2D boundary integral equations and the Nyström method

Alex Barnett[1] and **Fruzsina Agocs**[1]

Computational Tools 2024 BIE workshop. Day 1, 6/10/24

[1]Center for Computational Mathematics, Flatiron Institute, Simons Foundation

Integral equations on 1D interval

Given: i) function $\sigma(t)$ defined on interval $[0, 2\pi)$, periodic: $\sigma(2\pi) = \sigma(0)$, etc

ii) "kernel" function $k(t, s)$ defined on square $[0, 2\pi)^2$,

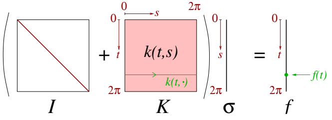
Integral *operator* K acts on σ to give another function $K\sigma$:

$$(K\sigma)(t) := \int_0^{2\pi} k(t,s)\sigma(s)ds, \quad t \in [0, 2\pi)$$

continuous analog of matrix-vector prod. $A\boldsymbol{x}$

Integral *equation*: $(I + K)\sigma = f$, ie

$$\sigma(t) + \int_0^{2\pi} k(t,s)\sigma(s)ds = f(t), \quad t \in [0, 2\pi)$$



analog of lin. sys. $A\boldsymbol{x} = \boldsymbol{b}$

Fredholm "second kind" (due to presence of I, otherwise called "first kind")

If kernel continuous, or "weakly" singular (integrable), K is *compact*:

- eigenvalues ($K\phi_k = \lambda_k\phi_k$) discrete, with $\lim_{k\to\infty}\lambda_k = 0$

  unless some $\lambda_k = -1$, 2nd kind IE has at most one soln: Nul $(I + K) = \{0\}$

- Nul $(I + K) = \{0\}$ $\Rightarrow$ *existence* of solution for *any* f Fredholm Alternative

  like square matrix (finite-dim), recall: uniqueness $\Rightarrow$ consistent for any RHS

Contrast 1st kind IE $K\sigma = f$ is ill-posed problem (unstable)!

See references for lots of beautiful theory, precise statements

Nyström discretization of 2nd kind IE on interval

Simplest quadrature for periodic funcs: periodic trapezoid rule (PTR)

$$\int_0^{2\pi} f(t)dt \approx \sum_{j=1}^{N} \frac{2\pi}{N} f\left(\frac{2\pi j}{N}\right) = \sum_{j=1}^{N} w_j f(t_j)$$ w_j=weights, t_j=nodes

For f smooth, superalgebraically convergent ("spectral"): error $= \mathcal{O}(N^{-p})$ for any p

Apply quad to integral in 2nd kind IE: call the resulting approx soln $\tilde{\sigma}$

$$\tilde{\sigma}(t) + \sum_{j=1}^{N} k(t,t_j) w_j \tilde{\sigma}(t_j) = f(t), \quad t \in [0, 2\pi) \qquad (*)$$

Holds for all t; in particular, holds at each t_i, $i = 1, \ldots, N$, giving:

$$\sigma_i + \sum_{j=1}^{N} k(t_i,t_j) w_j \sigma_j = f(t_i), \quad i = 1, \ldots, N$$ where $\sigma_j := \tilde{\sigma}(t_j)$

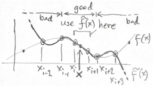
Write as: $A\boldsymbol{\sigma} = \boldsymbol{f}$ $\quad N \times N$ lin sys, entries $a_{ij} = \delta_{ij} + k(t_i,t_j)w_j$, and $f_j := f(t_j)$

solve? dense direct $\mathcal{O}(N^3)$; dense iter. $\mathcal{O}(N^2)$; fast iter. $\approx \mathcal{O}(N)$; fast direct $\approx \mathcal{O}(N^{(d+1)/2})$

Why 2nd kind? eigs(A) accumulate only at $+1$, iterative fast conv.

