Discretization of integral equations

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Overview

Introduction

Goal: Convert boundary integral equation (BIE) into a discrete equation

$$\int_\Gamma k(\mathbf{x},\mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y}) = f(\mathbf{x}), \mathbf{x}\in\Gamma \Rightarrow \mathbf{A}\boldsymbol{\sigma} = \mathbf{f}$$

Central task: How to numerically evaluate an integral such as

$$u(\mathbf{x}) = \int_\Gamma k(\mathbf{x},\mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y})$$

while most of the kernel functions $k(\mathbf{x},\mathbf{y})$ have singularities as $\mathbf{y}\to\mathbf{x}$

Parameterization of curves

Suppose our contour Γ can be parameterized using a piecewise smooth periodic function

$$\mathbf{G} : I \to \mathbb{R}^2$$

In other words, $\Gamma = \{\mathbf{G}(t) : t \in I\}$, then the BIE can be written as

$$u(\mathbf{x}) = \int_I k(\mathbf{x}, \mathbf{G}(t))\sigma(\mathbf{G}(t))|\mathbf{G}'(t)|dt$$

Parameterization of curves

Example of the behavior of the function $\phi(t) = k(\mathbf{x}, \mathbf{G}(t))|\mathbf{G}'(t)|$:

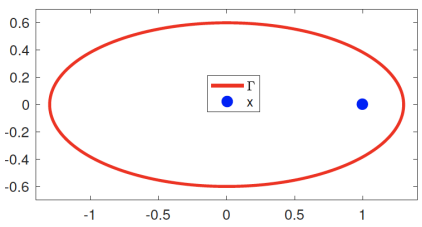
- The single-layer kernel: $k_1(\mathbf{x}, \mathbf{y}) = -\frac{1}{2\pi} \log |\mathbf{x} - \mathbf{y}|$
- The double-layer kernel: $k_2(\mathbf{x}, \mathbf{y}) = \frac{(\mathbf{x}-\mathbf{y})\cdot\mathbf{n}(\mathbf{y})}{2\pi|\mathbf{x}-\mathbf{y}|^2}$

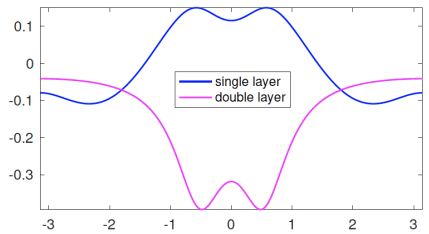
Remark: the double-layer kernel happens to be smooth when the contour is smooth.

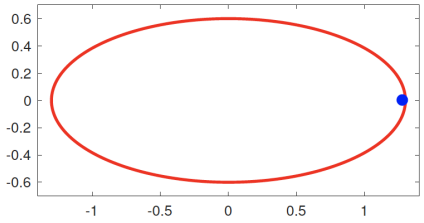
$$\mathbf{G}(t) = (G_1(t), G_2(t))$$

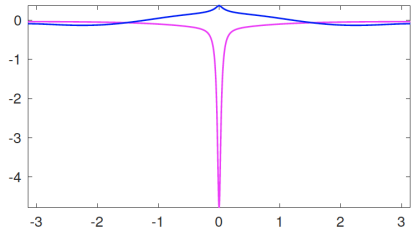
$$\lim_{t' \to t} k_2(\mathbf{G}(t), \mathbf{G}(t')) = \frac{G_2'(t)G_1''(t) - G_1'(t)G_2''(t)}{4\pi|\mathbf{G}'(t)|^3}$$

