A rational variant of Fejér's quadrature rule with arbitrary complex poles

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Outline

1. Preliminaries
   - Problem formulation
   - Rational interpolatory quadrature rule
   - Rational Chebyshev nodes and weights
2. Rational variant of Fejér's quadrature rule
   - Computing the weights
   - Special case: complex conjugate pairs of poles

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Problem formulation

Numerical integration

$$\int_a^b \mathbf{F}(x)dx \approx \sum_{k=1}^{N} A_{Nk}\mathbf{F}(x_{Nk}), \quad \{x_{Nk}\}_{k=1}^{N} \subset [a,b],$$

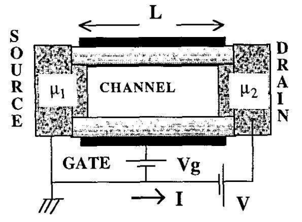
where

- $-\infty \leqslant a < b \leqslant \infty$,
- $\mathbf{F}(x)$ is a vector/matrix of non-smooth functions, caused by singularities close to $[a,b]$,
- the entries $F_j(x)$ are bounded on $[a,b]$,
- $F_j(x) = \mathcal{O}(x^{-2})$ for $x \to b$ $(x \to a)$ if $b = \infty$ $(a = -\infty)$.

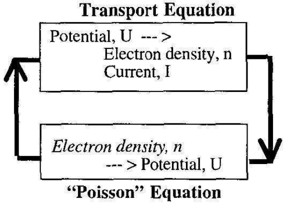
Problem formulation

Example from Nano device modeling [S. Datta, proc. IEDM, 2002]:

FET



Iterative loop



Transport equation

$$\rho = \left[\int_{-\infty}^{\infty} \left(\sum_{i=1}^{2} \frac{p_{2(n-1)}^{(i,j,k)}(x)}{|\pi_n(x)|^2} \cdot \frac{1}{e^{\frac{(x-\mu_i)}{kT}} + 1} \right) dx \right]_{j,k=1}^{n} .$$

Outline

Rational interpolatory quadrature rule

Given:

- $\{\alpha_1, \ldots, \alpha_{N-1}\} \subset (\mathbb{C} \cup \{\infty\}) \setminus [-1, 1]$, and
- distinct nodes $\{x_{Nk}\}_{k=1}^{N} \subset [-1, 1]$.

Rational interpolatory quadrature rule

There exist weights $\{A_{Nk}\}_{k=1}^{N}$ so that

$$\int_{-1}^{1} f(x)dx \approx \sum_{k=1}^{N} A_{Nk} f(x_{Nk}),$$

which is exact for (at least) every f of the form $f(x) = \frac{p_{N-1}(x)}{(1-x/\alpha_1)\cdot\ldots\cdot(1-x/\alpha_{N-1})}$.

$\forall k : \alpha_k = \infty \Rightarrow$ polynomial interpolation

Rational interpolatory quadrature rule

Rational non-orthogonal basis

$$J_m^{(\alpha)} := \int_{-1}^{1} f_m^{(\alpha)}(x)dx, \quad f_m^{(\alpha)}(x) := \left(\frac{1-x\alpha}{x-\alpha}\right)^m.$$

Then

$$J_0^{(\alpha)} = 2, \qquad J_1^{(\alpha)} = (\alpha^2-1)\log\left(\frac{\alpha+1}{\alpha-1}\right) - 2\alpha$$

$$\alpha^2 J_{m-1}^{(\alpha)} + 2\alpha J_m^{(\alpha)} + J_{m+1}^{(\alpha)} = (\alpha^2-1)\,\frac{1-(-1)^m}{m}, \quad m \geqslant 1.$$

Computing the weights

$$\mathbf{J}_f = \mathbf{F}\cdot\mathbf{a}.$$

$\mathbf{J}_f : \mathcal{O}(N)$ ops, $\mathbf{F} : \mathcal{O}(N^2)$ ops, and $\mathcal{O}(N^3)$ ops to solve the system
$\Rightarrow$ total: $O(N^3)$ ops.

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Rational Chebyshev nodes and weights

What?

