Quadrature By Zeta Correction

A Singular Quadrature Method For Integral Equations

Bowei (Bobbie) Wu
Per-Gunnar Martinsson

Sayas Numerics Seminar
Feb. 23, 2021

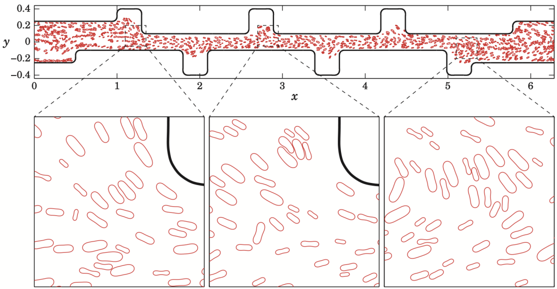
The University of Texas at Austin
Oden Institute for Computational Engineering and Sciences

Outline

1. Integral Equations And Singular Quadrature

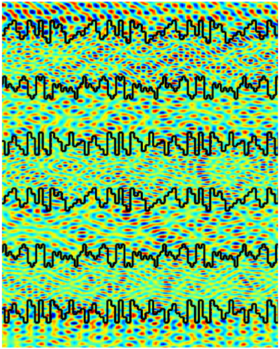
2. Zeta Quadrature On Curves And Surfaces

Integral Equation Method



Vesicle flow in periodic channel

Marple et al.(SISC,2016)



Multilayered media scattering

Zhang & Gillman(BIT,2020)

- Fredholm 2nd kind integral equation on surface $\Gamma \subset \mathbb{R}^n$

$$\sigma(x) + \int_\Gamma K(x,y)\sigma(y)\,\mathrm{d}S(y) = f(x), \quad x \in \Gamma$$

- Large number of unknowns N, complex geometry Γ
  - Want solvers that are **fast** (scales like $O(N)$), **robust**, **high-order accurate**, **adaptive**, and **easy to use**

Singular Integrals

- Nyström method (pick $\{x_i\}_{i=1}^N$ quadrature nodes = collocation points)

$$\sigma(x) + \int_\Gamma K(x,y)\sigma(y)\,\mathrm{d}S(y) = f(x)$$

$$\text{collocation} \longrightarrow \quad \sigma(x_i) + \int_\Gamma K(x_i,y)\sigma(y)\,\mathrm{d}S(y) = f(x_i), \quad 1 \le i \le N$$

$$\text{quadrature} \longrightarrow \quad \sigma(x_i) + \sum_{j=1}^{N} K(x_i,x_j)\sigma(x_j)w_j = f(x_i), \quad 1 \le i \le N$$

$$\longrightarrow \quad (\mathbf{I}+\mathbf{K})\boldsymbol{\sigma} = \mathbf{f}$$

- Quadrature nodes $\{x_i\}$ and weights $\{w_i\}$ for smooth integrands

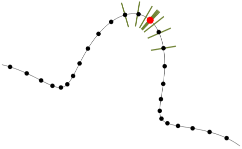
$$\mathbf{K}_{i,j} = K(x_i,x_j)w_j$$

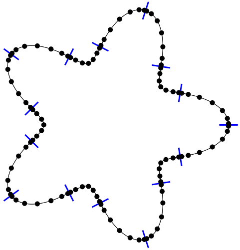
- However, $K(x,y)$ singular near diagonal $\implies K(x_i,x_i) = \infty$

$$\text{Laplace}\begin{cases}\text{(2D)} & \frac{1}{2\pi}\log\frac{1}{|x-y|}\\ \text{(3D)} & \frac{1}{4\pi}\frac{1}{|x-y|}\end{cases}$$

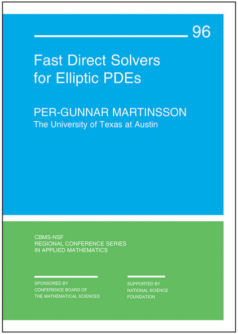
- Require specially designed quadratures (modify the entries of $\mathbf{K}$)

Singular Quadrature By Correcting The Regular



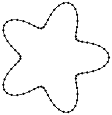
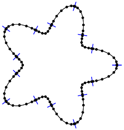
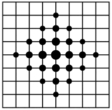
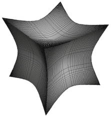
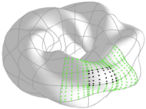


- global vs panel quadrature
- global vs local correction
- on-grid vs off-grid (auxiliary nodes) correction
- **Compatibility with fast algorithms**
  - Fast Multipole Method (FMM)
    $(\mathbf{I}+\mathbf{K})\boldsymbol{\sigma}$ in $O(N)$ time
    Fast Direct Solver (FDS)
    $(\mathbf{I}+\mathbf{K})^{-1}\mathbf{f}$ in $O(N)$ time
  - FMM/FDS-compatible:
    $\mathbf{K}_{i,j} = K(x_i, x_j)w_j$ except for $O(N)$ entries