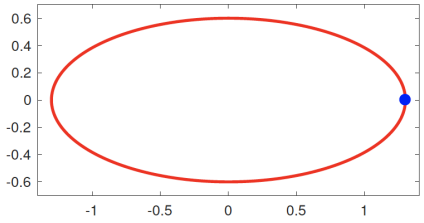
Parameterization of curves

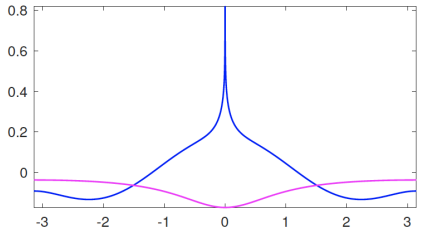


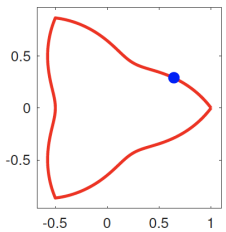


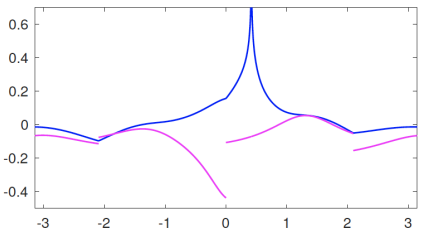












The trapezoidal rule

Suppose $\mathbf{G} : [0, T] \to \mathbb{R}^2$, $\Gamma = \{\mathbf{G}(t) : t \in [0, T]\}$
Given a positive integer N, pick N equispaced nodes $\{t_i\}_{i=1}^{N} \in [0, T]$, where $t_i = ih$ for $h = T/N$. Then apply the trapezoidal rule to parameterized BIE to obtain the approximation:

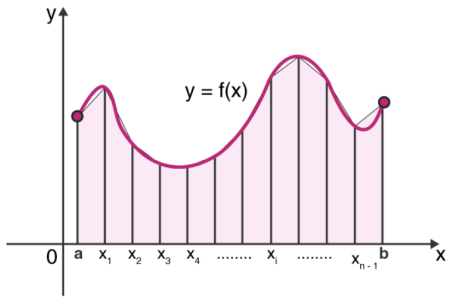
$$u(\mathbf{x}) \approx h \sum_{i=1}^{N} k(\mathbf{x}, \mathbf{G}(t_i))\sigma(\mathbf{G}(t_i))|\mathbf{G}'(t_i)|$$

Notice that since the integrand is periodic, all nodes have the same quadrature weight h

The trapezoidal rule

$$\text{Set } x_i = \mathbf{G}(t_i) \ , \ \omega_i = h|\mathbf{G}'(t_i)|$$

$$\Rightarrow u(\mathbf{x}) \approx \sum_{i=1}^{N} k(\mathbf{x}, \mathbf{x}_i)\sigma(\mathbf{x}_i)\omega_i$$



- When $x \notin \Gamma$, $u(\mathbf{x})$ is C^∞ periodic, so the error of the trapezoidal rule is $o(N^{-p})$ for any positive integer p. In fact, $|error| \leq \frac{2\pi M}{e^{aN}-1}$
- When $x \in \Gamma$, the double-layer kernel is still smooth, so the error converges superpolynomially fast to zero while a weakly singular (integrable singularity) kernel converges to zero slowly. For example, the singular kernel, with a logarithmic singularity, converges as $O(h \log(1/h))$

Panel-based quadrature rules

For a contour that is only piecewise smooth, it may lose smoothness at the corners. Then we need to split the contour Γ into disjoint pieces:

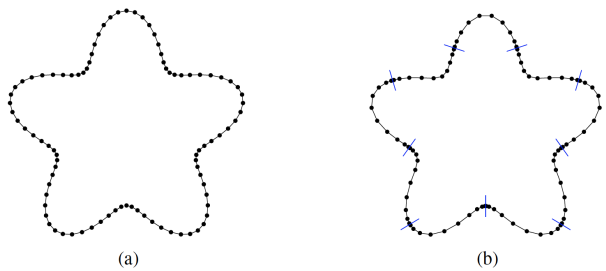
$$\Gamma = \Gamma_1 \cup \Gamma_2 \cup \cdots \cup \Gamma_m$$