Sometimes for BIE (eg, far-field eval), node values $\{\sigma_j\}_{j=1}^N$ suffice.
If not, interpolate from them to any $t \in [0, 2\pi)$. Two approaches:

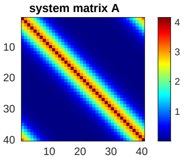
- either: rearrange (*) to give $\tilde{\sigma}(t) = \ldots$, called "Nyström interpolant" (rare)
- or (common): use local high-order Lagrange (or global spectral) interpolation:

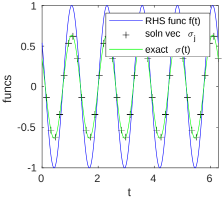


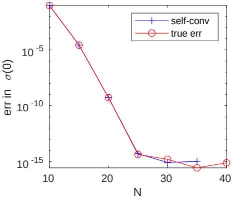
Demo Nyström on interval (1D)

day1/code/nyst1d_demos.m

```
kfun = @(s,t) exp(3*cos(t-s));                  % smooth convolutional kernel, periodic domain [0,2pi)
ffun = @(t) cos(5*t+1);                         % smooth data (RHS) func
N = 30;                                         % number of unknowns: should study convergence as N grows...
tj = 2*pi/N*(1:N); wj = 2*pi/N*ones(1,N);       % PTR nodes and weights, row vecs
A = eye(N) + bsxfun(kfun,tj',tj)*diag(wj);      % identity plus fill k(t_i,t_j)w_j for i,j=1..N
rhs = ffun(tj');                                % col vec
sigmaj = A\rhs;                                 % dense direct square solve (pivoted LU), gives col vec
```







"self-convergence": use N=40 as "true"

f and k smooth

$\Rightarrow$ σ smooth

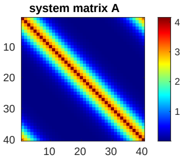
$\Rightarrow$ spectral conv?

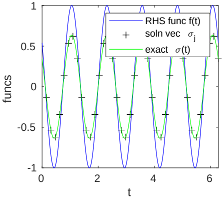
Thm. (Anselone, Kress,...): error at node values (and Nyström interpolant) same order as that of quadrature rule applied to integrand $k(t,\cdot)\sigma$.

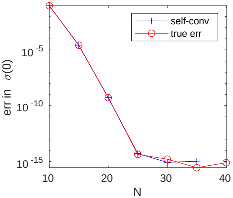
Demo Nyström on interval (1D)

day1/code/nyst1d_demos.m

```
kfun = @(s,t) exp(3*cos(t-s));               % smooth convolutional kernel, periodic domain [0,2pi)
ffun = @(t) cos(5*t+1);                       % smooth data (RHS) func
N = 30;                                       % number of unknowns: should study convergence as N grows...
tj = 2*pi/N*(1:N); wj = 2*pi/N*ones(1,N);     % PTR nodes and weights, row vecs
A = eye(N) + bsxfun(kfun,tj',tj)*diag(wj);    % identity plus fill k(t_i,t_j)w_j for i,j=1..N
rhs = ffun(tj');                              % col vec
sigmaj = A\rhs;                               % dense direct square solve (pivoted LU), gives col vec
```







"self-convergence": use $N{=}40$ as "true"

f and k smooth

$\Rightarrow$ σ smooth

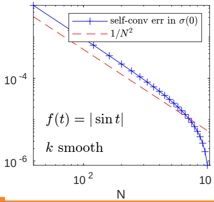
$\Rightarrow$ spectral conv?

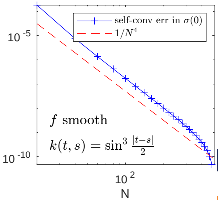
Thm. (Anselone, Kress,...): error at node values (and Nyström interpolant) same order as that of quadrature rule applied to integrand $k(t,\cdot)\sigma$.

- Then, f or k nonsmooth?

worse (here *algebraic*) convergence using plain PTR rule:

Qu: why does order appear to improve at end?





Fundamental solution in $\mathbb{R}^2$

Eg PDE: Poisson eqn $\Delta u = g$ $\quad$ $\Delta := (\partial/\partial x_1)^2 + (\partial/\partial x_2)^2$ Laplacian

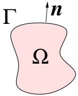
Notation: $\boldsymbol{x} := (x_1, x_2) \in \mathbb{R}^2$ is a point. This frees up $\boldsymbol{y} \in \mathbb{R}^2$ as another point (not y-coord!)

