1]$
$\mathring{w}(\theta)\mathrm{d}\theta = w(\cos\theta)\lvert\sin\theta\rvert\mathrm{d}\theta$	$w(x)\mathrm{d}x$

- $\int_{-1}^1 f(x)w(x)\mathrm{d}x = \frac{1}{2}\int_{-\pi}^{\pi} f(\cos\theta)\mathring{w}(\theta)\mathrm{d}\theta = \frac{1}{2}\int_{-\pi}^{\pi} \mathring{f}(e^{\mathrm{i}\theta})\mathring{w}(\theta)\mathrm{d}\theta, \quad \mathring{f} = f \circ \mathrm{j}$
- $\alpha_i \in \hat{\mathbb{C}}^{\mathbf{I}} \leftrightarrow \beta_i = \mathrm{j}^{inv}(\alpha_i) \in \mathbb{D}$
- $B_0 = 1$, $B_k = \prod_{j=1}^k \zeta_j$, $\zeta_j(z) = \frac{z - \beta_j}{1 - \overline{\beta}_j z}$
- $f \in \text{span}\{b_0, \ldots, b_n\} \Rightarrow f^*(z) = \frac{b_n(z)}{b_{n^*}(z)} f_*(z) \Rightarrow \mathcal{L}_n^* = \mathcal{L}_n$

Rational Chebyshev ORF

- Chebyshev weights on $\mathbf{I} = [-1, 1]$:
  $w^{(1)}(x) = (1 - x^2)^{-1/2}$, $w^{(2)}(x) = \left(\frac{1-x}{1+x}\right)^{1/2}$, $w^{(3)}(x) = (1 - x^2)^{1/2}$
- Define

i	c_i	d_i	p_i	q_i
1	1	1	1	-1
2	3/2	0	1	1
3	2	0	2	1

and $B_{n-1}(z) = \prod_{k=1}^{n-1} \frac{z - \beta_k}{1 - \overline{\beta}_k z}$

Theorem

The ORF for $w^{(i)}$ are ($x = \mathrm{j}^{inv}(z)$ and $\beta_k = \mathrm{j}^{inv}(\alpha_k)$)

$$\phi_n^{(i)}(x) = \frac{q_i N_i}{2z^{i-1} + q_i - 3}\left(\frac{z^i B_{(n-1)^*}(z)}{1 - \beta_n z} - \frac{q_i}{(z - \beta_n)B_{n-1}(z)}\right), \quad n \geq 1$$

$\phi_0^{(i)} = \sqrt{p_i/\pi}$, $N_i = \sqrt{2^i/\pi}\sqrt{1 - |\beta_n|^2}$.

Rational Gauss-Chebyshev qf

- Chebyshev weights on $\mathbf{I} = [-1, 1]$:
  $w^{(1)}(x) = (1 - x^2)^{-1/2}$, $w^{(2)}(x) = \left(\frac{1-x}{1+x}\right)^{1/2}$, $w^{(3)}(x) = (1 - x^2)^{1/2}$
- explicit expressions $\phi_n^{(i)} \leftrightarrow$ recurrence coefficients
- Standard: zeros of $\phi_n^{(i)}$ + IQF
  $x_{nk} = \cos\theta_{nk} \rightarrow \xi_{nk} = e^{\mathrm{i}\theta_{nk}}$.

Theorem

$f_n(\theta_{nk}^{(i)}) - (n - c_i)\theta_{nk}^{(i)} = \frac{\pi}{2}(2k - d_i)$, $k = 1, \ldots, n$

$f_n(\theta) = 2\sum_{j=1}^{n}{}' \arctan\frac{\sin\theta}{\cos\theta - \beta_j}$, ($\sum'$ *means last term halved)*

node $x = \cos\theta \rightarrow$ *weight* $\lambda = \frac{2\pi(1 - x^{i-1})}{i + g_n(x)}$, $g_n(x) = 2\sum_{k=1}^{n}{}' \frac{\sqrt{1 - 1/\alpha_k^2}}{1 - x/\alpha_k}$

Rational Gauss-Chebyshev qf

Some remarks:

- The functions $f_n(\theta)$ are very smooth so that efficient (Newton-based) algorithms exist for the nodes. Only $O(n^2)$ operations needed for the nodes.
- One may look at the zeros of QORFs as well
- One may consider general complex poles in $\hat{\mathbb{C}}^{\mathbf{I}}$

Rational modification of the measure

Another way to construct explicitly some ORFs

- Given ORF for $w(z)$, find ORF for $\tilde{w}(z) = |r(z)|^2 w(z)$, r rational
- Well studied in the polynomial case:
  Christoffel tf $r(z) = |z-\alpha| \to \langle f,g\rangle_{\tilde{w}} = \langle (z-\alpha)f,(z-\alpha)g\rangle_w$
  Geronimus tf $r(z) = 1/|z-\alpha| \to \langle f,g\rangle_{\tilde{w}} = \left\langle \frac{f}{z-\alpha}, \frac{g}{z-\alpha}\right\rangle_w$
  Uvarov tf $\tilde{w}(z) = w(z) + m\delta_\alpha(z) \to \langle f,g\rangle_{\tilde{w}} = \langle f,g\rangle_w + m\overline{f(\alpha)}g(\alpha)$

Rational modification of the measure

An example (for $\mathbb{T}$)