For each Γ_j we introduce a local parameter map:

$$\mathbf{G}_j : [0, 1] \to \Gamma_j$$

$$\Rightarrow u(\mathbf{x}) = \sum_{j=1}^{m} \int_{\Gamma_j} k(\mathbf{x}, \mathbf{y}) \sigma(\mathbf{y}) ds(\mathbf{y}) = \sum_{j=1}^{m} \int_0^1 k(\mathbf{x}, \mathbf{G}_j(t)) \sigma(\mathbf{G}_j(t)) |\mathbf{G}_j'(t)| dt$$

Panel-based quadrature rules



When $\mathbf{x}$ is away from the contour, each integrand is smooth. By the Gauss–Legendre quadrature rule, if we place p Legendre nodes on [0,1], then the quadrature has $N = mp$ total points, which leads to the approximation

$$u(\mathbf{x}) \approx \sum_{i=1}^{N} k(\mathbf{x}, \mathbf{x}_i)\sigma(\mathbf{x}_i)\omega_i$$

For the above figure, the quadrature error goes to zero as $O((1/m)^{2p-1})$. Panel-based quadratures offer more flexibility than a global quadrature such as the trapezoidal rule. They also adapt much more easily to 3D problems.

Nyström discretization

Suppose we are given an BIE such as:

$$b\sigma(x) + \int_\Gamma k(\mathbf{x}, \mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y}) = f(\mathbf{x}), x \in \Gamma$$

Use an quadrature scheme on the domain Γ, defined by nodes $\{\mathbf{x}_i\}_{i=1}^N \subset \Gamma$ and corresponding weights $\{\omega_i\}_{i=1}^N$, to construct an linear system that relates a given data vector $\mathbf{f} = \{f_i\}_{i=1}^N$, where $f_i = f(\mathbf{x}_i)$, to an unknown solution vector $\boldsymbol{\sigma} = \{\sigma_i\}_{i=1}^N$, where $\sigma_i \approx \sigma(\mathbf{x}_i)$

$$b\sigma(\mathbf{x}_i) + \int_\Gamma k(\mathbf{x}_i, \mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y}) = f(\mathbf{x}_i), i = 1, 2, \cdots, N$$

Nyström discretization

For a smooth function σ on Γ, the matrix $\mathbf{A}$ is constructed such that,

$$\int_{\Gamma} k(\mathbf{x}_i, \mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y}) \approx \sum_{j=1}^{N} \mathbf{A}(i,j)\sigma(\mathbf{x}_j)$$

So we obtain a square linear system that relates $\boldsymbol{\sigma}$ to $\mathbf{f}$:

$$b\sigma_i + \sum_{j=1}^{N} \mathbf{A}(i,j)\sigma_j = f_i, i = 1, 2, \cdots, N$$

$$\Rightarrow b\boldsymbol{\sigma} + \mathbf{A}\boldsymbol{\sigma} = \mathbf{f}$$

Once $\boldsymbol{\sigma}$ has been found, $\sigma(\mathbf{x})$ for general $\mathbf{x} \in \Gamma$ may be constructed by interpolation through the vector $\boldsymbol{\sigma}$

Nyström discretization

For a smooth kernel k, such as the double-layer function, matrix $\mathbf{A}$ can be chosen via the quadrature scheme:

$$\mathbf{A}(i,j) = k(\mathbf{x}_i, \mathbf{x}_j)\omega_j$$

and the error converges to zero of the same rate as the quadrature scheme.

Domains with corners

Consider a contour that is only piecewise smooth, with the pieces joined together to form a corner, then the function σ will lack regularity at the corner.