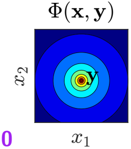
Not well-posed prob. unless add BC! BIEs are good for *homogeneous* PDEs (driving $g \equiv 0$)

Eg well-posed* BVP:

$$\Delta u = 0 \text{ in } \Omega \qquad \text{PDE (u harmonic)}$$
$$u = f \text{ on } \Gamma \qquad \text{Dirichlet BC}$$

*exists, unique, continuous w.r.t. data





Laplace fundamental soln: $\Phi(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{2\pi} \log \frac{1}{r}$ $\quad$ where $r := \|\boldsymbol{x} - \boldsymbol{y}\|$

obeys $-\Delta_{\boldsymbol{x}} \Phi = -\Delta_{\boldsymbol{y}} \Phi = \delta_{\boldsymbol{x}}$ $\quad$ Φ harmonic except unit point-mass at $\mathbf{0}$

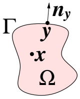
Normal $\boldsymbol{n}$ points outwards, $\|\boldsymbol{n}\| = 1$ $\quad$ normal deriv. notation $u_n := \boldsymbol{n} \cdot \nabla u$

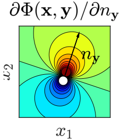
Green's 2nd identity: $\int_\Gamma v u_n - v_n u \, ds = \int_\Omega v \Delta u - (\Delta v) u \, d\boldsymbol{y}$ $\quad$ calculus

warm-up: set $u =$ BVP soln, $v \equiv 1$, G2I becomes $\int_\Gamma u_n ds \; - 0 = 0 - 0$: so u has zero *flux*
more fun: fix "target" $\boldsymbol{x} \in \Omega$, let $v = \Phi(\boldsymbol{x}, \cdot)$, G2I gives:

Green's representation formula:

$$\int_\Gamma \Phi(\boldsymbol{x}, \boldsymbol{y}) u_n(\boldsymbol{y}) - \frac{\partial \Phi(\boldsymbol{x}, \boldsymbol{y})}{\partial \boldsymbol{n}_{\boldsymbol{y}}} u(\boldsymbol{y}) \, ds_{\boldsymbol{y}} = u(\boldsymbol{x}) \qquad \text{for } \boldsymbol{x} \in \Omega$$



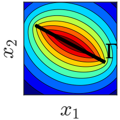


Gets soln from "Cauchy data" $(u, u_n)|_\Gamma$

also versions for Helmholtz, Stokes, Maxwell,...

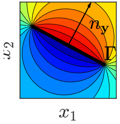
Layer potentials and their jump relations

Representations of harmonic functions off a curve Γ: "density" σ



Single-layer potential $(\mathcal{S}\sigma)(\boldsymbol{x}) := \int_\Gamma \Phi(\boldsymbol{x},\boldsymbol{y})\sigma(\boldsymbol{y})ds_{\boldsymbol{y}}$ charge sheet

Double-layer potential $(\mathcal{D}\sigma)(\boldsymbol{x}) := \int_\Gamma \frac{\partial\Phi(\boldsymbol{x},\boldsymbol{y})}{\partial \boldsymbol{n}_{\boldsymbol{y}}}\sigma(\boldsymbol{y})ds_{\boldsymbol{y}}$ dipole sheet



interior (-) / exterior (+) limits:

$$u^\pm(\boldsymbol{x}) := \lim_{h\to 0^+} u(\boldsymbol{x} \pm h\boldsymbol{n}_{\boldsymbol{x}})$$
$$u_n^\pm(\boldsymbol{x}) := \lim_{h\to 0^+} \boldsymbol{n}_{\boldsymbol{x}} \cdot \nabla u(\boldsymbol{x} \pm h\boldsymbol{n}_{\boldsymbol{x}})$$

Jump relations:

$(\mathcal{S}\sigma)^\pm = S\sigma$ — S (Roman font) means *restriction* of $\mathcal{S}$ to Γ: a bdry int. op.