Theorem

$\mathcal{A}_n = \{\alpha_1,\dots,\alpha_n\}$, $\mathcal{A}_n^\beta = \{\beta,\alpha_1,\dots,\alpha_n\}$
$\gamma \in \mathbb{D}\cup\mathbb{T}$, $\mathrm{d}\hat{\mu}(z) = \left|\frac{z-\gamma}{1-\overline{\beta}z}\right|^2 \mathrm{d}\mu(z)$
$\hat{\phi}_n$ *= ORF for* $\hat{\mu}$ *and poles in* $\mathcal{A}_n \leftrightarrow \phi_{n+1}$ *ORF for* μ *and poles in* $\mathcal{A}_n^\beta$

$$\left(\frac{z-\gamma}{1-\overline{\beta}z}\right)\hat{\phi}_n(z) = \overline{\eta}_\beta \frac{1-\gamma\overline{\alpha}_n}{1-\beta\overline{\alpha}_n}\left[\phi_{n+1}(z) - \frac{\phi_{n+1}(\gamma)}{k_n(\gamma,\gamma)}k_n(z,\gamma)\right]$$

$k_n(z,y)$ *is reproducing kernel for* $\mathcal{L}_n$ *with measure* μ *and poles* $\mathcal{A}_n^\beta$.
$\eta_\beta = \overline{\beta}/|\beta|$ *if* $\beta \neq 0$, *and 1 otherwise.*

Note $\gamma = 0$, $\beta = re^{\mathrm{i}\theta}$, $r<1$, $\mathrm{d}\mu = \mathrm{d}\lambda$, then $\mathrm{d}\hat{\mu}(z) = \frac{\mathrm{d}\lambda(z)}{1-2r\cos\theta+r^2}$ is the Poisson measure. The ORFs are $\hat{\phi}_n(z) = \frac{(r-z)B_n(z)}{z-\alpha_n}$.

Near best rational approximation

- L_∞ approximation on $\mathbf{I} = [-1,1]$ needs equi-oscillation of the error
- Polynomial interpolant in $x_1,\dots,x_n \in \mathbf{I}$ gives
  $|f(x)-p_n(x)| \le \max_{t\in\mathbf{I}}|f^{(n+1)}(t)|\frac{|x-x_0|\cdots|x-x_n|}{(n+1)!}$
- If $(x-x_0)\cdots(x-x_n) \sim T_{n+1}(x)$, then equi-oscillation. Thus interpolate in zeros of T_{n+1}.
- Rational case: $\pi_m(x) = \prod_{k=1}^m(1-x/\alpha_k)$ and p_n interpolates $\pi_m f$ in $\{x_0,\dots,x_n\} \subset \mathbf{I}$, then
  $\left|f(x) - \frac{p_n(x)}{\pi_m(x)}\right| \le \max_{t\in\mathbf{I}}|[\pi_m(t)f(t)]^{(n+1)}|\frac{|x-x_0|\cdots|x-x_n|}{|\pi_m(x)|(n+1)!}$
- Minimize $\max_{x\in\mathbf{I}}|\frac{(x-x_0)\cdots(x-x_n)}{\pi_m(x)}|$ then x_i are zeros of rational Chebyshev ORF.

Near best rational approximation

- For $w^{(1)}(x) = (1-x^2)^{-1/2}$ and $w^{(3)}(x) = (1-x^2)^{-1/2}$
  $\alpha_k = \mathrm{j}(\beta_k)$, $x = \mathrm{j}(z) = \frac{1}{2}(z+\frac{1}{z})$ ORFs are known:

$$\mathcal{T}_n(x) = \sqrt{\frac{1-|\beta_n|^2}{2\pi}}\left(\frac{zB_{(n-1)^\sharp}(z)}{1-\beta_n z} + \frac{1}{(z-\beta_n)B_{n-1}(z)}\right)$$

and

$$\mathcal{U}_n(x) = \sqrt{\frac{1-|\beta_n|^2}{\pi}}\frac{z\sqrt{2}}{z^2-1}\left(\frac{z^2B_{(n-1)^\sharp}(z)}{1-\beta_n z} - \frac{1}{z(z-\beta_n)B_{n-1}(z)}\right)$$

for $n = 1,2,\dots$, $\mathcal{T}_0 = 1/\sqrt{\pi}$, $\mathcal{U}_0 = \sqrt{2/\pi}$.

- Zeros can be found by an efficient iterative process or
  By solving a generalized eigenvalue problem of the form
  $z\Phi_n(x)(I_n - S_n + D_n^{-1}J_n) = \Phi_n(x)J_n$
  The extra matrix S_n has only elements on the first superdiagonal.
  The matrices in $(J_n, I_n - S_n + D_n^{-1}J_n)$ are both tridiagonal.
- for real poles or conjugate pairs $S_n = 0$.

Quadrature with preassigned nodes

QORF depend on a parameter that can be used to place one node at a particular place.

- We shall consider qf on $\mathbb{R}^+$ and on $\mathbf{I} = [-1,1]$
- Recall that we want 'good' QF
  - nodes to be on $\mathbb{R}^+$ or $\mathbf{I}$
  - weights to be positive
  - exact in largest possible space

preassigned nodes on $\mathbf{I}$

- n-point (Polynomial) Gauss qf exact in $\mathcal{P}_{2n-1}$
- Fix m nodes $\Rightarrow$ nodes = zeros of P with $\langle P, x^k\rangle = 0$,
  $k = 0,\dots,n-m-1$ and $\langle P, x^{n-m}\rangle \neq 0$.
  quasi-orthogonal polynomials of order m.
- $m=1$: Gauss-Radau qf; $m=2$: Gauss-Lobatto qf
  usually fixed nodes at end points of interval.
- Exact in $\mathcal{P}_{2n-m-1}$
- In general zeros may not be all in $\mathbf{I}$ and weights need not be all positive!