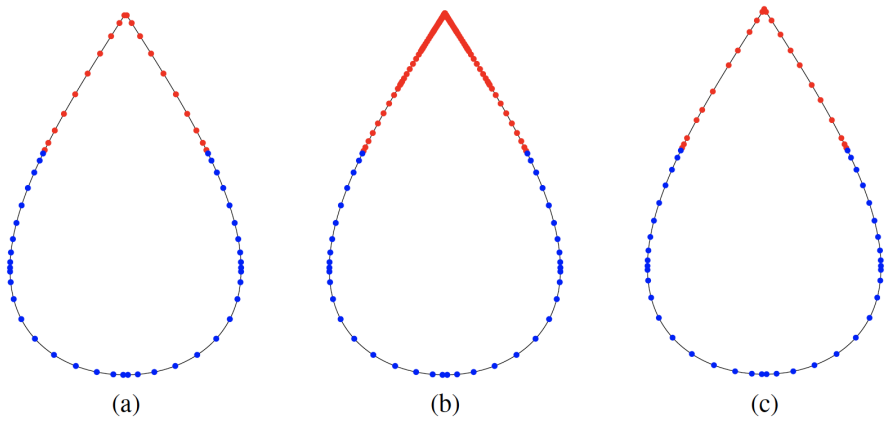


Figure 12.3. *A contour Γ with a corner.* (a) *The original Gaussian grid before refinement; red nodes are in Γ_1 and blue nodes are in Γ_2.* (b) *The locally refined grid.* (c) *The grid after local compression.*

Refinement: Partition $\Gamma = \Gamma_1 \cup \Gamma_2$ where Γ_1 is a small piece containing the corner. And then recursively cut the panel nearest the corner in half. Once the innermost panel is small enough that its contribution can be ignored, stop the refinement.

Weighted norms

1. Selection of nodes in Nyström discretization : accuracy of computing integral vs optimal collocation points.
2. With clusters of discretization points around singularities, is the discrete system as well conditioned as the continuous integral equation?

To solve BIE: Our paraphernalia - quadrature nodes $\{\mathbf{x}_i\}_{i=1}^N$, weights $\{w_i\}_{i=1}^N$ and $\int_\Gamma g(\mathbf{x})ds(\mathbf{x}) \approx \sum_{i=1}^N w_i g(\mathbf{x}_i)$ holds.

We associate for a given function g defined on Γ with a vector $\mathbf{g} \in \mathbb{R}^N$ as:

$$\mathbf{g}(i) = w_i^{\frac{1}{2}} g(\mathbf{x}_i)$$

Weighted norms

We observe:

$$||\mathbf{g}||_{l^2}^2 = \sum_{i=1}^{N} w_i |\mathbf{g}(\mathbf{x}_i)|^2 \approx \int_\Gamma |g(\mathbf{y})|^2 ds(\mathbf{y}) = ||g||_{L^2(\Gamma)}^2.$$

The idea: Weight the elements of the discretizing matrix $\mathbf{A}$ of our integral operator to get more faithful approximation.
Ex: As $\{$quadrature errors $\to 0\} \to \{$ spectral norm $\approx$ norm of op.$\}$

$$\mathbf{A}(i,j) = w_i^{1/2} k(\mathbf{x}_i, \mathbf{x}_j) w_j^{1/2}.$$

Weighted norms

If $\mathbf{f} = \mathbf{A}\mathbf{g}$ and $f(x) = \int_\Gamma k(\mathbf{x},\mathbf{y})g(\mathbf{y})ds(\mathbf{y})$, then:

$$
\begin{aligned}
||\mathbf{f}||_{l^2}^2 &= \sum_{i=1}^{N} w_i \Big(\sum_{j=1}^{N} k(\mathbf{x}_i, \mathbf{x}_j) w_j^{1/2} w_j^{1/2} \mathbf{g}(\mathbf{x}_j) \Big)^2 \\
&\approx \sum_{i=1}^{N} w_i \Big(\int_\Gamma k(\mathbf{x}_i, \mathbf{y}) g(\mathbf{y}) ds(\mathbf{y})) \Big)^2 \\
&= \sum_{i=1}^{N} w_i |f(\mathbf{x}_i)|^2 \approx ||f||_{L^2(\Gamma)}^2 .
\end{aligned}
$$

Modified trapezoidal quadrature rules for singular kernels

Evaluate accurately:

$$[K\sigma](\mathbf{x}) = \int_{\Gamma} k(\mathbf{x},\mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y}); x \in \Gamma$$

where, the kernel $k(\mathbf{x},\mathbf{y})$ is singular $|\mathbf{x}\text{-}\mathbf{y}| \to 0$.
The basic idea: Ex: take a smooth Γ, with a log singularity kernel: $k(\mathbf{x},\mathbf{y}) = \log|\mathbf{x}\text{-}\mathbf{y}|a(\mathbf{x},\mathbf{y}) + b(\mathbf{x},\mathbf{y})$, a and b are smooth and periodic. We have:

