Rational Gauss quadrature

Adhemar Bultheel

Dept. Computer Science, KU Leuven

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This is joint work with Maria-José Cantero, Ruyman Cruz Barroso, Leila Daruis, Karl Deckers, Pablo González-Vera, Erik Hendriksen, Andreas Lasarow, Olav Njåstad, Francisco Perdomo-Pío, Joris Van Deun, Patrick Van gucht.
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 $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$]
- $f \in \mathcal{L} \subseteq L_1^\mu$

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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 $\leq n$)

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

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

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

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

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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 $k \geq n$?
$\max k$ = 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):

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

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

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

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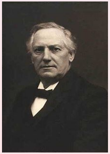
Some facts on $\mathbb{R}$

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

Notation

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

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



Jørgen Pedersen Gram

Herman Hankel

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

$\mathcal{L}_n = \mathcal{P}_n = \mathrm{span}\{1, z, z^2, \dots, z^n\} \to$ orthogonalize $\to$ OPs $\{\phi_k\}_{k=0,1,\dots}$
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 $m \geq n-1$ 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 $\operatorname{supp} \mu$
- Quadrature weights should be positive (stability and convergence)
- DoE as large as possible

Glory days!

Gauss qf have all these.

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QF = moment matching = interpolation

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

QF = moment matching

$\mathcal{I}_\mu\{p_* q\} = \mathcal{I}_n\{p_* q\}\ \forall p, q \in \mathcal{P}_n$, 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 $\Omega_\mu(z) - \Omega_n(z) = O(z^{-(2n+1)})$

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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

- $\text{supp}(\mu) = \hat{\mathbb{R}}$ all poles on $\hat{\mathbb{R}}$ or all in $\hat{\mathbb{C}} \setminus \mathbb{R}$ Hamburger
- $\text{supp}(\mu) = [0, +\infty]$ all poles on $[-\infty, 0]$ or in $\hat{\mathbb{C}} \setminus [0, +\infty)$ Stieltjes
- $\text{supp}(\mu) = [-1, 1]$ 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 $\alpha_k = \infty$.


Felix Hausdorff ($[0, 1]$)


Thomas Stieltjes ($[0, \infty)$)


Hans Hamburger ($\mathbb{R}$)

$$\boxed{\textbf{ORF on } \mathbb{R}}$$

Definitions and notation

- $\hat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$, $\hat{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$
  $\mathbb{U} = \{z \in \mathbb{C} : \mathrm{Im}\,(z) > 0\}$
- $f_*(z) = \overline{f(\overline{z})}$
- Cayley transform: (note factor $\mathbf{i}$)

$$z = \mathfrak{ic}(w) = \mathbf{i}\tfrac{1-w}{1+w} \leftrightarrow w = \mathfrak{ic}^{inv} = \tfrac{\mathbf{i}-z}{\mathbf{i}+z}, \quad w \in \left\{ \begin{array}{l} \mathbb{D} \\ \mathbb{T} \end{array} \right. \leftrightarrow z \in \left\{ \begin{array}{l} \mathbb{U} \\ \hat{\mathbb{R}} \end{array} \right.$$

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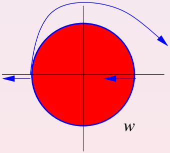

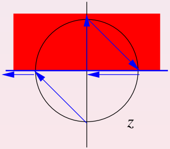

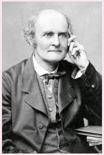

Arthur Cayley

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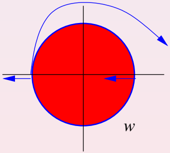

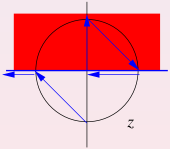

Henri Lebesgue

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relation

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

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

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Rolf Nevanlinna

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Augustin L. Cauchy

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- $\lim_{y \downarrow 0} \mathrm{Re}\, \Omega_{\mathring{\mu}}(x + \mathbf{i}y) = \mu'(x)$
- Remove factor $\mathbf{i}$ in the Nevanlinna and Cauchy kernel results in Ω in *Pick/Nevanlinna class* $= \{f \in H(\mathbb{U}) : f(\mathbb{U}) \subseteq \mathbb{U} \cup \mathbb{R}\}$

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: $\Omega_{\mu}(z) = \frac{1}{\mathbf{i}} \int \frac{\mathrm{d}\mu(x)}{x-z}$
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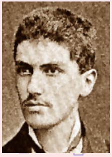
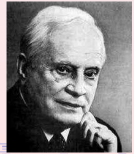
Georg A. Pick



Rolf Nevanlinna



The spaces $\mathcal{L}_n$

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

- set $b_0 = 1$, $b_n(z) = Z_n(z) b_{n-1}(z)$, $Z_n(z) = \frac{z}{1 - z/\alpha_n}$, $n \geq 1$,
- $\mathcal{L}_n = \operatorname{span}\{b_0, b_1, \ldots, b_n\}$
  $\mathcal{L}_n = \left\{ \frac{p_n}{\pi_n} : p_n \in \mathcal{P}_n; \pi_n(z) = \prod_{k=1}^{n} (1 - z/\alpha_k) \right\}$
- 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 $n - m$.