R-Gauss-Radau on $\mathbf{I}$

- Choose poles α_k in $\hat{\mathbb{R}}^{\mathbf{I}} = \hat{\mathbb{R}} \setminus [-1,1]$
- $(n+1)$-point qf with prefixed ξ.
  Nodes = zeros of QORF $Q_{n+1}(x) = \phi_{n+1}(x) + \tau_{n+1}\frac{Z_{n+1}(x)}{Z_n(x)}\phi_n(x)$,
  $\tau_{n+1} \in \mathbb{R}$
- Ensure ξ is zero by
  $\tau_{n+1} = -\frac{\phi_{n+1}(\xi)Z_n(\xi)}{\phi_n(\xi)Z_{n+1}(\xi)} = -\frac{\tilde{\phi}_{n+1}(\xi)}{\tilde{\phi}_n(\xi)} = -\frac{p_{n+1}(\xi)}{p_n(\xi)(1-\xi/\alpha_{n-1})}$.
- All nodes real and simple, but in $\mathbf{I}$? Weights > 0?
  No problem for all of $\hat{\mathbb{R}}$, but should not coincide with poles!

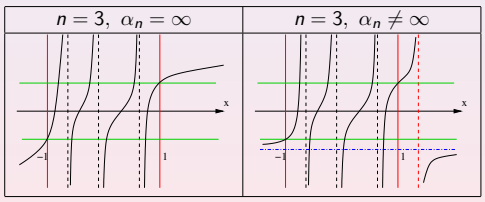
Theorem

If $\alpha_k \in \hat{\mathbb{R}}^{\mathbf{I}}$ *then at least* $n-1$ *zeros of* Q_n *are in* $\mathbf{I}$ *with positive weights.*

- Similar for qf on $[0,\infty)$. $\alpha_k \in \hat{\mathbb{C}}^{\mathbf{I}} \to$ complex nodes.
- 'good' R-Gauss-Radau may not always exist!!

R-Gauss-Radau on $\mathbf{I}$

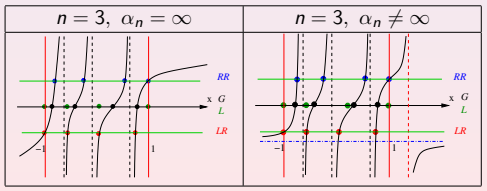
$Q_{n+1}(x) = \phi_{n+1}(x) + \tau \frac{1-x/\alpha_n}{1-x/\alpha_{n+1}}\phi_n(x) = 0$ & $\phi_k = \frac{p_k}{\pi_k} \Rightarrow$
$\tau(x) = -\frac{p_{n+1}(x)}{(1-x/\alpha_n)p_n(x)}$



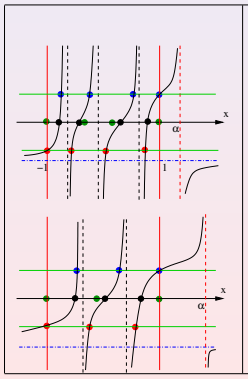
If the prefixed node ξ is too close to a zero of p_n, then one node may be outside $\mathbf{I}$!!
Similar observations hold for integrals over the half-line.

R-Gauss-Lobatto on $\mathbf{I}$

Terminology:
G: Gauss ($\tau = 0$)
RR: Right Radau ($x = 1$ is a node); RR^ξ: nodes $x = 1$ & $\xi \in (-1, 1)$
LR: Left Radau ($x = -1$ is a node); LR^ξ: nodes $x = -1$ & $\xi \in (-1, 1)$
L: Lobatto ($x = -1$ and $x = 1$ are nodes); L^ξ: 3rd node $\xi \in (-1, 1)$



R-Gauss-Radau on $\mathbf{I}$

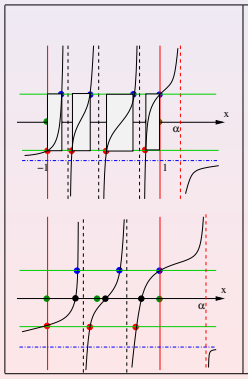


top: $n = 3,\ \alpha = \alpha_3$
bottom: $n = 2,\ \alpha = \alpha_2$

curve = zeros of
$P_{n+1}(x, \xi) = p_{n+1}(x) - \frac{p_{n+1}(\xi)}{\tilde{p}_n(\xi)}\tilde{p}_n(x)$
$\tilde{p}_n(x) = (1 - \frac{x}{\alpha_n})p_n(x)$

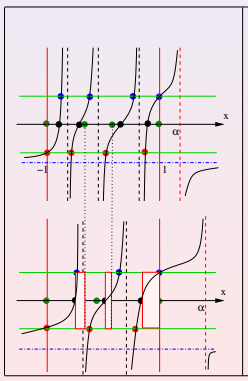
$\phi_n(x) = \frac{p_n(x)}{\pi_n(x)}$
assuming $p_n(\alpha_n) \neq 0$
otherwise replace α_n by some α

