Quadrature by Expansion: Evaluating Nearly Singular Integrals

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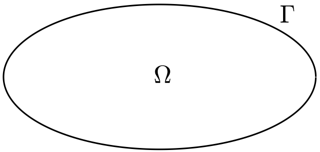
Outline

1. **Boundary Integral Equations**
2. **Quadrature by Expansion**
3. **Stepping off the Boundary**

Solving an Elliptic PDE

Say we want to solve the Dirichlet Laplace problem on some interior $\Omega \subset \mathbb{R}^2$

$$\begin{cases} \Delta u = 0, & \text{in } \Omega \\ u = f, & \text{on } \partial\Omega = \Gamma \end{cases}$$



Numerically, we have options:

- Finite Difference Methods
- Finite Element Methods
- Boundary Integral Methods

Either discretize a **differential operator** or an **integral operator**.

Solving an Elliptic PDE

Using a finite difference method would give us a linear system like

$$Ax = b$$

$$A = \frac{1}{h^2}\begin{bmatrix} T & I & & & \\ I & T & I & & \\ & \ddots & \ddots & \ddots & \\ & & I & T & I \\ & & & I & T \end{bmatrix} \qquad T = \begin{bmatrix} -4 & 1 & & & 0 \\ 1 & -4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -4 & 1 \\ 0 & & & 1 & -4 \end{bmatrix}$$

Discretizing the derivative operator leads to a **sparse** matrix with a condition number like $O(h^{-2})$ as mesh size $h \to 0$.

Solving an Elliptic PDE

Boundary integral equations (BIEs) give us a alternative recipe for solving elliptic PDEs:

1. Formulate the problem as a BIE
2. Discretize the equation
3. Solve for the density layer on the boundary
4. Evaluate the BIE for all points in the domain

Solving an Elliptic PDE

The same problem can be formulated as an integral equation using a *density layer* σ and the fundamental solution in 2D

$$k(z,w) = \frac{1}{2\pi} \log|z-w|$$

The solution can be written using the **double layer potential**

$$u(z) = D\sigma(z) = \int_\Gamma \frac{\partial k(z,w)}{\partial n_w} \sigma(w)\, ds(w), \qquad z \in \Omega$$

Limiting to the boundary gives us (for reasonably smooth σ)

$$\frac{1}{2}\sigma(z) + \int_\Gamma \frac{\partial k(z,w)}{\partial n(w)} \sigma(w)\, ds(w) = f(z)$$

Our 2D PDE is now a 1D integral equation. Using an IE **reduces the dimensions** of the problem by one.

Solving an Elliptic PDE

$$u(z) = \int_\Gamma \frac{\partial k(z,w)}{\partial n(w)}\,\sigma(w)\,ds(w), \qquad z \in \Omega$$

This can be written in complex notation [1]

$$u(z) = \text{Re}\, v(x)$$
$$v(z) = \frac{1}{2\pi}\int_\Gamma k(z,w)\,\sigma(w)\,ds(w), \qquad k(z,w) = \frac{n(w)}{z-w}$$

The corresponding BIE

$$\frac{1}{2}\sigma(z) + \frac{1}{2\pi}\int_\Gamma \frac{n(w)}{z-w}\,\sigma(w)\,ds(w) = f(z)$$

is a *Fredholm equation of the second kind*.

Discretizing a Boundary Integral Equation

Use the **Nyström technique** to discretize the BIE. Assume we have some quadrature scheme defined on Γ with nodes $\{z_i\}_{i=1}^N$ and weights $\{w_i\}_{i=1}^N$. We use the nodes as **collocation** points

$$\frac{1}{2}\sigma(z_i) + \int_\Gamma k(z_i, w)\,\sigma(w)\,ds(w) = f(z_i), \qquad i = 1, \dots, N$$

Now we can approximate the integral with the quadrature scheme

$$\int_\Gamma k(z_i, w)\,\sigma(w)\,ds(w) = \sum_{j=1}^N k(z_i, z_j)\,\sigma(z_j)\,w_j$$

This gives us a system of linear equations

$$\frac{1}{2}\sigma(z_i) + \sum_{j=1}^N k(z_i, z_j)\,\sigma(z_j)\,w_j = f(z_i), \qquad i = 1, \dots, N$$

Discretizing a Boundary Integral Equation

This leads to the matrix equation

$$\left(\frac{1}{2}I + A\right)\sigma = \mathbf{f}$$

A is **dense**, but has structured representations!