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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 $m_{k,l} = \int b_{k*}(x) b_l(x) \mathrm{d}\mathring{\mu}(x)$
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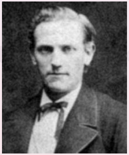
- $\langle f, g \rangle_{\mathring{\mu}} = \langle f, g \rangle_{\mathring{\nu}}$, $\forall f, g \in \mathcal{L}_n$ iff $\Omega_{\mathring{\mu}}$ is an Hermite int…or $\Omega_{\mathring{\nu}}$ for the points $\{\mathbf{i}, -\mathbf{i}, \alpha_1, \alpha_1, \alpha_2, \alpha_2, \ldots, \alpha_n, \alpha_n\}$
- The $\mathbf{i}$ appears because $D(t, \mathbf{i}) = 1$ and $1 = \int \mathrm{d}\mathring{\mu}(t) = \int \frac{\mathrm{d}\mu(x)}{1+x^2} = \int D(x, \mathbf{i})\mathrm{d}\mathring{\mu}(x) = \Omega_{\mathring{\mu}}(\mathbf{i}) = \overline{\Omega_{\mathring{\mu}}(-\mathbf{i})}$

Jørgen Pedersen Gram



- (QF =) moment matching = interpolation

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Charles Hermite

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The ORF ϕ_n

- ORF $\mathcal{L}_{n-1} \perp_\mu \phi_n \in \mathcal{L}_n$
- $\phi_n(z) = a_{nn} b_n(z) + a_{n,n-1} b_{n-1}(z) + \cdots + a_{n0} b_0$,
  $a_{nn} = \kappa_n > 0, \quad a_{n,n-1} = \kappa'_n$
- We may assume all functions are real ☺ + ☹ = ☺
- Note that $\mathcal{L}_{n*} = \mathcal{L}_n$ if the α_k are real (recall $f_*(z) = \overline{f(\overline{z})}$)
- $\phi_n = \frac{p_n}{\pi_n}$ 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)
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Recurrence for ORF ϕ_n

- Define $\phi_{-1} = 0$, $\phi_0 = 1$ (assuming $\int \mathrm{d}\mathring{\mu} = 1$), $\alpha_{-1} = \alpha_0 = \infty$, 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)

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

Recurrence for ORF ϕ_n

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

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

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

Theorem

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

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

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

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

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Skip proof

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Functions of the second kind

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

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

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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 $x \to y$

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

Elwin B. Christoffel

Gaston Darboux

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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

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Rational qf

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

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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.

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

Skip proof

- Let $p_n = c\prod_{i=1}^{l}(x-x_i)^{2m_i+1}\prod_{j=1}^{k}(x-\xi_j)^2, \quad n = 2M+l+2k$
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- $\therefore$ 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 $\mathcal{L}_{n,n-1}$

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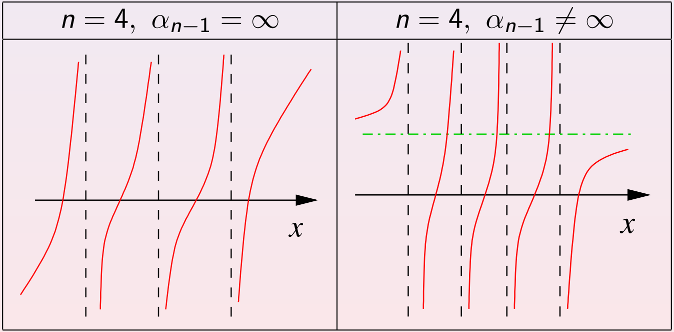
Proof

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



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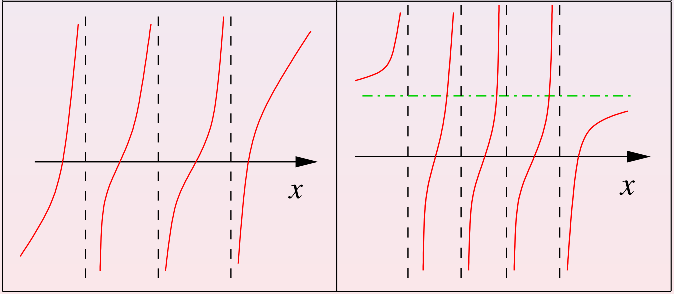

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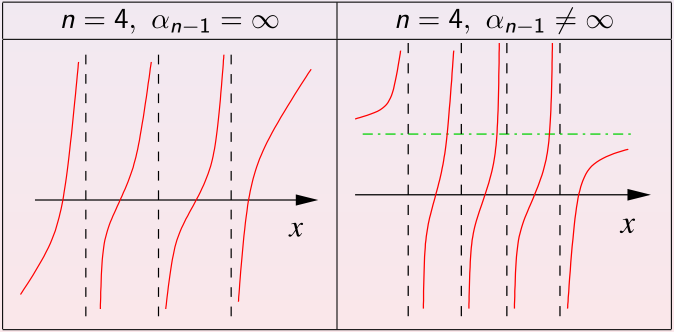