R-Gauss-Radau on $\mathbf{I}$



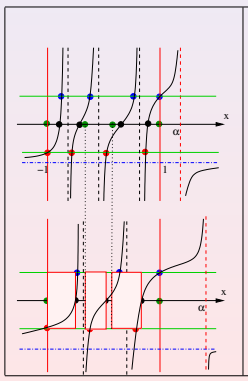
top: $n = 3,\ \alpha = \alpha_3$
bottom: $n = 2,\ \alpha = \alpha_2$
R-Gauss-Radau: all nodes in $[-1, 1]$
one node ξ fixed in $(-1, 1)$
all weights positive
$\xi \in \bigcup_{j=1}^{n+1} (x^{LR}_{n+1,j}, x^{RR}_{n+1,j})$
zeros of $P_{n+1}(x, \xi)$

R-Gauss-Lobatto on $\mathbf{I}$



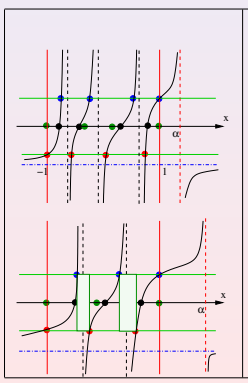
top: $n = 3,\ \alpha = \alpha_3$
bottom: $n = 2,\ \alpha = \alpha_2$
LR^ξ:
one node is -1
second node $\xi \in (-1, 1)$
all weights positive
$\xi \in \bigcup_{j=1}^{n} (x^G_{n,j}, x^L_{n+1,j})$
zeros of $P^{(1)}_n(x, \xi)$
$d\mu^{(1)}(x) = (x + 1)d\mu(x)$

R-Gauss-Lobatto on $\mathbf{I}$



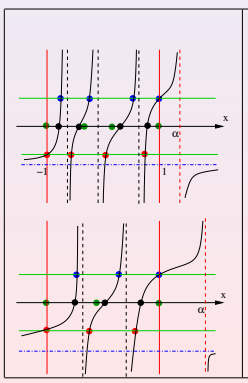
top: $n = 3,\ \alpha = \alpha_3$
bottom: $n = 2,\ \alpha = \alpha_2$
RR^ξ:
one node is 1
second node $\xi \in (-1, 1)$
all weights positive
$\xi \in \bigcup_{j=1}^{n} (x^L_{n+1,j}, x^G_{n,j})$
zeros of $P^{(2)}_n(x, \xi)$
$d\mu^{(2)}(x) = (1 - x)d\mu(x)$

R-Gauss-Lobatto on $\mathbf{I}$



top: $n = 3,\ \alpha = \alpha_3$
bottom: $n = 2,\ \alpha = \alpha_2$
Gauss-Lobatto L^ξ:
both -1 and 1 are nodes
3rd node $\xi \in (a, b)$
all weights positive
$\xi \in \bigcup_{j=1}^{n-1} (x^{RR}_{n,j}, x^{LR}_{n,j+1})$
zeros of $P^{(3)}_{n-1}(x, \xi)$
$d\mu^{(3)}(x) = (1 - x^2)d\mu(x)$

R-Gauss-Lobatto on $\mathbf{I}$



Gauss-Lobatto: $\xi, \hat{\xi} \in (-1, 1)$
def. $\hat{X}^G_{n+1} = X^G_n \cup \{\xi\}$
$\hat{X}^R_{n+1}$ nodes RR^ξ & $\hat{X}^L_{n+1}$ nodes LR^ξ
all weights positive
either
$\xi \in \bigcup_{j=1}^{n} (x^G_{n,j-1}, x^L_{n+1,j})$ & $\hat{\xi} \in \bigcup_{i=1}^{n} [\hat{x}^L_{n+1,i}, \hat{x}^G_{n+1,i})$
or
$\xi \in \bigcup_{j=1}^{n} (x^L_{n+1,j}, x^G_{n,j})$ & $\hat{\xi} \in \bigcup_{i=1}^{n} (\hat{x}^G_{n+1,i}, \hat{x}^R_{n+1,i}]$
ξ can be anywhere & $\hat{\xi}$ is restricted

R-Gauss-Lobatto on $\mathbf{I}$ Computations

All computations can be done by GEP $\widehat{J}_{n+1} v_\xi = \xi \hat{B}_{n+1} v_\xi$,
$\hat{B}_{n+1} = I_{n+1} + \hat{D}_{n+1}^{-1} \widehat{J}_{n+1}$
Only the last elements (a_n, b_{n+1}) need to be changed

$$\widehat{J}_{n+1} = \left[\begin{array}{c|c} J_n & \begin{matrix} 0_{n-1} \\ \times \end{matrix} \\ \hline \begin{matrix} 0_{n-1}^T & \times \end{matrix} & \times \end{array}\right], \quad \hat{B}_{n+1} = \left[\begin{array}{c|c} B_n & \begin{matrix} 0_{n-1} \\ \times \end{matrix} \\ \hline \begin{matrix} 0_{n-1}^T & \times \end{matrix} & \times \end{array}\right].$$

Possibly need to replace α_n by another α to avoid singular situation.
$\hat{D}_{n+1} = \mathrm{diag}(\alpha_0, \ldots, \alpha_{n-1}, \alpha)$

R-Gauss-Radau and -Lobatto on $\mathbf{I}$ Alternative

- n-point R-Gauss qf exact in $\mathcal{L}_n \cdot \mathcal{L}_{n-1}$
- n-point R-Gauss-Radau qf (1 prefixed node) exact in $\mathcal{L}_{n-1} \cdot \mathcal{L}_{n-1}$
- n-point R-Gauss-Lobatto qf (2 prefixed nodes) exact in $\mathcal{L}_{n-1} \cdot \mathcal{L}_{n-2}$
- One might choose different spaces: e.g. $\mathcal{L}_n \cdot \mathcal{L}_{n-2}$ for Radau and $\mathcal{L}_n \cdot \mathcal{L}_{n-3}$ for Lobatto.