Consider the rational Gauss-Chebyshev quadrature formula:

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx \approx \sum_{k=1}^{N} \lambda_{Nk} f(x_{Nk}),$$

which is exact for every f of the form
$f(x) = \frac{p_{2N-1}(x)}{|(1-x/\alpha_1)\cdot\ldots\cdot(1-x/\alpha_{N-1})|^2(1-x/\alpha_N)}$, where
$\alpha_N \in (\mathbb{R} \cup \{\infty\}) \setminus [-1,1]$.

$$\longrightarrow \quad \begin{aligned} x_{Nk}\text{'s} &= \text{rational Chebyshev nodes} \\ \lambda_{Nk}\text{'s} &= \text{rational Chebyshev weights} \end{aligned}$$

Rational Chebyshev nodes and weights

What?

Rational Chebyshev nodes are zeros of Chebyshev orthonormal rational function (CORF) $\varphi_N(x) = \frac{p_N(x)}{(1-x/\alpha_1)\cdot\ldots\cdot(1-x/\alpha_N)}$, for which

$$\langle \varphi_N , \varphi_j \rangle = \int_{-1}^{1} \varphi_N(x)\overline{\varphi_j(x)} \frac{dx}{\sqrt{1-x^2}} = \begin{cases} 0, & j \neq N \\ 1, & j = N \end{cases} .$$

Rational Chebyshev nodes and weights

Why?

1. Explicit expressions are known for the CORFs, and given in [K. Deckers, J. Van Deun and A. Bultheel, Math. Comp. 77(262), 2008];
2. MATLAB-function `rcheb` to compute the rational Chebyshev nodes and weights (complexity $= \mathcal{O}(mN)$) [J. Van Deun, K. Deckers, A. Bultheel and J.A.C. Weideman, ACM Trans. Math. Software 35(2), 2008];
3. Possible to reduce computational effort to construct the quadrature formula;
4. Near best for rational interpolation [J. Van Deun, K. Deckers, A. Bultheel and J.A.C. Weideman, ACM Trans. Math. Software 35(2), 2008].

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Rational Fejér's quadrature rule

Theorem

Set

$$A_{Nk} = \lambda_{Nk} \sum_{j=1}^{N-1} \overline{\varphi_j(x_{Nk})} \int_{-1}^{1} \varphi_j(x)dx.$$

Then the quadrature formula:

$$\int_{-1}^{1} f(x)dx \approx \sum_{k=1}^{N} A_{Nk} f(x_{Nk})$$

is exact for every f of the form $f(x) = \frac{p_{N-1}(x)}{(1-x/\alpha_1)\cdot\ldots\cdot(1-x/\alpha_{N-1})}$.

Rational Fejér's quadrature rule

- $\mathbf{J}_\varphi = \left(\int_{-1}^{1} \varphi_0(x)dx \quad \dots \quad \int_{-1}^{1} \varphi_{N-1}(x)dx \right)^T$
- $\mathbf{\Phi} = \begin{pmatrix} \varphi_0(x_{N1}) & \dots & \varphi_0(x_{NN}) \\ \vdots & \ddots & \vdots \\ \varphi_{N-1}(x_{N1}) & \dots & \varphi_{N-1}(x_{NN}) \end{pmatrix}$
- $\mathbf{\Lambda} = \text{diag}\left(\lambda_{N1} \quad \dots \quad \lambda_{NN} \right), \qquad \mathbf{I} = [\langle \varphi_j , \varphi_k \rangle]_{j,k=0}^{N-1}$

Proof of Theorem

$$\left.\begin{array}{l} \mathbf{J}_\varphi = \mathbf{\Phi} \cdot \mathbf{a} \Leftrightarrow \mathbf{a} = \mathbf{\Phi}^{-1} \cdot \mathbf{J}_\varphi \\ \\ \mathbf{\Phi} \cdot \mathbf{\Lambda} \cdot \mathbf{\Phi}^H = \mathbf{I} \Leftrightarrow \mathbf{\Phi}^{-1} = \mathbf{\Lambda} \cdot \mathbf{\Phi}^H \end{array}\right\} \Rightarrow \mathbf{a} = \mathbf{\Lambda} \cdot \mathbf{\Phi}^H \cdot \mathbf{J}_\varphi.$$

Assume $\mathbf{J}_\varphi$ is known
$\Rightarrow$ constructing $\mathbf{\Phi}$: $\mathcal{O}(N^2)$ ops, and computing $\mathbf{a}$: $\mathcal{O}(N^2)$ ops.