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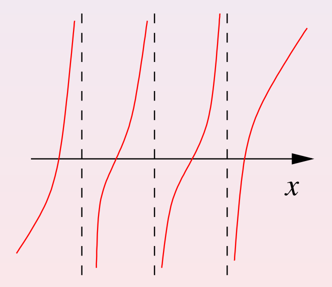	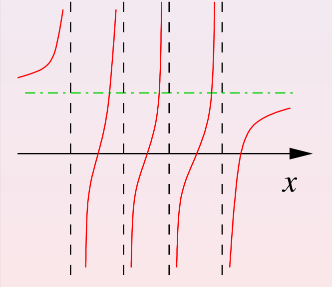

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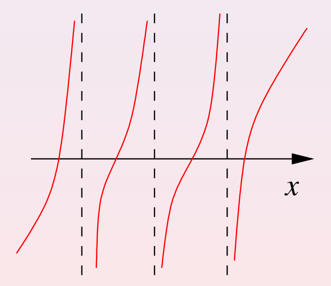	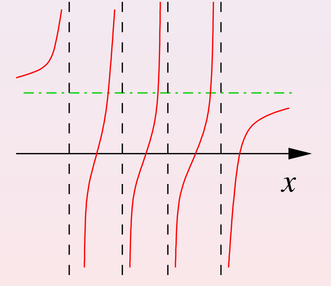

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Interpolation

- 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 $\mathcal{A}^{\mathbf{i}}_{n-1} = \{\mathbf{i}, -\mathbf{i}, \alpha_1, \alpha_1, \alpha_2, \alpha_2, \ldots, \alpha_{n-1}, \alpha_{n-1}\}$.
- What is $\Omega_{\mathring{\mu}_n}$?

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- QORF: $Q_n(z) = \phi_n(z) + \tau \frac{Z_n(z)}{Z_{n-1}(z)} \phi_{n-1}(z)$
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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
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Interpolation and kernels

- Define

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

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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 $\Omega_{\mathring{\mu}_n}$.
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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:
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- polynomials = poles at $\infty \to$ poles near ∞
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Thomas Stieltjes

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- 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 $(\sigma_{-1}, \sigma_0) = (1, 0)$.

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

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where $F_n = E_n Z_{n-1} + B_n$.

- Note that singularity is excluded!

The half-line

- Suppose we work with μ and $D(x,y)$ replaced by $C(x,y)=\frac{1}{x-y}$, i.e. $\Omega_\mu(z)=\int\frac{\mathrm{d}\mu(x)}{x-z}$.
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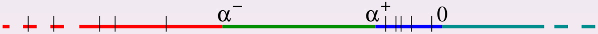

- Suppose $-\infty < \alpha_{2m} \le \alpha^- < x < \alpha^+ \le \alpha_{2m+1} < 0$
- The QF in zeros of ϕ_n (nodes and weights positive) exact in $\mathcal{L}_{n,n-1}$
- $\Omega_n = \frac{\sigma_n}{\phi_n}$ then Ω_n interpolates Ω_μ in $\{\alpha_0, \alpha_1, \alpha_1, \alpha_2, \alpha_2, \ldots, \alpha_n\}$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

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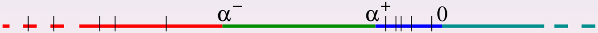

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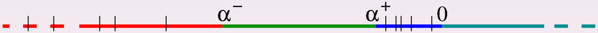

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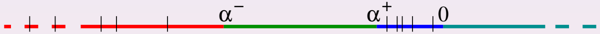

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The finite interval $\mathbf{I} = [-1, 1]$

- 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 $x = \cos\theta$, $\theta \in [-\pi, \pi]$, $z = e^{\mathrm{i}\theta}$
- $w(x), \quad x = \cos\theta \in \mathbf{I} \Leftrightarrow \mathring{w}(z) = w(\cos\theta)|\sin\theta|, \quad z = e^{\mathrm{i}\theta}$
- There are other possibilities e.g. $x \in [0, \infty) \leftrightarrow y = \frac{1-x}{1+x} \in [-1, 1]$

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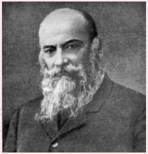
Nikolai Joukowski



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- inner product $\langle f, g\rangle_\mu = \int_{\mathbb{T}} \overline{f(z)} g(z) \mathrm{d}\mu(z)$
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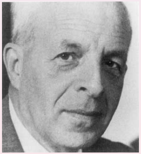
Gabor Szegő