Error estimate on $\mathbb{R}$

The problem is to estimate $E_n\{f\} = \mathcal{I}_\mu\{f\} - \mathcal{I}_n\{f\}$.

- R-Gauss qf (exact in $\mathcal{L}_{n,n-1}$) via Hermite interpolation.
- IQF: take $R_{2n-1} \in \mathcal{L}_{n,n-1}$ that interpolates f twice in each point of $\{t_1, \ldots, t_n\}$: $R_{2n-1}(t_i) = f(t_i)$ and $R'_{2n-1}(t_i) = f'(t_i)$.
- $R_{2n-1} = \frac{P_{2n-1}}{D_{2n-1}}$, $D_{2n-1} = \pi_n \pi_{n-1}$, $\pi_k = \prod_{j=1}^k (1 - \frac{x}{\alpha_j})$.
- $P_{2n-1}(x) = \sum_{j=1}^n [H_j(x) f(t_j) + \tilde{H}_j(x) f'(t_j)]$
  with $\begin{cases} H_j(x) = L_j(x) D_{2n-1}(t_j) + \tilde{L}_j(x) D'_{2n-1}(t_j) \\ \tilde{H}_j(x) = \tilde{L}_j(x) D_{2n-1}(t_j) \end{cases}$
  Lagrange polynomials: $\begin{cases} L_j(t_k) = \delta_{jk}, & L'_j(t_k) = 0 \\ \tilde{L}_j(t_k) = 0, & \tilde{L}'_j(t_k) = \delta_{jk} \end{cases}$.
- IQF: $\mathcal{I}_n\{f\} = \sum_{j=1}^n [A_j f(t_j) + \tilde{A}_j f'(t_j)]$ with $\begin{cases} A_j = \mathcal{I}_\mu\{H_j / D_{2n-1}\} \\ \tilde{A}_j = \mathcal{I}_\mu\{\tilde{H}_j / D_{2n-1}\} \end{cases}$.

Error estimate on $\mathbb{R}$

The problem is to estimate $E_n\{f\} = \mathcal{I}_\mu\{f\} - \mathcal{I}_n\{f\} = \mathcal{I}_\mu\{f - R_{2n-1}\}$.

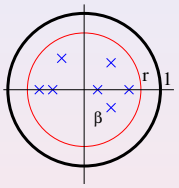
- If $\{t_k\}$ are zeros of ORF ϕ_n then
  $\tilde{A}_j = \int \phi_n(x) r_{n-1}(x) \mathrm{d}\mu(x) = 0$ since $r_{n-1} \in \mathcal{L}_{n-1}$
- $E_n\{f\} = \mathcal{I}_\mu\{f - R_{2n-1}\} = c \frac{(f D_{2n-1})^{(2n)}(\theta(x))}{(2n)!} \int \phi_n^2(x)(1 - \frac{x}{\alpha_n}) \mathrm{d}\mu(x)$.
- Example: related interpolation error, $\mathrm{supp}\,(\mu) = [0, +\infty]$,
  $\alpha_k \in (-\infty, 0)$
  $\Omega_\mu(z) - \Omega_n(z) = \mathcal{I}_\mu\{\frac{\mathrm{d}(\mu - \mu_n)}{z - x}\} = \frac{1}{(1 - \frac{z}{\alpha_n}) \phi_n^2(z)} \int \frac{\phi_n^2(x)(1 - \frac{x}{\alpha_n})}{z - x} \mathrm{d}\mu(x)$,
  $z \notin [0, +\infty]$.

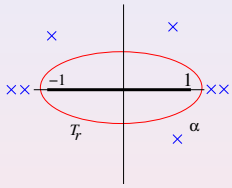
Theorem

f analytic in $G \supset [0, +\infty]$, $\partial G = \Gamma$

$$|E_n\{f\}| \le \frac{C(\Gamma, f)}{\inf_{z \in \Gamma} |\phi_n^2(z)(1 - \frac{z}{\alpha_n})|} \int_0^\infty \phi_n^2(x)(1 - \frac{x}{\alpha_n}) \mathrm{d}\mu(x)$$

Error estimate on I





use Joukowski
$\pi_n(x) = \prod_1^n (1 - x/\alpha_k)$
$\tilde{\pi}_n(z) = \prod_1^n (1 - \beta_i z)$
$\beta_i = \mathrm{j}^{inv}(\alpha_i)$
$T_r = \{|\mathrm{j}^{inv}(z)| = r\}$
$\|\mu\| = \int \mathrm{d}\mu$
$\|\mathcal{I}_n\| = \sum_k |w_k|$

Theorem

$\mathcal{I}_n$ exact in $\mathcal{L}_{m+1}$,

$$|E_n\{f\}| \le \|\pi_n f\|_{T_r} \frac{2 r^{m+1}}{1 - r^2} (\|\mu\| + \|\mathcal{I}_n\|) \prod_{i=1}^m |1 + \beta_i^2| g(r)$$

$g(r) = \frac{1}{2\pi} \int_0^{2\pi} \frac{\mathrm{d}t}{|\tilde{\pi}_m(r e^{\mathrm{i}t})|^2}$

Convergence of qf on $\mathbb{R}$

It will depend on the smoothness of f and the choice of the poles that will determinate the density of the rationals and hence convergence.