$(\mathcal{D}\sigma)^\pm = (D \pm I/2)\sigma$ — jump in potential equal to σ; D restriction to Γ in P.V. sense

$(\mathcal{S}\sigma)_n^\pm = (D^T \mp I/2)\sigma$ — jump in normal derivative

$(\mathcal{D}\sigma)_n^\pm = T\sigma$ — T hypersingular, kernel $\partial^2\Phi(\boldsymbol{x},\boldsymbol{y})/\partial\boldsymbol{n}_{\boldsymbol{x}}\partial\boldsymbol{n}_{\boldsymbol{y}} \sim 1/r^2$

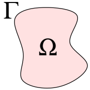
- D smooth kernel on smooth Γ, while S always log (weakly) singular

Recap GRF in LP notation: u harmonic in $\Omega \Rightarrow \mathcal{S}u_n^- - \mathcal{D}u^- = u$ in Ω

Converting BVP to BIE and solving

Say wish to solve interior Dirichlet Laplace BVP:

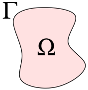
$$\Delta u = 0 \text{ in } \Omega \qquad \text{PDE}$$
$$u^- = f \text{ on } \Gamma \qquad \text{BC}$$



Converting BVP to BIE and solving

Say wish to solve interior Dirichlet Laplace BVP:

$$\Delta u = 0 \text{ in } \Omega \qquad \text{PDE}$$
$$u^- = f \text{ on } \Gamma \qquad \text{BC}$$

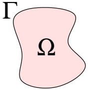


Pick **representation**: $u = \mathcal{D}\sigma$, look up its **JR** for BC: $u^- = (D - I/2)\sigma$

Converting BVP to BIE and solving

Say wish to solve interior Dirichlet Laplace BVP: $\Delta u = 0$ in Ω PDE

$u^- = f$ on Γ BC



Pick **representation**: $u = \mathcal{D}\sigma$, look up its **JR** for BC: $u^- = (D - I/2)\sigma$

Insert the BC to get BIE: $$(I - 2D)\sigma = -2f$$ scaled to 2nd kind form

This shows: let σ solve BIE, then $u = \mathcal{D}\sigma$ solves BVP (i.e., no spurious solns)

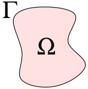
But how know *all* solns u of this form?

Converting BVP to BIE and solving

Say wish to solve interior Dirichlet Laplace BVP:

$\Delta u = 0$ in Ω PDE

$u^- = f$ on Γ BC



Pick **representation**: $u = \mathcal{D}\sigma$, look up its **JR** for BC: $u^- = (D - I/2)\sigma$

Insert the BC to get BIE: $(I - 2D)\sigma = -2f$ scaled to 2nd kind form

This shows: let σ solve BIE, then $u = \mathcal{D}\sigma$ solves BVP (i.e., no spurious solns)

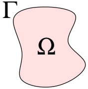
But how know *all* solns u of this form? Fred. Alt.: BIE *has* soln $\forall f$! BVP & BIE equivalent ☺

(had we picked $u = \mathcal{S}\sigma$, would get 1st kind, poorly conditioned but can have its uses)

Converting BVP to BIE and solving

Say wish to solve interior Dirichlet Laplace BVP: $\Delta u = 0$ in Ω PDE

$u^- = f$ on Γ BC



Pick **representation**: $u = \mathcal{D}\sigma$, look up its **JR** for BC: $u^- = (D - I/2)\sigma$

Insert the BC to get BIE: $(I - 2D)\sigma = -2f$ scaled to 2nd kind form

This shows: let σ solve BIE, then $u = \mathcal{D}\sigma$ solves BVP (i.e., no spurious solns)

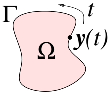
But how know *all* solns u of this form? Fred. Alt.: BIE *has* soln $\forall f$! BVP & BIE equivalent ☺

(had we picked $u = \mathcal{S}\sigma$, would get 1st kind, poorly conditioned but can have its uses)

Above BIE expressed on Γ using arc-length measure ds. Usually not how Γ described...