Issai Schur

Samuel Verblunsky

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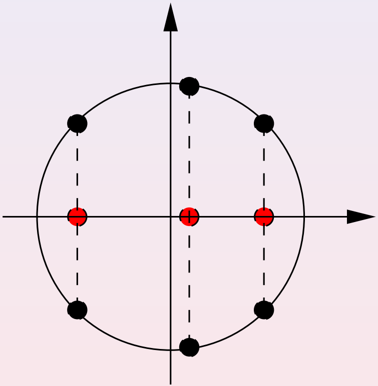
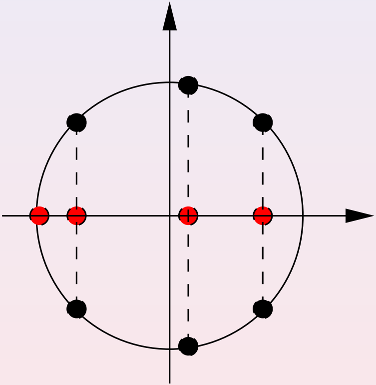


Carl F. Gauss

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

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Gauss-Radau qf on $\mathbb{I}$

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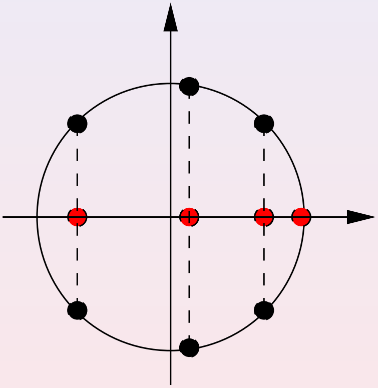


Carl F. Gauss

Rodolphe Radau

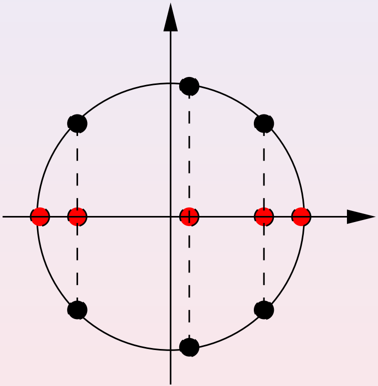
Szegő qf with PORF

$Q_n(z) = \phi_n(z) + \tau\phi_n^*(z)$ with

n odd and $\tau = -1 \rightarrow$

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

Symmetric case



Carl F. Gauss

Rehuel Lobatto

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Polynomials (Golub-Welsch algorithm)

- $x\phi_{n-1}(x) = a_{n-1}\phi_{n-2}(x) + b_n\phi_{n-1}(x) + a_n\phi_n(x), \quad \phi_0 = 1, \phi_{-1} = 0$
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$$J_n = \text{tridiag}\begin{pmatrix} a_1, \ldots, a_{n-1} \\ b_1, b_2, \ldots, b_{n-1}\, b_n \\ a_1, \ldots, a_{n-1} \end{pmatrix} \quad \text{(Jacobi matrix)}$$

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 $1/\sum_{j=0}^{n-1}|\phi_j(\xi)|^2 = 1/\|\Phi_n(\xi)\|^2$
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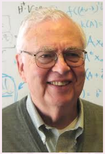
Gene Golub



John H. Welsch

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Carl G. Jacobi

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ORFs

- $x\phi_{n-1}(x) = \frac{1}{E_n}\tilde{\phi}_n(x) - \frac{B_{n-1}}{E_n}\tilde{\phi}_{n-1}(x) + \frac{1}{E_{n-1}}\tilde{\phi}_{n-2}(x)$
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  J_∞ is not representation of the shift in $\mathcal{L}_\infty$.

ORFs One way to write the TTRR

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- $\Phi_n(x) = [\phi_0, \ldots, \phi_{n-1}(x)]$, $\Delta_n(x) = \mathrm{diag}(1 - \frac{x}{\alpha_0}, \ldots, 1 - \frac{x}{\alpha_{n-1}})$

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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 $d\lambda$ on $\mathbb{T}$:

$$\phi_n(z) = \frac{\sqrt{1-|\alpha_n|^2}}{1-\overline{\alpha}_n z} z \prod_{j=1}^{n-1} \frac{z-\alpha_j}{1-\overline{\alpha}_j z}$$

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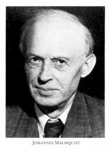
Satoru Takenaka

F. Malmquist



Rational Gauss-Chebyshev qf

- Recall $\mathsf{I} = [-1,1]$, $\mathcal{A} = \{\alpha_1, \alpha_2, \ldots\} \subset \hat{\mathbb{C}}^{\mathsf{I}} = \hat{\mathbb{C}} \setminus \mathsf{I}$
- $b_0 = 1$, $b_k = \prod_{j=1}^{k} Z_j$, $Z_j(x) = \frac{x}{1 - x/\alpha_j}$
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on $\mathbb{T} \leftrightarrow$ on $[-\pi, \pi]$	on $[-1, 1]$
$\mathring{w}(\theta)\mathrm{d}\theta = w(\cos\theta)\lvert\sin\theta\rvert\mathrm{d}\theta$	$w(x)\mathrm{d}x$

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- Chebyshev weights on $\mathbf{I} = [-1, 1]$:

$$w^{(1)}(x) = (1-x^2)^{-1/2}, \quad w^{(2)}(x) = \left(\frac{1-x}{1+x}\right)^{1/2}, \quad w^{(3)}(x) = (1-x^2)^{1/2}$$

Pafnuty L. Chebyshev

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

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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 $\hat{\mathbb{C}}$!