Rational Fejér's quadrature rule

Computing $\mathbf{J}_\varphi$

$$\mathbf{J}_f = \mathbf{F} \cdot \mathbf{a} = \mathbf{B} \cdot \mathbf{\Phi} \cdot \mathbf{a} = \mathbf{B} \cdot \mathbf{J}_\varphi,$$

where

$$\mathbf{B} = \mathbf{F} \cdot \mathbf{\Lambda} \cdot \mathbf{\Phi}^H = [b_{i,j}]_{i,j=0}^{N-1}$$

with

$$b_{i,j} = \left\langle f_{m_i}^{(\alpha_i)}, \varphi_j \right\rangle, \quad 0 \leqslant j \leqslant i \leqslant N-1$$

and $b_{i,j} = 0$, $0 \leqslant i < j \leqslant N-1$.

constructing $\mathbf{B}$: $\mathcal{O}(N^3)$ ops, and computing $\mathbf{J}_\varphi$: $\mathcal{O}(N^2)$ ops

Rational Fejér's quadrature rule

Constructing **B**

- the first column $b_{i,0}$, $i = 0, \ldots, N-1$, can be computed analytically,
- if $\alpha_i \notin \{\alpha_1, \ldots, \alpha_{i-1}\}$, then the $(i+1)-$th row can be computed recursively: $b_{i,j} = R(b_{i,j-1})$, $j = 2, \ldots, i$,
- the diagonal can be computed recursively: $\alpha_i = \alpha_k$, $i > k$, $\Rightarrow b_{i,i} = R(b_{k,k})$.

$\Rightarrow \mathcal{O}(N^2) - \mathcal{O}(N^3)$ ops

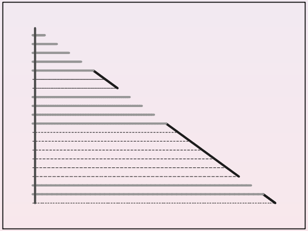

Figure: 20 poles from which 11 are different

Rational Fejér's quadrature rule

Automatic integrator

```
automatic_int(f,α's)
    Initialization
    construct N-point qf
    approximate ∫_{-1}^{1} f(x)dx
    while not converged and not stop criterion do
        choose pole and increase N → N+1
        construct N-point qf
        approximate ∫_{-1}^{1} f(x)dx
        check convergence/stop criterion
    end
```

Rational Fejér's quadrature rule

Automatic integrator: for $N = 1, \ldots, M$

1. $\mathbf{J}_f = \mathbf{F} \cdot \mathbf{a} \Rightarrow \mathcal{O}(M^4)$ ops
2. Based on rational Chebyshev nodes and weights:
   - $\mathbf{B}^N = \begin{pmatrix} \mathbf{B}^{N-1} & \mathbf{0} \\ b_{N,0} \ldots b_{N,N-1} & b_{N,N} \end{pmatrix} \rightarrow \mathcal{O}(M^2) - \mathcal{O}(M^3)$ ops
   - $\mathbf{J}_\varphi^N = \begin{pmatrix} \mathbf{J}_\varphi^{N-1} & \int_{-1}^{1} \varphi_N(x) dx \end{pmatrix}^T \rightarrow \mathcal{O}(M^2)$ ops
   - $\mathbf{\Phi} : \mathcal{O}(M^3)$ ops, and $\mathbf{a} : \mathcal{O}(M^3)$ ops

   $\Rightarrow \mathcal{O}(M^3)$ ops

In the polynomial case: $\mathcal{O}(M^2)$ ops

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Rational Fejér's quadrature rule

Complex conjugate pairs of poles $\Rightarrow A_{Nk}$ are all real

- $\varphi_k(x) \longrightarrow \Re\{\varphi_k(x)\}$ for $x \in [-1,1]$
- $\alpha_k = \text{real} \Rightarrow \Re\{\varphi_k(x)\} = \varphi_k(x)$
- $\alpha_k = \overline{\alpha}_{k-1} \Rightarrow \Re\{\mathbf{\Phi}_k(x)\} = \mathbf{A}_k \cdot \mathbf{\Phi}_k(x)$, with:

