FLATIRON INSTITUTE
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Introduction to Integral Equation Methods

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Outline

- Introduction
- Mathematical preliminary
- Numerical methods
  - Discretization
  - Numerical quadratures
  - Fast algorithms
- Numerical examples

Setting

Solving linear BVPs:

$$\begin{aligned} Lu &= 0, \ \textit{in } \Omega \\ u &= g, \ \textit{on } \Gamma := \partial\Omega, \end{aligned}$$

- L is a 2^{nd} order diff. op. (elliptic/parabolic).
- $\Omega \in \mathbb{R}^d$ ($d = 2, 3$) can be interior or exterior (decay conditions at ∞ for the exterior case).
- Other boundary conditions: $\partial u / \partial \boldsymbol{n} = g$, or mix.

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- Other boundary conditions: $\partial u / \partial \boldsymbol{n} = g$, or mix.
- For simplicity, consider $\Delta u = 0$.

Mathematical preliminary: potential theory

Review: PDE I

Definition (fundamental solution)

The function

$$G(\boldsymbol{x}, \boldsymbol{y}) = \begin{cases} \frac{1}{2\pi} \ln \frac{1}{|\boldsymbol{x}-\boldsymbol{y}|}, & d = 2 \\ \frac{1}{4\pi} \frac{1}{|\boldsymbol{x}-\boldsymbol{y}|}, & d = 3 \end{cases}$$

is called the fundamental solution of Laplace's equation. For fixed $\boldsymbol{y} \in \mathbb{R}^d$ it is harmonic in $\mathbb{R}^d \backslash \{\boldsymbol{y}\}$.

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Theorem (Green's identity)

Let Ω be a bounded domain of class C^1, and let $u \in C^2(\Omega) \cap C^1(\overline{\Omega})$ satisfy $\Delta u = 0$. Then u satisfies

$$u(x) = \int_\Gamma G(\boldsymbol{x}, \boldsymbol{y}) \frac{\partial u(\boldsymbol{y})}{\partial \boldsymbol{n}} ds_{\boldsymbol{y}} - \int_\Gamma \frac{\partial}{\partial \boldsymbol{n}_{\boldsymbol{y}}} G(\boldsymbol{x}, \boldsymbol{y}) u(\boldsymbol{y}) ds_{\boldsymbol{y}} \,,$$

where $\Gamma = \partial\Omega$ is the boundary of Ω, and $\boldsymbol{x} \in \Omega$.

Review: PDE I

Definition (layer potentials)

The integral operators

$$\mathcal{S}[\sigma] := \int_\Gamma G(\boldsymbol{x}, \boldsymbol{y})\sigma(\boldsymbol{y})ds_{\boldsymbol{y}}$$

$$\mathcal{D}[\mu] := \int_\Gamma \frac{\partial}{\partial \boldsymbol{n}_{\boldsymbol{y}}} G(\boldsymbol{x}, \boldsymbol{y})\mu(\boldsymbol{y})ds_{\boldsymbol{y}}$$

are called a single layer potential and a double layer potential respectively.

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are called a single layer potential and a double layer potential respectively.

Green's identity:

$$u(\boldsymbol{x}) = \mathcal{S}[\frac{\partial u}{\boldsymbol{n}}] - \mathcal{D}[u]. \ \boldsymbol{x} \in \Omega$$

Potential theory

Theorem (the jump relation)

Let Γ be of class C^2 and $\sigma \in C(\Gamma)$. Then the single layer potential $u = \mathcal{S}[\sigma]$ is continuous throughout $\mathbb{R}^d$. It satisfies $\Delta u = 0$ for $\boldsymbol{x} \notin \Gamma$. On the boundary there holds:

$$\lim_{\substack{\boldsymbol{x} \to \boldsymbol{x}_0 \in \Gamma \\ \boldsymbol{x} \in \Omega}} \frac{\partial u(\boldsymbol{x})}{\partial \boldsymbol{n}} = \frac{1}{2}\sigma(\boldsymbol{x}_0) + \frac{\partial}{\partial \boldsymbol{n}} \mathcal{S}[\sigma](\boldsymbol{x}_0)$$

$$\lim_{\substack{\boldsymbol{x} \to \boldsymbol{x}_0 \in \Gamma \\ \boldsymbol{x} \notin \Omega}} \frac{\partial u(\boldsymbol{x})}{\partial \boldsymbol{n}} = -\frac{1}{2}\sigma(\boldsymbol{x}_0) + \frac{\partial}{\partial \boldsymbol{n}} \mathcal{S}[\sigma](\boldsymbol{x}_0)$$