Once we have built A, we can solve for σ, and move onto the next step: evaluation.

Unfortunately, the kernels arising from BIEs often have a singularity. This leads to **specialized quadrature**. For now, assume we have solved for σ and it is well resolved.

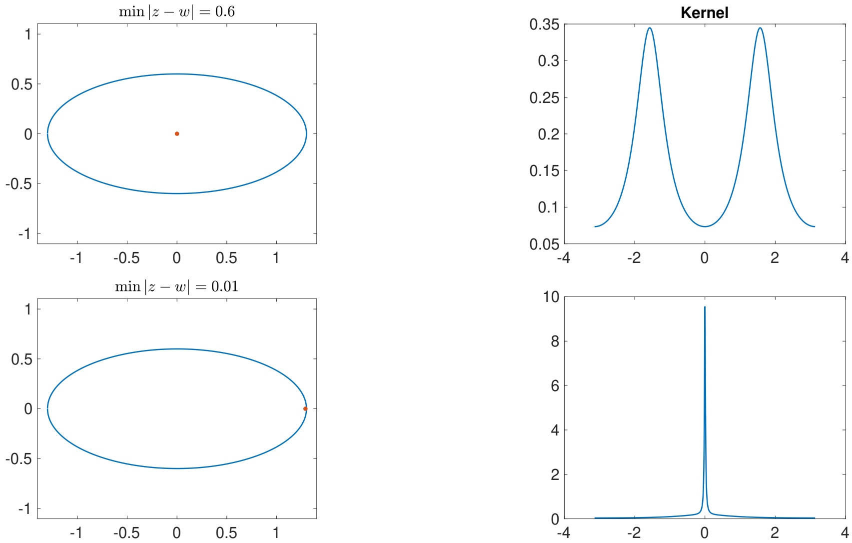
Evaluating a BIE

Once we have σ well resolved, we can use it in the integral formulation to compute the solution at any point in our domain. Now we have an IE with target point z and source points w.

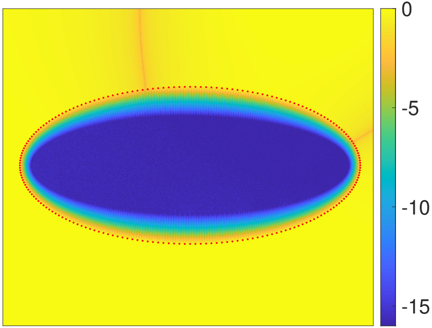
$$v(z) = \int_{\Gamma} k(z, w)\, \sigma(w)\, ds(w)$$

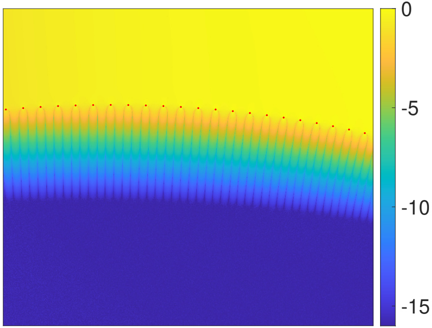
Now, this is just a matter of quadrature. But the kernel has a pesky singularity. As our target gets close to the boundary, the kernel becomes **nearly singular**.