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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 $r(z) = |z - \alpha| \to \langle f, g \rangle_{\tilde{w}} = \langle (z-\alpha) f, (z-\alpha) g \rangle_w$
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Elwin B. Christoffel

Yakov Geronimus

Vasily Borisovich Uvarov

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

Theorem

$\mathcal{A}_n = \{\alpha_1, \ldots, \alpha_n\}$, $\mathcal{A}_n^\beta = \{\beta, \alpha_1, \ldots, \alpha_n\}$
$\gamma \in \mathbb{D} \cup \mathbb{T}$, $\mathrm{d}\hat{\mu}(z) = \left|\frac{z-\gamma}{1-\overline{\beta}z}\right|^2 \mathrm{d}\mu(z)$
$\hat{\phi}_n$ = *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 $\hat{\phi}_n(z) = \frac{(r-z)B_n(z)}{z-\alpha_n}$.

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Siméon D. Poisson

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Near best rational approximation

- L_∞ approximation on $\mathbb{I} = [-1, 1]$ needs equi-oscillation of the error
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- If $(x - x_0)\cdots(x - x_n) \sim T_{n+1}(x)$, then equi-oscillation. Thus interpolate in zeros of T_{n+1}.
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for $n = 1, 2, \ldots$, $\mathcal{T}_0 = 1/\sqrt{\pi}$, $\mathcal{U}_0 = \sqrt{2/\pi}$.

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

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- n-point (Polynomial) Gauss qf exact in $\mathcal{P}_{2n-1}$
- Fix m nodes $\Rightarrow$ nodes $=$ zeros of P with $\langle P, x^k \rangle = 0$, $k = 0, \ldots, n-m-1$ 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
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R-Gauss-Radau on $\mathbb{I}$

- Choose poles α_k in $\hat{\mathbb{R}}^{\mathbb{I}} = \hat{\mathbb{R}} \setminus [-1, 1]$
- $(n+1)$-point qf with prefixed ξ.
  Nodes = zeros of QORF $Q_{n+1}(x) = \phi_{n+1}(x) + \tau_{n+1} \frac{Z_{n+1}(x)}{Z_n(x)} \phi_n(x)$, $\tau_{n+1} \in \mathbb{R}$
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If $\alpha_k \in \hat{\mathbb{R}}^{\mathbb{I}}$ then at least $n-1$ zeros of Q_n are in $\mathbb{I}$ with positive weights.

- Similar for qf on $[0, \infty)$. $\alpha_k \in \hat{\mathbb{C}}^{\mathbb{I}} \to$ complex nodes.
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  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!

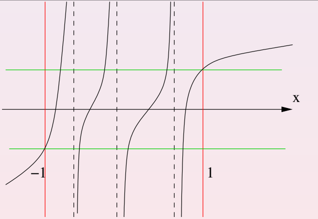
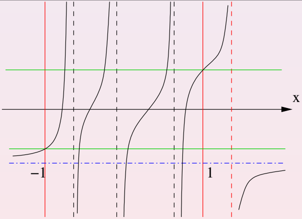
Theorem

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 $\mathbb{I}$

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

$n=3,\ \alpha_n = \infty$	$n=3,\ \alpha_n \neq \infty$
	

If the prefixed node ξ is too close to a zero of p_n, then one node may be outside $\mathbb{I}$!!

Similar observations hold for integrals over the half-line.

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

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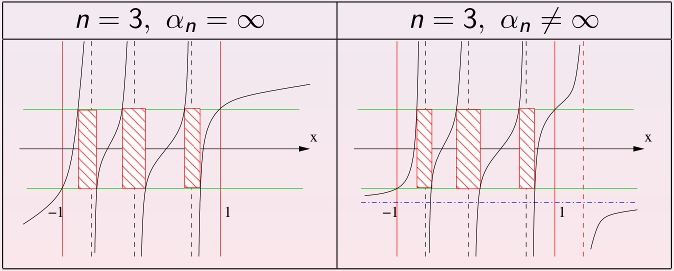

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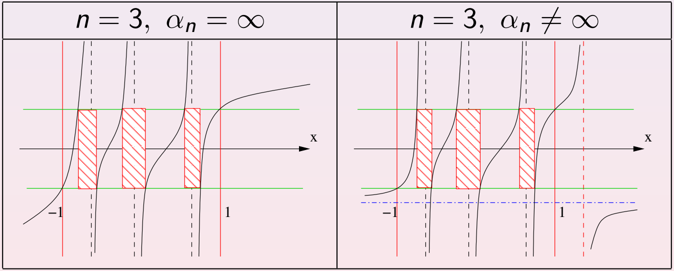
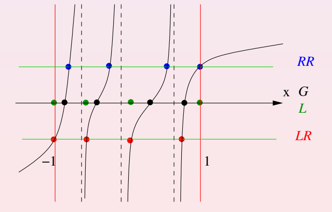
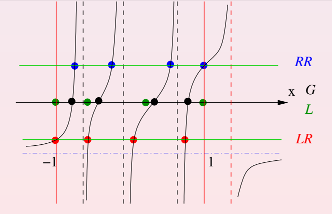