Martinsson (SIAM,2019)

Existing Singular Quadrature Methods

 uniform grid	 panels	 uniform mesh ($\mathbb{R}^2$)
`Kapur-Rokhlin,1997` `Kress,1991` (global) `Alpert,1999` (off-grid)	`Kolm-Rokhlin,2001` `Helsing-Ojala,2008`	`Duan-Rokhlin,2009` `Marin-Runborg-Tornberg,2014`
 triangular panels	 rectangular panels	Other popular techniques: • local change of variable • spherical quadrature • extrapolation
`Bremer-Gimbutas,2012`	`Barnett-Greengard-Hagstrom,2019`	

- Goal: *facilitate* the development of FDS (esp. in 3D)
- *Simplest* to implement: global quadrature with local, on-grid correction

Outline

1. Integral Equations And Singular Quadrature

2. Zeta Quadrature On Curves And Surfaces

Corrected Trapezoidal Rule on $\mathbb{R}$

Zeta quadrature: local, on-grid correction to the trapezoidal rule

$$\int_{-a}^{a} \log \frac{1}{|x|} \varphi(x)\, \mathrm{d}x = \sum_{\substack{n=-N/2 \\ n\neq 0}}^{N/2-1} \log \frac{1}{|nh|}\, \varphi(nh)\, h + E_h[\varphi]$$

where $h = 2a/N$. (φ smooth & with compact support in $(-a, a)$.)

$$\int_{-a}^{a} \log \frac{1}{|x|} \varphi(x)\, \mathrm{d}x = \sum_{\substack{n=-N/2 \\ n\neq 0}}^{N/2-1} \log \frac{1}{|nh|}\, \varphi(nh)\, h + \varphi(0) h \log(1/h)$$
$$+ h \sum_{j=0}^{M} \tilde{w}_j \big(\varphi(jh) + \varphi(-jh)\big) + O(h^{2M+3})$$

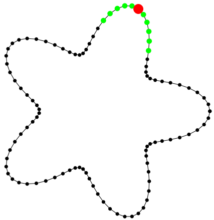
- $\tilde{w}_j$ same as one of the quadrature rules in `Kapur,Rokhlin(1997)`

Zeta Quadrature On Curves

- Let Γ be parameterized by $\mathbf{r}(x)$ on $[-a, a)$. (WLOG, $\mathbf{r}(0) = \mathbf{0}$)
- Regular weights $w_n = |\mathbf{r}'(nh)|\, h$ (arc length elements)

$$\int_\Gamma \log \frac{1}{|\mathbf{r}|} \varphi(\mathbf{r})\, \mathrm{d}s = \sum_{\substack{n=-N/2 \\ n\neq 0}}^{N/2-1} \log \frac{1}{|\mathbf{r}(nh)|}\, \varphi(\mathbf{r}(nh))\, w_n + \varphi(\mathbf{0}) w_0 \log(1/w_0)$$

$$+ \sum_{j=0}^{M} \tilde{w}_j \big(\varphi(jh) w_j + \varphi(-jh) w_{-j}\big) + O(h^{2M+3})$$



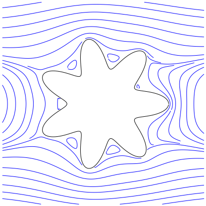
- Geometric analysis: $\log |\mathbf{r}(x)| \approx \log |\mathbf{r}'(0) x|$ for $x \approx 0$

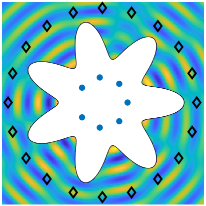
Numerical Examples

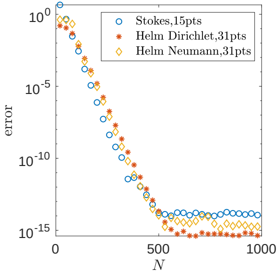
- Generalization to kernels of the Helmholtz equation $(\Delta u + \kappa^2 u = 0)$ and Stokes equation $(-\mu\Delta\mathbf{u} + \nabla p = 0)$

Helmholtz:	$\frac{i}{4}H_0^{(1)}(\kappa\lvert\mathbf{r}\rvert) = \frac{1}{2\pi}J_0(\kappa\lvert\mathbf{r}\rvert)\log\frac{1}{\lvert\mathbf{r}\rvert} +$ smooth
Stokes:	$\frac{1}{4\pi\mu}\left(\left(\log\frac{1}{\lvert\mathbf{r}\rvert}\right)\mathbf{I} + \frac{\mathbf{r}\otimes\mathbf{r}}{\lvert\mathbf{r}\rvert^2}\right)$