Evaluating a BIE



Evaluating a BIE





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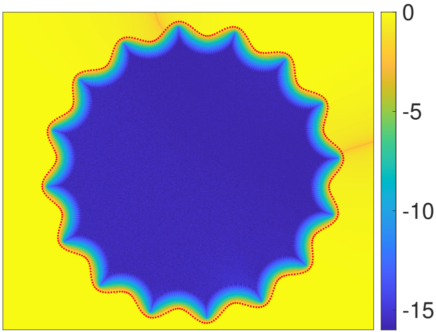
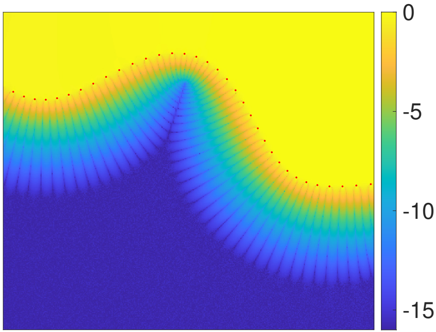
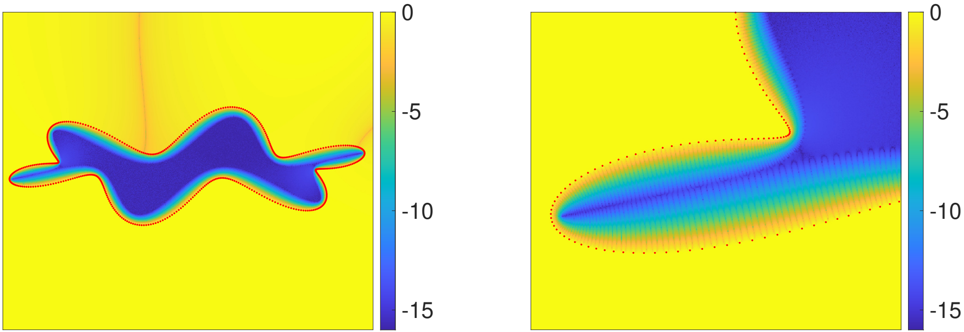




Evaluating a BIE



Outline

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- More Quadrature Nodes
- Singularity Subtraction
- Interpolation/Extrapolation
- **Quadrature by Expansion**

Quadrature by Expansion

Quadrature by Expansion (QBX) [5] is a specialized quadrature technique for nearly-singular integrals.

QBX hinges on being able to split the kernel into a series valid inside some radius r, about an expansion center z_0 using an *addition theorem*[1]

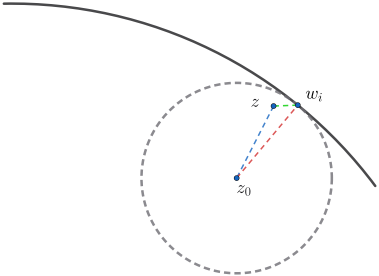
$$k(z, w) = \sum_{m=0}^{\infty} A_m^r(w, z_0) \cdot B_m^r(z, z_0)$$

where r is chosen as

$$r = \min_{w \in \Gamma} |w - z_0|$$

The interaction between z and the boundary is now *through* the point z_0 which is **further from the boundary** than z.

Quadrature by Expansion



$$k(z, w_i) = \sum_{m=0}^{\infty} A_m^r(w_i, z_0) \cdot B_m^r(z, z_0)$$

Quadrature by Expansion

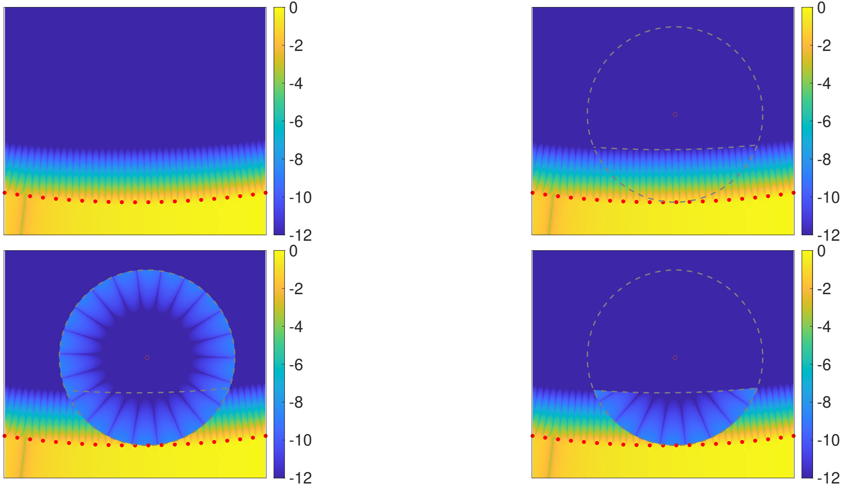
As defined, r means that the expansion is valid up to the boundary.

In [4] it was shown that the expansion is valid **including** the boundary for Laplace and Helmholtz kernels.

And in [2], Barnett showed that the expansion is valid for some $R > r$ for the same kernels as long as σ is analytic in the ball with radius R.

Quadrature by Expansion

QBX is like carving out and punching a hole in the near boundary.