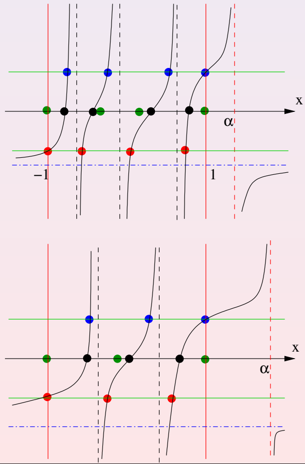
If the prefixed node ξ is too close to a zero of p_n, then one node may be outside $\mathbb{I}$!!
Similar observations hold for integrals over the half-line.

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

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

$n = 3,\ \alpha_n = \infty$	$n = 3,\ \alpha_n \neq \infty$
	

R-Gauss-Radau on I



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

curve = zeros of

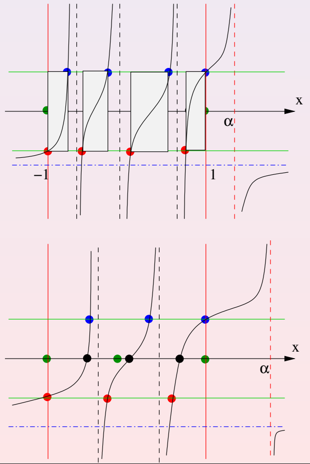
$$P_{n+1}(x,\xi) = p_{n+1}(x) - \frac{p_{n+1}(\xi)}{\tilde{p}_n(\xi)}\tilde{p}_n(x)$$

$$\tilde{p}_n(x) = (1 - \frac{x}{\alpha_n})p_n(x)$$

$$\phi_n(x) = \frac{p_n(x)}{\pi_n(x)}$$

assuming $p_n(\alpha_n) \neq 0$
otherwise replace α_n by some α

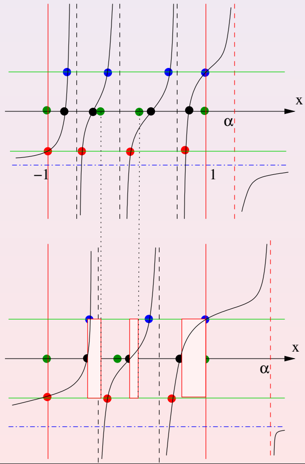
R-Gauss-Radau on I



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 $P_{n+1}(x, \xi)$



top: $n = 3, \ \alpha = \alpha_3$

bottom: $n = 2, \ \alpha = \alpha_2$

LR^ξ:

one node is -1

second node $\xi \in (-1, 1)$

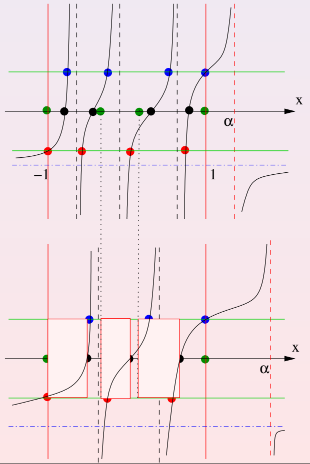
all weights positive

$$\xi \in \bigcup_{j=1}^{n} (x_{n,j}^G, x_{n+1,j}^L)$$

zeros of $P_n^{(1)}(x, \xi)$

$$\mathrm{d}\mu^{(1)}(x) = (x+1)\mathrm{d}\mu(x)$$

R-Gauss-Lobatto on I



top: $n = 3, \ \alpha = \alpha_3$

bottom: $n = 2, \ \alpha = \alpha_2$

RR$^\xi$:

one node is 1

second node $\xi \in (-1, 1)$

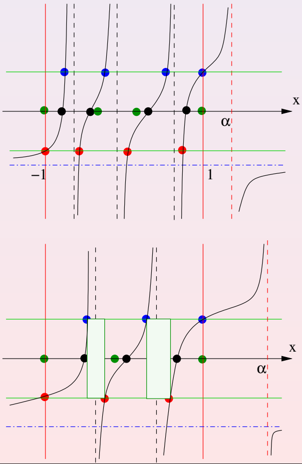
all weights positive

$$\xi \in \bigcup_{j=1}^{n} (x^L_{n+1,j}, x^G_{n,j})$$

zeros of $P_n^{(2)}(x, \xi)$

$$\mathrm{d}\mu^{(2)}(x) = (1 - x)\mathrm{d}\mu(x)$$

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



top: $n = 3$, $\alpha = \alpha_3$

bottom: $n = 2$, $\alpha = \alpha_2$

Gauss-Lobatto L^{ξ}:

both -1 and 1 are nodes

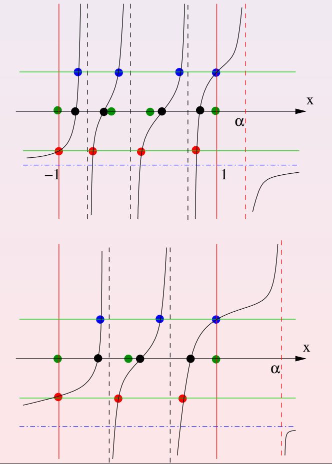
3rd node $\xi \in (a, b)$

all weights positive

$$\xi \in \bigcup_{j=1}^{n-1} (x_{n,j}^{RR}, x_{n,j+1}^{LR})$$

zeros of $P_{n-1}^{(3)}(x, \xi)$

$$\mathrm{d}\mu^{(3)}(x) = (1 - x^2)\mathrm{d}\mu(x)$$



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

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

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

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 $\mathbb{I}$ 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.