$$\mathbf{A}_k = \frac{1}{2}\begin{pmatrix} a_k & b_k \\ b_k & a_k \end{pmatrix}, \qquad \mathbf{\Phi_k}(x) = \begin{pmatrix} \varphi_{k-1}(x) \\ \varphi_k(x) \end{pmatrix},$$

  where $a_k = 1 + \frac{1-|\beta_k|^2}{1-\beta_k^2}$ and $b_k = \frac{2i\Im\{\beta_k\}}{1-\beta_k^2}$, with $\alpha_k = \frac{1}{2}(\beta_k + 1/\beta_k)$ and $|\beta_k| < 1$.
- set $\mathbf{K} = [\langle \Re\{\varphi_j\}, \Re\{\varphi_k\}\rangle]_{j,k=0}^{N-1} = \text{diag}\begin{pmatrix} 1 & \mathbf{K}_1 & \dots & \mathbf{K}_m \end{pmatrix}$, where

$$\mathbf{K}_j = \begin{cases} 1, & \alpha_j = \text{real} \\ \mathbf{A}_j \cdot \mathbf{A}_j^H, & \alpha_j = \overline{\alpha}_{j-1} \end{cases}.$$

Rational Fejér's quadrature rule

Then:

$$\left.\begin{array}{l}\mathbf{J}_{\Re\{\varphi\}} = \Re\{\mathbf{\Phi}\} \cdot \mathbf{a} \Leftrightarrow \mathbf{a} = \Re\{\mathbf{\Phi}\}^{-1} \cdot \mathbf{J}_{\Re\{\varphi\}} \\ \Re\{\mathbf{\Phi}\} \cdot \mathbf{\Lambda} \cdot \Re\{\mathbf{\Phi}\}^T = \mathbf{K} \Leftrightarrow \Re\{\mathbf{\Phi}\}^{-1} = \mathbf{\Lambda} \cdot \Re\{\mathbf{\Phi}\}^T \cdot \mathbf{K}^{-1}\end{array}\right\}$$

$$\Rightarrow \mathbf{a} = \mathbf{\Lambda} \cdot \Re\{\mathbf{\Phi}\}^T \cdot \mathbf{K}^{-1} \cdot \mathbf{J}_{\Re\{\varphi\}}.$$

Computing $\mathbf{J}_{\Re\{\varphi\}}$

- $f_m^{(\alpha)},\ f_m^{(\overline{\alpha})} \to \Re\left\{f_m^{(\alpha)}\right\},\ \Im\left\{f_m^{(\alpha)}\right\}$, $\mathbf{F} \to \hat{\mathbf{F}}$ and $\mathbf{J}_f \to \mathbf{J}_{\hat{f}}$
- $\mathbf{J}_{\hat{f}} = \hat{\mathbf{B}} \cdot \mathbf{J}_{\Re\{\varphi\}}$, where $\hat{\mathbf{B}} = \hat{\mathbf{F}} \cdot \mathbf{\Lambda} \cdot \Re\{\mathbf{\Phi}\}^T$ is lower Hessenberg (lower block-triangular).

Rational Fejér's quadrature rule

Constructing $\hat{\mathbf{B}}$

Let

$$a_{i,j} = \left\langle f_{m_i}^{(\alpha_i)}, \Re\{\varphi_j\} \right\rangle = \begin{cases} \hat{b}_{i,j}, & \alpha_i = \text{ real} \\ \hat{b}_{i-1,j} + \mathbf{i}\hat{b}_{i,j}, & \alpha_i = \overline{\alpha}_{i-1} \end{cases}.$$

- $\alpha_j = \text{real}$: $a_{i,j} = b_{i,j}$
- $\alpha_j = \overline{\alpha}_{j-1}$:

$$\begin{aligned} \begin{pmatrix} a_{i,j-1} \\ a_{i,j} \end{pmatrix} &= \mathbf{A}_j \cdot \begin{pmatrix} 1 \\ \frac{\beta_i - \beta_{j-1}}{1-\beta_i\beta_{j-1}} \end{pmatrix} \cdot b_{i,j-1} \\ b_{i,j} &= \begin{pmatrix} 0 & 1 \end{pmatrix} \cdot \mathbf{A}_j^{-1} \cdot \begin{pmatrix} a_{i,j-1} \\ a_{i,j} \end{pmatrix}. \end{aligned}$$

References

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Thank you …