Quadrature by Expansion

Recall

$$u(z) = \frac{1}{2\pi} \int_\Gamma \frac{n(w)}{z-w} \sigma(w) \, ds(w)$$

The **Cauchy kernel** has a Taylor series

$$\frac{-1}{z-w} = \sum_{m=0}^{\infty} \frac{(z-z_0)^m}{(w-z_0)^{m+1}}$$

Plug this into the integral

$$u(z) = \frac{1}{2\pi} \int_\Gamma \sum_{m=0}^{\infty} \frac{-(z-z_0)^m}{(w-z_0)^{m+1}} \, n(w) \, \sigma(w) \, ds(w)$$

Quadrature by Expansion

$$u(z) = \sum_{m=0}^{\infty} \frac{1}{2\pi} \int_{\Gamma} \frac{-(z-z_0)}{(w-z_0)^{m+1}}\, n(w)\, \sigma(w)\, ds(w)$$

$$= \sum_{m=0}^{\infty} \int_{\Gamma} \frac{n(w)\, \sigma(w)\, r^m}{(w-z_0)^{m+1}}\, ds(w)\, \frac{-(z-z_0)^m}{r^m}$$

Now we need to evaluate the coefficient integrals

$$\int_{\Gamma} \frac{n(w)\, \sigma(w)\, r^m}{(w-z_0)^{m+1}}\, ds(w)$$

Quadrature by Expansion

QBX effectively turns a single bad integral into a series of milder ones.

$$\int_\Gamma \frac{n(w)}{z-w}\,\sigma(w)\,ds(w) \to \int_\Gamma \frac{n(w)\,\sigma(w)\,r^m}{(w-z_0)^{m+1}}\,ds(w), \qquad |z-w| < |w-z_0|$$

The coefficient integrals a_m are evaluated using a general quadrature rule applicable to the geometry of Γ.

In this way, QBX is a *regularization* scheme.

Quadrature by Expansion

Error Analysis: There are two main sources of error in QBX:

- Truncation error e_T
- Coefficient error e_C

Quadrature by Expansion

Truncation Error: The series representation must be truncated to some order p to be practical.

The truncation error depends on the local geometry of Γ and the regularity of the density layer σ

In practice, the truncation error usually decays exponentially [1]. Estimate the truncation error

$$|e_T| \approx |a_{p+1} \cdot B^r_{p+1}(z, z_0)| \leq |a_{p+1}|$$

- e_T: $\uparrow$ with r, $\downarrow$ with p

Quadrature by Expansion

Coefficient Error: Each QBX coefficient requires an integral evaluation. And Quadrature = Error.

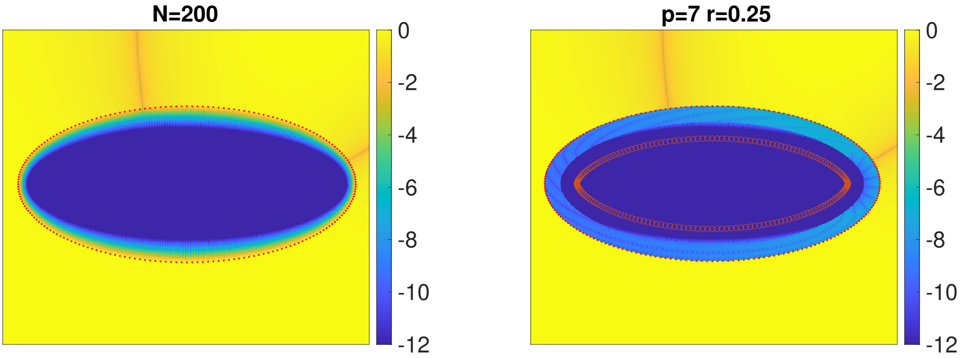
The coefficient error is the sum of all of the errors when evaluating these coefficient integrals and depends on the strength of the singularity in the kernel expansion, the type of quadrature used, and the number of nodes.

In general, the quadrature on Γ will need to be **upsampled** by some factor κ [1].

- e_C: $\uparrow$ with p, $\downarrow$ with r and κ

Quadrature by Expansion

QBX can then paint in the near boundary.



Outline

Stepping off the Boundary

As long as we have a *meromorphic* function, we can think about QBX.

For an arbitrary kernel, a series expansion would need to be found, and any error analysis would be specific to that kernel.