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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 $R'_{2n-1}(t_i) = f'(t_i)$.
- $R_{2n-1} = \frac{P_{2n-1}}{D_{2n-1}}$, $D_{2n-1} = \pi_n \pi_{n-1}$, $\pi_k = \prod_{j=1}^k (1 - \frac{x}{\alpha_j})$.
- $P_{2n-1}(x) = \sum_{j=1}^n [H_j(x) f(t_j) + \tilde{H}_j(x) f'(t_j)]$

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  Lagrange polynomials: $\begin{cases} L_j(t_k) = \delta_{jk}, & L'_j(t_k) = 0 \\ \tilde{L}_j(t_k) = 0, & \tilde{L}'_j(t_k) = \delta_{jk} \end{cases}$.
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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 $r_{n-1} \in \mathcal{L}_{n-1}$
- $E_n\{f\} = \mathcal{I}_\mu\{f - R_{2n-1}\} = c\frac{(fD_{2n-1})^{(2n)}(\theta(x))}{(2n)!} \int \phi_n^2(x)(1 - \frac{x}{\alpha_n})\mathrm{d}\mu(x)$.
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f analytic in $G \supset [0, +\infty]$, $\partial G = \Gamma$

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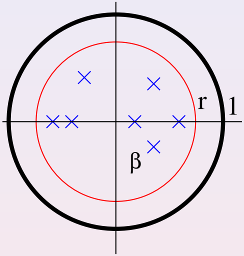

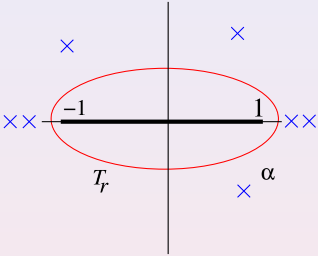

use Joukowski

$\pi_n(x)=\prod_1^n(1-x/\alpha_k)$

$\tilde{\pi}_n(z)=\prod_1^n(1-\beta_i z)$

$\beta_i=\mathrm{j}^{inv}(\alpha_i)$

$T_r=\{|\mathrm{j}^{inv}(z)|=r\}$

$\|\mu\|=\int \mathrm{d}\mu$

$\|\mathcal{I}_n\|=\sum_k |w_k|$

Theorem

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

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

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

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.

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$\operatorname{supp}(\mu) = [0, +\infty]$ *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)*
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The following convergence result is a direct consequence of the error estimate

Theorem

If $\int \frac{|\rho(\theta)|^2}{w(\theta)} \mathrm{d}\theta < \infty$ for pos. weight w and $\sum_{j=1}^{\infty}(1-|\alpha_j|) = \infty$ then $\forall f$ continuous on $\mathbb{T}$ and $\mathcal{I}_n$ an R-Szegő 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 $\mathbb{I} = [-1, 1]$

Theorem

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

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- 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 $(I - cA^T)x = \mathbf{1}$
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- If A too large then project it onto a lower dimensional subspace:
  $\mathcal{K}_{n-1} = \text{colsp}\, V_n = \text{colsp}[v_0, v_1, \ldots, v_{n-1}]$, $v_k = b_k(A)v$
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  $Q_n = \Phi_n(A)v$
- recurrence $\quad x\Phi_n(x)(I_n + D_n^{-1}J_n) = \Phi_n(x)J_n + [0\ldots,0,*]$
  translates as $\quad AQ_n(I_n + D_n^{-1}J_n) = Q_nJ_n + [0,\ldots,0,*]$
- 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 $f(A_n) = \widehat{U}_n f(\Lambda_n) \widehat{U}_n^H$, $\widehat{U}_n^H \widehat{U}_n = I_n$
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- $\mathcal{I}_\mu\{f\} \approx \mathcal{I}_n\{f\} = \sum_{k=0}^{n-1} |u_k^H v|^2 f(\lambda_k) = \sum_{k=0}^{n-1} w_k f(\lambda_k)$, $w_k = |u_k^H v|^2$
- $=$ R-Gauss qf exact for $f \in \mathcal{L}_{n,n-1}$
- Also Radau and Lobatto variants are possible.