Potential theory

Theorem (the jump relation)

Let Γ be of class C^2 and $\mu \in C(\Gamma)$. Then the double layer potential $v = \mathcal{D}[\mu]$ satisfies $\Delta v = 0$ for $\boldsymbol{x} \notin \Gamma$, and can be continuously extended to the boundary from the interior or the exterior, with limiting values

$$\lim_{\substack{\boldsymbol{x}\to\boldsymbol{x}_0\in\Gamma \\ \boldsymbol{x}\in\Omega}} v(\boldsymbol{x}) = -\frac{1}{2}\mu(\boldsymbol{x}_0) + \mathcal{D}[\mu](\boldsymbol{x}_0)$$

$$\lim_{\substack{\boldsymbol{x}\to\boldsymbol{x}_0\in\Gamma \\ \boldsymbol{x}\notin\Omega}} v(\boldsymbol{x}) = \frac{1}{2}\mu(\boldsymbol{x}_0) + \mathcal{D}[\mu](\boldsymbol{x}_0).$$

Boundary integral equation (BIE)

Turning back to the Green's identity

$$u(\boldsymbol{x}) = \mathcal{S}[\frac{\partial u}{\boldsymbol{n}}] - \mathcal{D}[u] \quad (if\ \Delta u = 0\ in\ \Omega),$$

letting $\boldsymbol{x} \to \Gamma$, we obtain (e.g. for the interior Dirichlet problem)

$$\mathcal{S}[\sigma] = \frac{1}{2}g(\boldsymbol{x}) + \mathcal{D}[g].$$

- An integral equation (first kind Fredholm) for the unkown density function σ.
- Once σ is obtained, the solution can be recovered by

$$u(\boldsymbol{x}) = \mathcal{S}[\sigma] - \mathcal{D}[g].$$

- Unkowns on the boundary only.

Boundary integral equation (BIE)

Alternatively, we seek solution of the form $u(\boldsymbol{x}) = \mathcal{D}[\mu]$, where μ is an unkown density function supported on the boundary. $u(\boldsymbol{x})$ satisfies $\Delta u = 0$ automatically for $\boldsymbol{x} \in \Omega$. It only remains to enforce the boundary condition. Letting $\boldsymbol{x} \to \Gamma$, we obtain (e.g. for the interior Dirichlet problem)

$$-\frac{1}{2}\mu + \mathcal{D}[\mu] = g.$$

- An integral equation (second kind Fredholm) for the unkown density function μ, well conditioned. $Cond(\mathcal{P}) = ||\mathcal{P}|| \cdot ||\mathcal{P}^{-1}||$.
- Once μ is obtained, the solution can be recovered by

$$u(\boldsymbol{x}) = \mathcal{D}[\mu].$$

- Unkowns on the boundary only.

Numerical methods

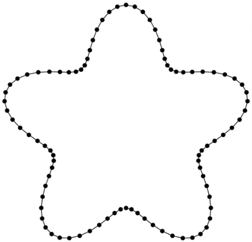
Discretization of the BIE

Consider the BIE

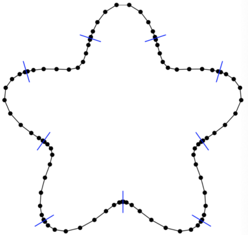
$$(I + \mathcal{K})\sigma = f,$$

where $\mathcal{K}\sigma = \int_\Gamma K(\boldsymbol{x}, \boldsymbol{y})\sigma ds_{\boldsymbol{y}}$, K is weakly singular when $\boldsymbol{x} = \boldsymbol{y}$.
Task I: representation of Γ

- global (simple smooth geoms)
- local (adaptive and/or CAD geoms)



peri. trap. rule



G-L panels

Discretization of the BIE

Three types of discretization

- Nyström: replace the integral by quadrature and impose the BIE at nodes (points$\rightarrow$ points)

$$\sigma_i + \sum_j w_j K(\boldsymbol{x}_i, \boldsymbol{x}_j)\sigma_j = f(\boldsymbol{x}_i)$$