But if we encounter a known kernel... we're in business.

Stepping off the Boundary

One problem that appears in scattering theory and solving the acoustic wave equation via frequency-time-hybrid techniques, is evaluating integrals like

$$I(\sigma_n) = \int_{W_1}^{W_2} \frac{A(\omega)}{\omega - \sigma_n} e^{-i\omega t} d\omega$$

where $A(\omega)$ is analytic, σ_n is in the lower half plane, and t could be large [3].

$\implies$ $I(\sigma_n)$ could be **nearly-singular** and **highly oscillatory**.

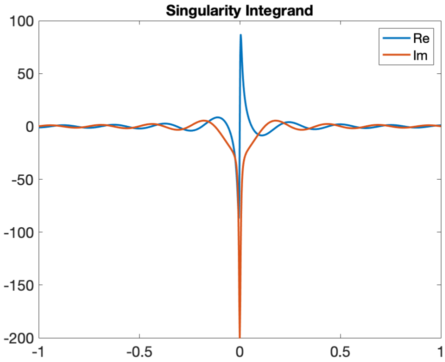
Stepping off the Boundary

This is just the Laplace kernel in disguise. We can do the same Cauchy kernel expansion.

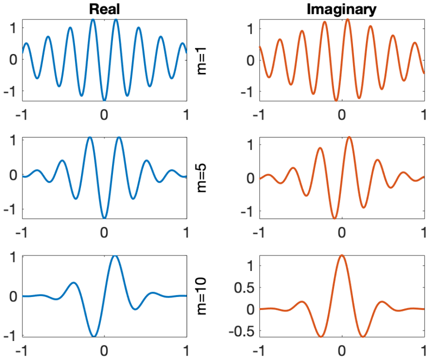
$$I(\sigma_n) = \sum_{m=0}^{\infty} b_m \frac{(\sigma_n - \sigma_c)^m}{r^m}, \qquad b_m = \int_{W_1}^{W_2} \frac{A(\omega)\, r^m}{(\omega - \sigma_c)^{m+1}}\, e^{-i\omega t}\, d\omega$$

The expansion center σ_c is further from the real-axis so the near-singularity is less severe, and our job becomes computing b_m.

Stepping off the Boundary



(a) Integrand (without QBX) for $t = 25$, $W_1 = -1, W_2 = 1$, and $\sigma_n = -i0.005$.



(b) QBX integrands when $t = 25$, $\sigma_n = -i0.005$, and a radius $r = 0.75$, corresponding to an expansion center of $\sigma_c = -i0.755$.

Stepping off the Boundary

QBX took care of the singularity, now how about the oscillations?

For simplicity

$$B(\omega) := \frac{A(\omega)\, r^m}{(\omega - \sigma_c)^{m+1}}$$

Like in [6] make the change of variables $\omega = Py + W_1$ where $P = W_2 - W_1$ and $y \in [0, 1]$. Write $B(Py + W_1)$ as a Fourier series

$$B(Py + W_1) = \frac{1}{2m+1} \sum_{j=-m}^{m} C_j\, e^{2\pi i j y}$$

$$C_j = \int_0^1 B(Py + W_1) e^{-2\pi i j y}\, dy$$

Stepping off the Boundary

Plug the Fourier series into the expression for a QBX coefficient integral b_m and we get the representation

$$b_m = \frac{Pe^{-it(W_1+P/2)}}{2m+1} \sum_{j=-m}^{m} C_j \, (-1)^j \operatorname{sinc}\left(j - \frac{Pt}{2\pi}\right)$$

This can be done quickly, with the **fast sinc transform** [6].

Takeaways

- If a kernel function omits a Taylor series, *exploit* this to try and push the target away from the singularity
- If you encounter a Cauchy or Laplace kernel in the wild, think about QBX as a regularization scheme.

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[1] Ludvig Af Klinteberg and Anna-Karin Tornberg. "Adaptive Quadrature by Expansion for Layer Potential Evaluation in Two Dimensions". en. In: *SIAM Journal on Scientific Computing* 40.3 (Jan. 2018), A1225–A1249. ISSN: 1064-8275, 1095-7197. DOI: 10.1137/17M1121615. URL: https://epubs.siam.org/doi/10.1137/17M1121615 (visited on 02/07/2026).

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