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Rational Krylov method

- Project on n-dimensional subspace of $\mathbb{C}^N$ ($n \ll N$)
  $\mathcal{K}_n(A, v) = \mathrm{span}\{v, Av, A^2v, \ldots, A^nv\} = \{p_n(A)v : p_n \in \mathcal{P}_n\}$
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- Orthogonal basis: $Q_n = [q_0, \ldots, q_n]$, $q_k = \phi_k(A)v$, $\phi_k =$ ORF.
- By $Z_k(A) = A(I - A/\alpha_k)^{-1}$ a shift and invert
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- $\sigma(A_n) \approx \sigma(A)$: Ritz values

Aleksey Krylov

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Walter Ritz

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

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$C^H \neq B$, $A^H \neq A$, $f(A) = (zI - A)^{-1}$

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project on subspaces of
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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):
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- 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!)

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Convergence via logarithmic potential

Cornelius Lanczos

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.

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  $\lim_{tN\to\infty} \frac{1}{tN}\sum_{k=1}^{tN} \delta_{\alpha_k} = \nu_t + (1-s)\delta_\infty$
  $t = n/N \in (0,1)$, 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.

Convergence via logarithmic potential

Connection with Lanczos: (= a Krylov method)

- Asymptotic distribution of eigenvalues of A_N:
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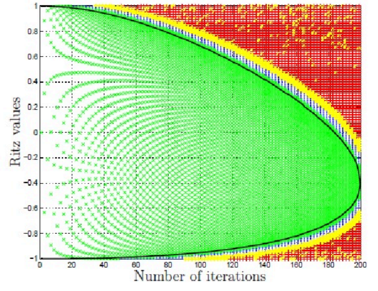
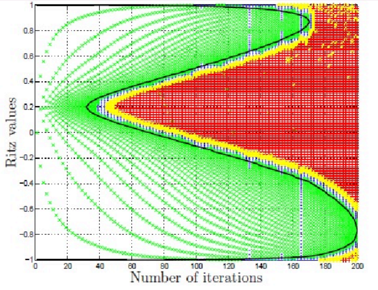
Rational Krylov

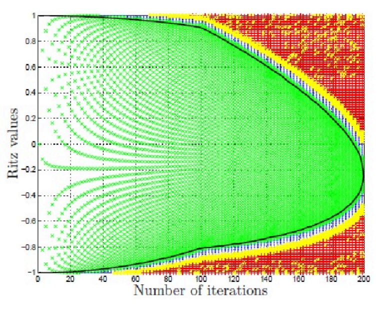
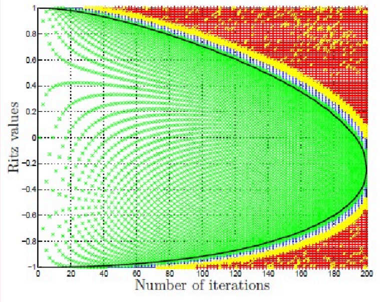
$A \in \mathbb{C}^{200\times 200}$, $\lambda_k = -1 + 2(k-1)/199$ $\mathrm{d}\lambda(x) = \frac{1}{2}\mathrm{d}x$

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

Convergence faster near α

Rational Krylov

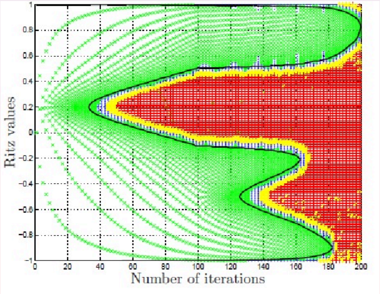
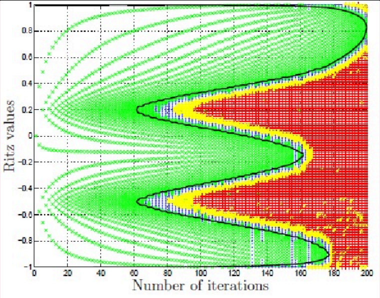
$A \in \mathbb{C}^{200\times 200}$, $\lambda_k = -1 + 2(k-1)/199$, $\alpha_1 = -5, \alpha_2 = 1.2$

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

Convergence faster near α_1, α_2

Rational Krylov

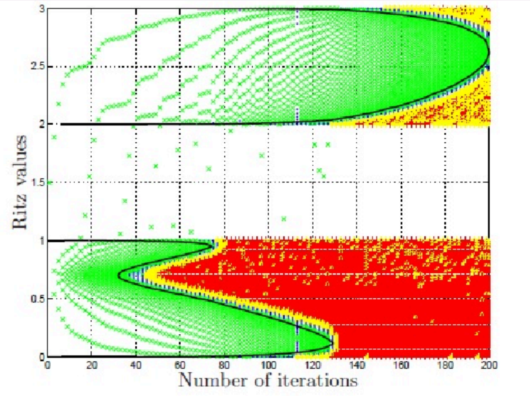
$A \in \mathbb{C}^{200\times 200}$, $\lambda_k = -1 + 2(k-1)/199$,
$\alpha_1 = -0.2 + 0.2\mathbf{i}, \alpha_2 = -0.5 + 0.1\mathbf{i}$

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

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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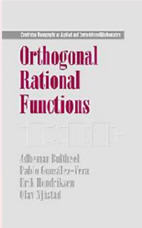

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