1. Equispaced nodes $\{\mathbf{x}_i\}_{i=1}^{N}$ in parameter domain $[0, T]$.
2. $\mathbf{x}_j = \mathbf{G}(t_j) = \mathbf{G}(jh)$
3. Grid spacing $h = T/N$ & $t_j = jh$ are the nodes in parameter space.

Modified trapezoidal quadrature rules for singular kernels

To evaluate:

$$I(f) = \int_0^T f(t)dt$$

where f has log singularity:

$$f(t) = \log\left(\sin\left(\frac{t\pi}{T}\right)\right)\phi(t) + \psi(t); t \in (0, T)$$

ϕ & ψ are smooth, periodic and we would need $\phi(0) = \phi(T) \& \phi'(0) = \phi'(T)$.... Now use trapezoidal rule:

$$I_N^{Trap}(f) = \sum_{j=1}^{N-1} hf(t_j)$$

Note: Error $|I_N^{Trap}(f) - I(f)|$ can't converge faster than $O(h)$

Modified trapezoidal quadrature rules for singular kernels

For higher accuracy, similar to boundary corrections in Gregory rules we amend say 4 weights, 2 on either sides. Here, Kapur and Rokhlin method (SIAM Journal on Numerical Analysis **34** (1997)), giving the choice of η_1 and η_2, let's us write:

$$I_N^{KR(2)}(f) = \eta_1 h(f(t_1) + f(T_{N-1})) + \eta_2 h(f(t_2) + f(T_{N-2})) + \underbrace{\sum_{j=1}^{N-1} hf(t_j)}_{= I_N^{Trap}(f)}$$

such that,

$$|I_N^{KR(2)}(f) - I(f)| = O(h^2) \to h \to 0$$

Modified trapezoidal quadrature rules for singular kernels

Higher order m-point K&R corrections:

$$I_N^{KR(m)}(f) = \underbrace{\sum_{j=1}^{m} \eta_j h(f(t_j) + f(t_{n-j}))}_{\text{correction terms}} + \underbrace{\sum_{j=1}^{N-1} hf(t_j)}_{= I_N^{Trap}(f)}$$

gives an accuracy of :

$$|I_N^{KR(m)}(f) - I(f)| = O(h^m) \to h \to 0$$

Note: K&R is slightly numerically unstable. η's alter in signs and grow larger with higher order corrections becomes ill-conditioned. Works well for $m \leq 6$ and not to be used for $m > 10$.

Modified trapezoidal quadrature rules for singular kernels

Now using K&R to the above integral equation, placing a node x_N at $t_N = T$:

$$[K\sigma](\mathbf{x}) = \int_\Gamma k(\mathbf{x},\mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y})$$

$$\approx \underbrace{\sum_{j=1}^{m} \eta_j h(k(x_N, \mathbf{G}(t_j))|\mathbf{G}'(t_j)|\sigma(\mathbf{x}_j) + k(x_N, \mathbf{G}(t_{N-j}))|\mathbf{G}'(t_{N-j})|\sigma(\mathbf{x}_{N-j}))+}_{\text{correction terms}}$$

$$+ \underbrace{\sum_{j=1}^{N-1} hk(x_N, \mathbf{G}(t_j))|\mathbf{G}'(t_j)|.}_{\text{Trap Rule}}$$

Modified trapezoidal quadrature rules for singular kernels

Now move the node to an interior point, i.e. $x_N \to x_j$, hence, $(t = 0) \to t_j$, equivalent transformation is $t' = t - t_j$ (A cyclic shift of quadrature weights.) Now take an $N \times N$ matrix $\mathbf{A}$ of Nyström discretization and apply K&R:

1. Diagonal elements set to 0 (blue).
2. m closest elements around the diagonal are modified (red).
3. Other elements remain un-modified (black).