- Example:

Theorem

$\mathrm{supp}\,(\mu) = [0, +\infty]$ *poles in* $(-\infty, 0)$
Poles α_k stay away from 0 and $-\infty$, or do not approach too fast:

$$\sum_{k=1}^\infty \frac{\sqrt{|\alpha_k|}}{1 + |\alpha_k|} = +\infty \quad \text{or} \quad \sum_{k=1}^\infty \frac{\sqrt{|\beta_k|}}{1 + |\beta_k|} = +\infty, \quad \beta_k = 1/\alpha_k$$

$\mathcal{S} = \{f : \text{continuous on } [0, +\infty) \text{ and finite at } +\infty\}$.
Then $\cup_{k=0}^\infty \mathcal{L}_k$ dense in $\mathcal{S}$ (uniform norm)
and the R-Gauss qf converges $\forall f \in \mathcal{S}$.

Convergence of qf on $\mathbb{T}$

The following convergence result is a direct consequence of the error estimate ($\beta_k = \mathrm{j}^{inv}(\alpha_k)$)

Theorem

If $\int \frac{|\rho(\theta)|^2}{w(\theta)} \mathrm{d}\theta < \infty$ for pos. weight w and $\sum_{j=1}^\infty (1 - |\beta_j|) = \infty$ then $\forall f$ continuous on $\mathbb{T}$ and $\mathcal{I}_n$ an R-Szegő-like qf w.r.t. w:
$\lim_{n \to \infty} \mathcal{I}_n\{f\} = \int_{-\pi}^{\pi} f(e^{\mathrm{i}\theta}) \rho(\theta) \mathrm{d}\theta$ *and*
$\lim_{n \to \infty} \sum_{j=1}^n |\lambda_{nj}| f(z_j) = \int_{-\pi}^{\pi} f(e^{\mathrm{i}\theta}) |\rho(\theta)| \mathrm{d}\theta$.

With Joukowski this can be translated in a corresponding result for $\mathbf{I} = [-1, 1]$

Theorem

If $\sum_{k=1}^\infty (1 - |\beta_k|) = \infty$ then the R-Gauss qf on $\mathbf{I}$ converge $\forall f$ continuous on $\mathbf{I}$ if and only if $\|\mathcal{I}_n\| = \sum_{k=1}^n |\lambda_{nk}| \le M < \infty$.

Application

- matrix functions $f(A)$ for large networks (A = adjacency matrix)
- Google's PageRank = eigenvalue problem for A of directed graph
- Communicability = function of e^A
- important hubs $(I - cA)x = \mathbf{1}$, authorities $(I - cA^T)x = \mathbf{1}$
- $f(A) = \int_\Gamma f(z)(zI - A)^{-1} \mathrm{d}z$, $\Gamma = \partial\Omega$, Ω contains spectrum of A

Application

- Suppose $A \in \mathbb{C}^{N\times N}$ is Hermitian positive definite, $v \in \mathbb{C}^N$, N large
- Linear functional $\mathcal{M}\{x^k\} = v^H A^k v$ (moment problem $\to \mu$)
- $\mathcal{M}\{f\} = \int f(x)\mathrm{d}\mu(x) = v^H f(A)v$ and $\langle f, g\rangle = \int \overline{f(x)}g(x)\mathrm{d}\mu(x)$
- $p = f(A)v$, $q = g(A)v$ then $\langle f, g\rangle_\mu = p^H q$
- Suppose $A = \widetilde{U}\widetilde{\Lambda}\widetilde{U}^H$. Then

$$\mathcal{I}_\mu\{f\} = v^H f(A)v = v^H \widetilde{U} f(\widetilde{\Lambda})\widetilde{U}^H v = \sum_{k=0}^{N-1} \tilde{w}_k f(\tilde{\lambda}_k), \quad \tilde{w}_k = |\tilde{u}_k^H v|^2.$$

$$\mu = \sum_{k=0}^{N-1} \tilde{w}_k \delta_{\tilde{\lambda}_k}$$

Application

- If A too large then project it onto a lower dimensional subspace:
  $\mathcal{K}_{n-1} = \mathrm{colsp}\, V_n = \mathrm{colsp}[v_0, v_1, \ldots, v_{n-1}]$, $v_k = b_k(A)v$
  Set $\mathcal{L}_{n-1} = \mathrm{span}\{b_k(x) : k = 0, \ldots, n-1\}$, then
  $\mathcal{K}_{n-1} = \mathrm{span}\{f(A)v : f \in \mathcal{L}_{n-1}\}$
- Construct an orthonormal basis $\mathcal{K}_{n-1} = \mathrm{colsp} Q_n$ and $Q_n^H Q_n = I_n$
  define $A_n = Q_n^H A Q_n \in \mathbb{C}^{n\times n}$
  and set $\mathcal{I}_\mu\{f\} = v^H f(A)v \approx \mathcal{I}_n\{f\} = v^H Q_n f(A_n) Q_n^H v$
- Note if $q_k = \phi_k(A)v$ then $q_k^H q_l = \delta_{kl}$ iff $\langle \phi_k, \phi_l\rangle_\mu = \delta_{kl}$
  $Q_n = [\phi_0(A), \ldots, \phi_{n-1}(A)]v = \Phi_n(A)v$.