Converting BVP to BIE and solving

Say wish to solve interior Dirichlet Laplace BVP: $\Delta u = 0$ in Ω PDE
$u^- = f$ on Γ BC



Pick **representation**: $u = \mathcal{D}\sigma$, look up its **JR** for BC: $u^- = (D - I/2)\sigma$

Insert the BC to get BIE: $(I - 2D)\sigma = -2f$ scaled to 2nd kind form

This shows: let σ solve BIE, then $u = \mathcal{D}\sigma$ solves BVP (i.e., no spurious solns)

But how know *all* solns u of this form? Fred. Alt.: BIE *has* soln $\forall f$! BVP & BIE equivalent ☺

(had we picked $u = \mathcal{S}\sigma$, would get 1st kind, poorly conditioned but can have its uses)

Above BIE expressed on Γ using arc-length measure ds. Usually not how Γ described...

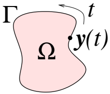
Parameterize the bdry $\boldsymbol{y}(t)$ $\boldsymbol{y} : \mathbb{R} \to \mathbb{R}^2$, 2π-periodic, $\Gamma = \{\boldsymbol{y}(t) : t \in [0, 2\pi)\}$

change variable $ds_{\boldsymbol{y}} = \|\boldsymbol{y}'(t)\| dt$ abuse notation $\sigma(t) = \sigma(\boldsymbol{y}(t))$

Converting BVP to BIE and solving

Say wish to solve interior Dirichlet Laplace BVP: $\Delta u = 0$ in Ω PDE

$u^- = f$ on Γ BC



Pick **representation**: $u = \mathcal{D}\sigma$, look up its **JR** for BC: $u^- = (D - I/2)\sigma$

Insert the BC to get BIE: $(I - 2D)\sigma = -2f$ scaled to 2nd kind form

This shows: let σ solve BIE, then $u = \mathcal{D}\sigma$ solves BVP (i.e., no spurious solns)

But how know *all* solns u of this form? Fred. Alt.: BIE *has* soln $\forall f$! BVP & BIE equivalent ☺

(had we picked $u = \mathcal{S}\sigma$, would get 1st kind, poorly conditioned but can have its uses)

Above BIE expressed on Γ using arc-length measure ds. Usually not how Γ described...

Parameterize the bdry $\boldsymbol{y}(t)$ $\boldsymbol{y} : \mathbb{R} \to \mathbb{R}^2$, 2π-periodic, $\Gamma = \{\boldsymbol{y}(t) : t \in [0, 2\pi)\}$

change variable $ds_{\boldsymbol{y}} = \|\boldsymbol{y}'(t)\| dt$ abuse notation $\sigma(t) = \sigma(\boldsymbol{y}(t))$

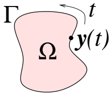
Get 1D IE: $\sigma(t) - 2\int_0^{2\pi} \frac{\partial \Phi(\boldsymbol{y}(t), \boldsymbol{y}(s))}{\partial \boldsymbol{n}_{\boldsymbol{y}(s)}} \sigma(s) \|\boldsymbol{y}'(s)\| ds = -2f(t), \quad t \in [0, 2\pi)$

familiar form $(I + K)\sigma = -2f$, with kernel $k(s,t) = \frac{-2}{2\pi} \frac{\boldsymbol{n}_{\boldsymbol{y}(s)} \cdot (\boldsymbol{y}(t) - \boldsymbol{y}(s))}{\|\boldsymbol{y}(t) - \boldsymbol{y}(s)\|^2} \|\boldsymbol{y}'(s)\|$

formula on diagonal: $k(t,t) = \lim_{s \to t} k(t,s) = \kappa(t)/2\pi$, κ curvature of Γ (check!)