If we define a "distance to the diagonal" as $l(i,j) = |mod(i-j, N)|$, where $mod(i-j, N)$ is an integer between $-N/2$ and $N/2$.

$$\mathbf{L} = \begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix}$$

Modified trapezoidal quadrature rules for singular kernels

$$\mathbf{A}(i,j) = \begin{cases} 0 & i = j \\ 1 + \eta_{l(i,j)} hk((\mathrm{x_i}, \mathrm{x_j}))|\mathrm{G}'(t_j)| & l(i,j) \in \{1, 2.., m\} \\ hk((\mathrm{x_i}, \mathrm{x_j}))|\mathrm{G}'(t_j)| & l(i,j) > m \end{cases}$$

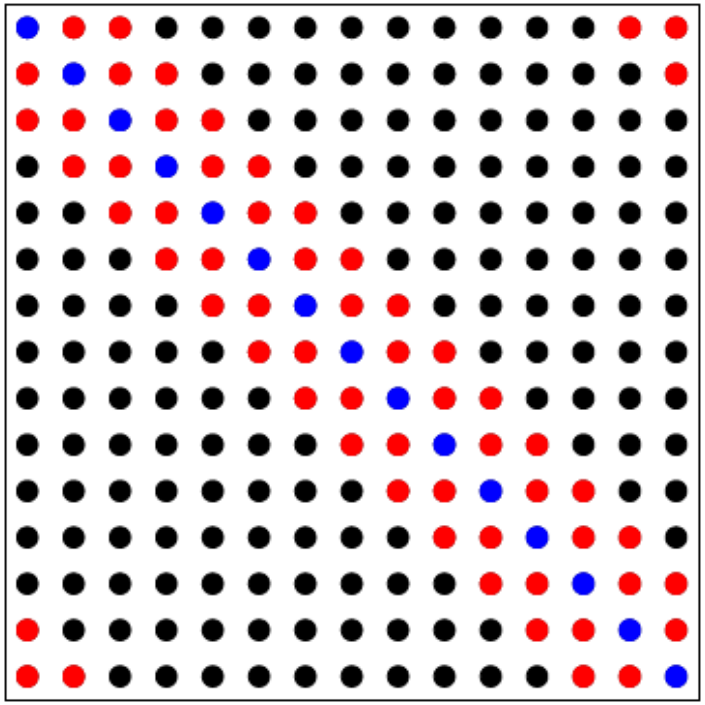


Figure: $N = 15$ and $m = 2$

Modified trapezoidal quadrature rules for singular kernels

K&R is numerically unstable for higher m. However once can look at **Alpert Quadrature method** (numerically more stable for higher m, than K&R):

$$I_N^{Alp}(f) = \underbrace{\sum_{j=1}^{m} \eta_j h(f(h\xi_j) + f(T - h\xi_j)}_{\text{correction terms}} + \underbrace{\sum_{j=1}^{N-1} hf(t_j)}_{= I_N^{Trap}(f)}$$

New nodes that $\{\xi_j\}_{j=1}^m \notin \{x_j\}_{j=1}^N$. Only k is singular but global σ is smooth. So these new nodes effect some local interpolation for higher accuracy. (S.Hao et al., Advances in Computational Mathematics **40** (2014), 245–272.)

Modified panel-based quadrature rules for singular kernels

Let us consider the standard BIE with a weakly singular kernel:

$$\alpha\sigma(\mathbf{x}) + \int_\Gamma k(\mathbf{x},\mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y}) = f(\mathbf{x}), x \in \Gamma$$