Application

- $\mathcal{I}_n\{f\} = v^H Q_n f(A_n) Q_n^H v$, $A_n = Q_n^H A Q_n$
  $Q_n = \Phi_n(A)v$
- recurrence $\quad x\Phi_n(x)(I_n + D_n^{-1}J_n) = \Phi_n(x)J_n + [0\ldots, 0, *]$
  translates as $\quad AQ_n(I_n + D_n^{-1}J_n) = Q_n J_n + [0, \ldots, 0, *]$
- Hence $A_n = Q_n^H A Q_n = J_n(I_n + D_n^{-1}J_n)^{-1}$
  eigenvalues of A_n = generalized eigenvalues of $(I_n + D_n^{-1}J_n, J_n)$
  = zeros of ϕ_n
- set $A_n = \widehat{U}_n \Lambda_n \widehat{U}_n^H$ then $f(A_n) = \widehat{U}_n f(\Lambda_n)\widehat{U}_n^H$, $\widehat{U}_n^H \widehat{U}_n = I_n$
  $\mathcal{I}_n\{f\} = v^H U_n f(\Lambda_n) U_n^H v$ with $U_n = Q_n \widehat{U}_n \in \mathbb{C}^{N\times n}$, $U_n^H U_n = I_n$
- $\mathcal{I}_\mu\{f\} \approx \mathcal{I}_n\{f\} = \sum_{k=0}^{n-1} |u_k^H v|^2 f(\lambda_k) = \sum_{k=0}^{n-1} w_k f(\lambda_k)$, $w_k = |u_k^H v|^2$
- = R-Gauss qf exact for $f \in \mathcal{L}_{n,n-1}$
- Also Radau and Lobatto variants are possible.

Application

Rational Krylov method

- Project on n-dimensional subspace of $\mathbb{C}^N$ ($n \ll N$)
  $\mathcal{K}_n(A, v) = \mathrm{span}\{v, Av, A^2v, \ldots, A^n v\} = \{p_n(A)v : p_n \in \mathcal{P}_n\}$
- polynomial $p_n(A)v \to$ rational $r_n(A)v$
  $\mathcal{K}_n(A, v) = \mathrm{span}\{v, b_1(A)v, \ldots, b_n(A)v\} = \{f_n(A)v : f_n \in \mathcal{L}_n\}$
- Orthogonal basis: $Q_n = [q_0, \ldots, q_n]$, $q_k = \phi_k(A)v$, ϕ_k = ORF.
- By $Z_k(A) = A(I - A/\alpha_k)^{-1}$ a shift and invert
  converges faster to eigenvalues near α_k
- In classical Krylov all $\alpha_k = \infty \Rightarrow$ cvg to 'largest' eigenvalues
- $\sigma(A_n) \approx \sigma(A)$: Ritz values

Application Model reduction

$H(z) = C(zI - A)^{-1}B + D$, $A \in \mathbb{C}^{N\times N}$, $C \in \mathbb{C}^{p\times N}$, $B \in \mathbb{C}^{N\times q}$, $D \in \mathbb{C}^{p\times q}$
$C^H = B$, $A^H = A$, $f(A) = (zI - A)^{-1}$

$$\begin{bmatrix} U_N^{-1} & 0 \\ 0 & I_p \end{bmatrix} \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} U_N & 0 \\ 0 & I_q \end{bmatrix}, \quad U_N \in \mathbb{C}^{N\times N}$$

project on subspace of
$\mathrm{colsp} U_n \subset \mathcal{K}(A, B) = \mathrm{span}\{B, AB, A^2B, \ldots\}$, $\quad U_n^H U_n = I_n$

$$\begin{bmatrix} U_n{}^H & 0 \\ 0 & I_p \end{bmatrix} \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} U_n & 0 \\ 0 & I_q \end{bmatrix}, \quad U_n \in \mathbb{C}^{N\times n}$$

Application Model reduction

$H(z) = C(zI - A)^{-1}B + D$, $A \in \mathbb{C}^{N\times N}$, $C \in \mathbb{C}^{p\times N}$, $B \in \mathbb{C}^{N\times q}$, $D \in \mathbb{C}^{p\times q}$
$C^H \neq B$, $A^H \neq A$, $f(A) = (zI - A)^{-1}$

$$\begin{bmatrix} U_N^{-1} & 0 \\ 0 & I_p \end{bmatrix} \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} U_N & 0 \\ 0 & I_q \end{bmatrix}, \quad U_N \in \mathbb{C}^{N\times N}$$

project on subspaces of
$\mathrm{colsp} Q_n \subset \mathcal{K}(A, B) = \mathrm{span}\{B, AB, A^2B, \ldots\}$, $Q_n^H Q_n = I_n$
$\mathrm{colsp} P_n \subset \mathcal{K}(A, C) = \mathrm{span}\{C^H, (CA)^H, (CA^2)^H, \ldots\}$, $P_n^H P_n = I_n$

$$\begin{bmatrix} (P_n^H Q_n)^{-1} P_n^H & 0 \\ 0 & I_p \end{bmatrix} \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} Q_n & 0 \\ 0 & I_q \end{bmatrix}, \quad P_n, Q_n \in \mathbb{C}^{N\times n}$$

Application Model reduction

Implementation in IRKA (Iterative Rational Krylov Algorithm)

S. Gugercin, A.C. Antoulas, C. Beattie.
H^2 Model reduction for large-scale linear dynamical systems.
SIAM. J. Matrix Anal. & Appl., vol.30, no.2, pp.609-638, 2008.