Converting BVP to BIE and solving

Say wish to solve interior Dirichlet Laplace BVP: $\Delta u = 0$ in Ω PDE
$u^- = f$ on Γ BC



Pick **representation**: $u = \mathcal{D}\sigma$, look up its **JR** for BC: $u^- = (D - I/2)\sigma$

Insert the BC to get BIE: $(I - 2D)\sigma = -2f$ scaled to 2nd kind form

This shows: let σ solve BIE, then $u = \mathcal{D}\sigma$ solves BVP (i.e., no spurious solns)

But how know *all* solns u of this form? Fred. Alt.: BIE *has* soln $\forall f$! BVP & BIE equivalent ☺

(had we picked $u = \mathcal{S}\sigma$, would get 1st kind, poorly conditioned but can have its uses)

Above BIE expressed on Γ using arc-length measure ds. Usually not how Γ described...

Parameterize the bdry $\boldsymbol{y}(t)$ $\boldsymbol{y} : \mathbb{R} \to \mathbb{R}^2$, 2π-periodic, $\Gamma = \{\boldsymbol{y}(t) : t \in [0, 2\pi)\}$

change variable $ds_{\boldsymbol{y}} = \|\boldsymbol{y}'(t)\|dt$ abuse notation $\sigma(t) = \sigma(\boldsymbol{y}(t))$

Get 1D IE: $\sigma(t) - 2\int_0^{2\pi} \frac{\partial\Phi(\boldsymbol{y}(t),\boldsymbol{y}(s))}{\partial \boldsymbol{n}_{\boldsymbol{y}(s)}}\sigma(s)\|\boldsymbol{y}'(s)\|ds = -2f(t), \quad t \in [0, 2\pi)$

familiar form $(I + K)\sigma = -2f$, with kernel $k(s,t) = \frac{-2}{2\pi}\frac{\boldsymbol{n}_{\boldsymbol{y}(s)}\cdot(\boldsymbol{y}(t)-\boldsymbol{y}(s))}{\|\boldsymbol{y}(t)-\boldsymbol{y}(s)\|^2}\|\boldsymbol{y}'(s)\|$

formula on diagonal: $k(t,t) = \lim_{s\to t} k(t,s) = \kappa(t)/2\pi$, κ curvature of Γ (check!)

Now Nyström discretize with PTR, solve lin. sys. for $\boldsymbol{\sigma} := \{\sigma_j\}_{j=1}^N$

Finally evaluate soln: $u(\boldsymbol{x}) = (\mathcal{D}\sigma)(\boldsymbol{x}) \overset{\text{PTR}}{\approx} \sum_{j=1}^N \frac{\boldsymbol{n}_{\boldsymbol{y}(t_j)}\cdot(\boldsymbol{x}-\boldsymbol{y}(t_j))}{\|\boldsymbol{x}-\boldsymbol{y}(t_j)\|^2}\|\boldsymbol{y}'(t_j)\|w_j\sigma_j$

Testing your codes

Test GRF first for a known soln

Indirect vs direct formulations

Above was indirect: pick representation,
Table: direct vs indirect pros/cons
we prefer indirect

Exterior Laplace

subtlety of decay in 2D

mixed rep

Helmholtz

$(\Delta + \kappa^2)u = 0$ arises from scalar wave equation $u_{tt} - \Delta u = 0$
κ "wavenumber"; wavelength $\lambda = 2\pi/\kappa$
Also used for 2D Maxwell (z-invar); TE vs TM

Recap

TO DO

Several steps: write out yourself + try HW exercises in repo

-
- Nyström discretization gets $\sigma(t_j)$ interpolate from them to other t
- Fancier quadratures needed for singular kernels and/or close eval
- Nyström is not the only discr. meth: Galerkin, collocation. but: simplest and no less accurate

Resources

Many numerical analysis (mathematical flavor), particularly:

- *Linear Integral Equations*, R. Kress, (1999, Springer). Ch. 6 & 12.
- *The Numerical Solution of Integral Equations of the Second Kind*, K. E. Atkinson, (1997, CUP).

Fewer on the practical/tutorial side:

- "High-order accurate methods for Nyström discretization of integral equations on smooth curves in the plane", S Hao, AH Barnett, PG Martinsson, P Young. *Adv. Comput. Math.* **40**, 245–272 (2014).

  goes beyond these slides for logarithmic singularities, eg SLP

- `https://users.flatironinstitute.org/~ahb/BIE/`
- `https://github.com/ahbarnett/BIEbook` in progress...