- **Examples:** BVP solve. Stokes flow & Helmholtz, $(\mathbf{I}+\mathbf{K})\boldsymbol{\sigma} = \mathbf{f}$



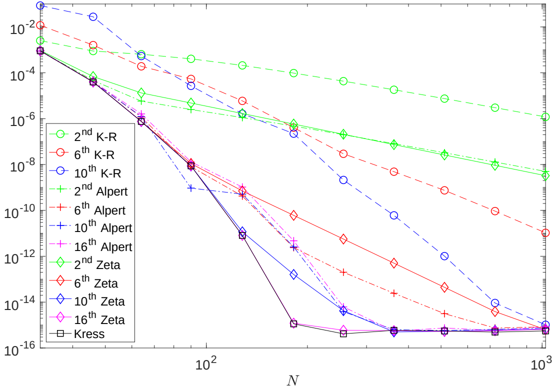




W & Martinsson(2020,arXiv:2007.13898)

Comparison

Zeta quadrature compared with Kapur-Rokhlin, Alpert, and Kress quadratures in the solution of the Stokes BVP



- K-R has large correction weights, thus bigger errors
- Zeta performs similarly to Alpert's hybrid Gauss-trapezoidal rule
- High-order zeta is as good as Kress's spectral quadrature

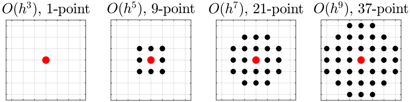
W & Martinsson(2020,arXiv:2007.13898)

Zeta Quadrature in 3D

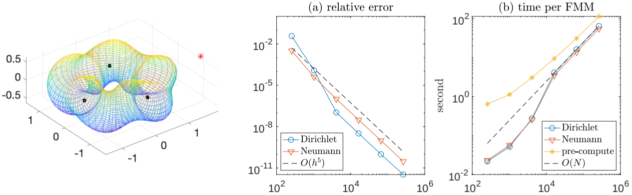
- Torus-like surface $\Gamma \subset \mathbb{R}^3$, double-trapezoidal rule for $\int \frac{1}{|\mathbf{r}|}\,\mathrm{d}S$
  1. error: Epstein zeta function (and derivatives) P.Epstein(1903,1906)

$$Z(s;Q) = \sum_{\substack{(i,j)\in\mathbb{Z}^2 \\ i,j\neq 0}} \frac{1}{Q(i,j)^{s/2}}, \quad Q(u,v) = Eu^2 + 2Fuv + Gv^2$$

  2. moment fitting: local 2D stencils

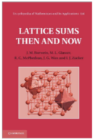


- **Example**: Laplace BVP. FMM iterative solve, $O(h^5)$ zeta quadrature



Details see **W** & Martinsson(2020,arXiv:2007.02512)

Historical Comments

- I.Navot (J.Math.Phys.,1961 & 1962)
  - extended Euler-Maclaurin formula for $\int_0^1 x^{-s} g(x)\,\mathrm{d}x$ and $\int_0^1 g(x)\log x\,\mathrm{d}x$
- A.Sidi,M.Israeli (J.Sci.Comput.,1988)
  - high-order quadrature for $\int_0^1 g(x)\log x\,\mathrm{d}x$ via extrapolation
- Celorrio,Sayas (BIT,1998) 
  - a proof for $\int_{-1/2}^{1/2} g(x)\log x^2\,\mathrm{d}x$; mentioned Navot & ζ in the end.
- Kapur,Rokhlin (1997): another proof of the Navot(1962) result
- Marin,Runborg,Tornberg (2014)
  - another proof of the Navot(1961) result; partial proof for $\int \frac{1}{|\mathbf{r}|}$ in $\mathbb{R}^2$.
- Looks like Navot's results had been rediscovered many times! (us included!)
  - **Our path:** surfaces (Epstein zeta) $\longrightarrow$ curves (Riemann zeta)
  - Borwein et al.(2013) *Lattice sums then and now*
    - 

      Epstein zeta function, Wigner limits.

Conclusion

- Zeta functions are connected to trapezoidal quadrature errors
- Geometric analysis is the key to zeta quadratures on curves & surfaces
- Zeta quadratures are simple & robust, ideal for developing FDS
- Currently non-adaptive
- Codes available:

  (2D) https://github.com/bobbielf2/ZetaTrap2D
  (3D) https://github.com/bobbielf2/ZetaTrap3D
- More at the SIAM CSE21 conference

backup slides

stability

Helmholtz integral operator evaluation (with random σ). Fast decay of correction weights (3rd fig)