V. Druskin and C. Lieberman and M. Zaslavsky.
On adaptive choice of shifts in rational Krylov subspace reduction of evolutionary problems.
SIAM. J. Sci,. Comp., vol. 32, no. 5, pp.2485-2496, 2010.

Convergence via logarithmic potential

- $\mathcal{M}(E)$ = measures with support in $E \subset \mathbb{C}$
- logarithmic potential $U^\mu(z) = \int \log \frac{1}{|z-x|}\mathrm{d}\mu(x)$, $\mu \in \mathcal{M}(E)$
  Energy: $I(\mu) = \iint \log \frac{1}{|z-x|}\mathrm{d}\mu(x)\mathrm{d}\mu(z)$
- minimize weighted energy $I(\mu - \nu)$, $\mathrm{supp}(\nu) \subset \mathbb{C} \setminus E$,
  $\nu(\mathbb{C}) = s \in [0, 1]$
- Constrained weighted energy problem (CWEP):
  $\sigma \in \mathcal{M}(E)$: $\min_{\mu\in\mathcal{M}(E)} I(\mu - \nu)$ such that $t\mu \le \sigma$, $t \in (0, 1)$
- Unique solution μ_t^ν with $U^{\mu_t^\nu - \nu}(z) =$ constant C_t^ν on $\mathrm{supp}(\sigma - \mu_t^\nu)$
  and smaller everywhere else: = equilibrium measure.
- There is an algorithm to compute the solution approximately
  (discretization!)

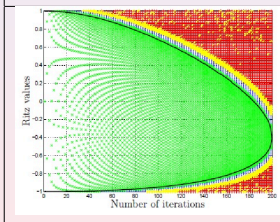
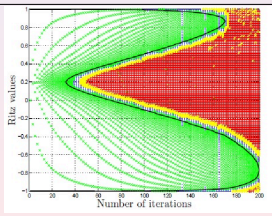
Convergence via logarithmic potential

Connection with Lanczos: (= a Krylov method)

- Asymptotic distribution of eigenvalues of A_N:
  $\sigma = \lim_{N\to\infty} \frac{1}{N} \sum_{k=0}^{N-1} \delta_{\lambda_{N,k}}$
- Asymptotic distribution of poles α_k:
  $\lim_{tN\to\infty} \frac{1}{tN} \sum_{k=1}^{tN} \delta_{\alpha_k} = \nu_t + (1-s)\delta_\infty$
  $t = n/N \in (0,1)$, s is ratio of poles at ∞
- Ritz values $\theta_{n,k}$: $\lim_{N\to\infty} \frac{1}{n(N)} \sum_{k=1}^{n} \delta_{\theta_{nk}} = \mu_t$
  This minimizes $I(\mu - \nu_t)$ and satisfies $t\mu_t \leq \sigma$.
- Solution of CWEP gives asymptotic distribution of the Ritz values.

Rational Krylov

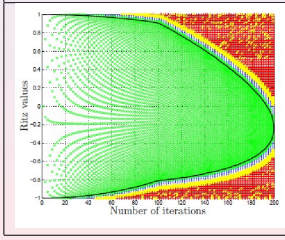
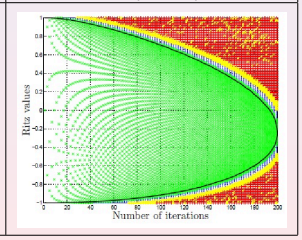
$A \in \mathbb{C}^{200\times 200}$, $\lambda_k = -1 + 2(k-1)/199$ $\mathrm{d}\lambda(x) = \frac{1}{2}\mathrm{d}x$

$\alpha = 2$	$\alpha = 0.2 + 0.1\mathbf{i}$
	

Convergence faster near α

Rational Krylov

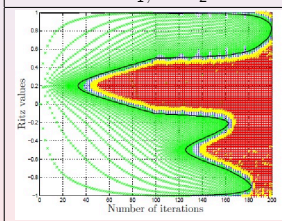
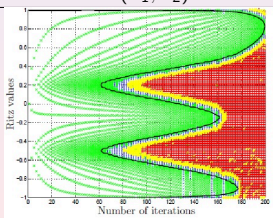
$A \in \mathbb{C}^{200\times 200}$, $\lambda_k = -1 + 2(k-1)/199$, $\alpha_1 = -5, \alpha_2 = 1.2$

$100\alpha_1, 100\alpha_2$	$100(\alpha_1, \alpha_2)$
	

Convergence faster near α_1, α_2

Rational Krylov

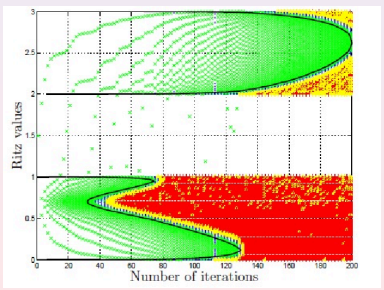
$A \in \mathbb{C}^{200\times 200}$, $\lambda_k = -1 + 2(k-1)/199$,
$\alpha_1 = -0.2 + 0.2\mathbf{i}, \alpha_2 = -0.5 + 0.1\mathbf{i}$

$100\alpha_1, 100\alpha_2$	$100(\alpha_1, \alpha_2)$
	

Convergence faster near α_1, α_2

Rational Krylov

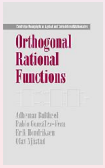
Eigenvalues of A in $E = [0,1] \cup [2,3]$
$\alpha = 0.7 + 0.1\mathbf{i}$



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K. Deckers, A. Bultheel, and F. Perdomo-Pío.
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