- Galerkin: project into basis: $\sigma = \sum_{m=1}^{N} \alpha_m \varphi_m$ (basis $\rightarrow$ basis)

$$\sum_{n=1}^{N} [(\varphi_m, \varphi_n) + (\varphi_m, \mathcal{K}\varphi_n)]\alpha_n = (\varphi_m, f)$$

- Collocation: project σ into basis, impose the BIE at nodes (basis $\rightarrow$ points).

$$\sum_{n=1}^{N} (\varphi_n(\boldsymbol{x}_m) + \mathcal{K}\varphi_n(\boldsymbol{x}_m))\alpha_n = f(\boldsymbol{x}_m).$$

At the same order, accuracy basically the same. Nyström is the simplest to implement, and is naturally compatible with fast algorithms.

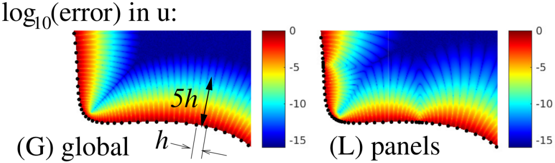
Quadrature tasks and challenges

Consider Nyström: $\sigma_i + (\mathcal{K}\sigma)(\boldsymbol{x}_i) = f_i$.

- Begin with a smooth ("native") quadrature rule

$$\int_\Gamma g(\boldsymbol{x}) ds_{\boldsymbol{x}} = \sum_{j=1}^{N} w_j g(\boldsymbol{x}_j). \quad g \in C^\infty(\Gamma)$$

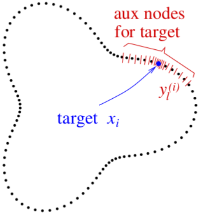
- Challenge 1: filling in the matrix. i.e. approx $\mathcal{K}\sigma(\boldsymbol{x}_i)$ on surface Γ. weak singularity of $K(\boldsymbol{x}, \boldsymbol{y})$ when $\boldsymbol{x} = \boldsymbol{y}$.
- Challenge 2: recovering the solution. i.e. approx $\mathcal{K}\sigma(\boldsymbol{x})$ off surface Γ.



Exponential in N, but rate depends on target x (Barnett '14)

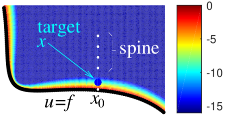
Quadrature: ideas

- on-surface (Review in 2D:(Hao–Barnett–Martinsson–Young '14)) auxiliary nodes, (analytic) complex Cauchy integrals, etc.

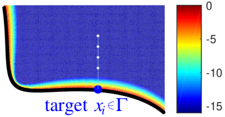


- off-surface: QBX, hedgehog, etc.

Interpolate for close eval:



Can also extrapolate for Nyström surf quadr:



Fast algorithms

Discretization of $(I + \mathcal{K})\sigma = f$ leades to a dense $N \times N$ linear system.

- Fast multipole methods (FMM) reduces the cost of applying $\mathcal{K}\sigma$ to $O(N)$.
  - (Greengard-Rokhlin '87; Greengard-Rokhlin '97; Cheng-Greengard-Rokhlin '99)
  - 3D FMM lib develeped at Flatiron: https://fmm3d.readthedocs.io
  - Combine with GMRES. Well conditioning $\Rightarrow O(1)$ iterations.
- Fast direct solvers.
  - Talk by Manas Rachh.
  - Suitable for: low rank perturbation of $\mathcal{K}$, multiple RHS, MFS, etc.

Numerical examples

Example 1: Inhomogeneous heat equation on a unit box with periodic boundary condition: automatic adaptivity

Numerical examples

Example 2: suspensions of rigid ellipses in shearing viscous flow

Summary

Integral equation methods have become powerful tools for the numerical solution of PDEs. They have the remarkable benefits:

- High accuracy
- Optimal/Near optimal complexity
- Ability to handle complex geometry
- Compatibility with automatic adaptivity

Requires a lot of machinery:

- Well conditioned integral formulation
- Efficient numerical quadratures
- Fast algorithms