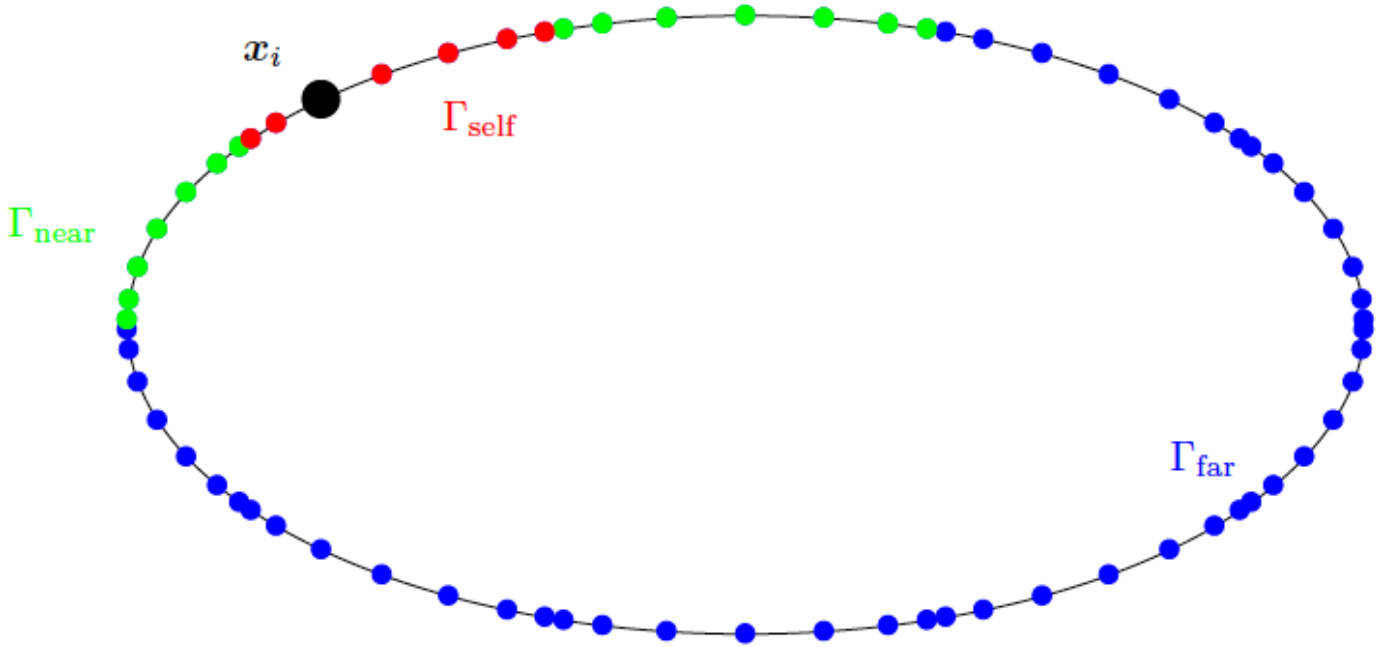
$k(\mathbf{x},\mathbf{y})$ is smooth except $x \neq y$ and $k(\mathbf{x},\mathbf{y}) \sim \log|\mathbf{x}-\mathbf{y}|$ as $\mathbf{y} \to \mathbf{x}$. Here, we use a panel based quadrature rule: We place p Gauss-Legendre nodes in a m panels, i.e $N = mp$. Now setting collocation points we get:

$$\alpha\sigma(\mathbf{x}_i) + \int_\Gamma k(\mathbf{x}_i,\mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y}) = f(\mathbf{x}_i), x \in \Gamma; i = 1,2,3...N$$

Our aim is to obtain an $N \times N$ matrix $\mathbf{A}$ such that:

$$\sum_{j=1}^{N} \mathbf{A}(i,j)\sigma(\mathbf{x}_j) \approx \int_\Gamma k(\mathbf{x}_i,\mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y})$$

Modified panel-based quadrature rules for singular kernels



Note: The solution to σ is smooth though k is not.
Now to determine elements of $\mathbf{A}$, first let us one index i and build the row $\mathbf{A}$(i, ;), i.e. evaluate integral op at $\mathbf{x} = \mathbf{x}_i$. For this we split contour into 3 parts:

$$\Gamma = \Gamma_{self} \cup \Gamma_{near} \cup \Gamma_{far}$$

Modified panel-based quadrature rules for singular kernels

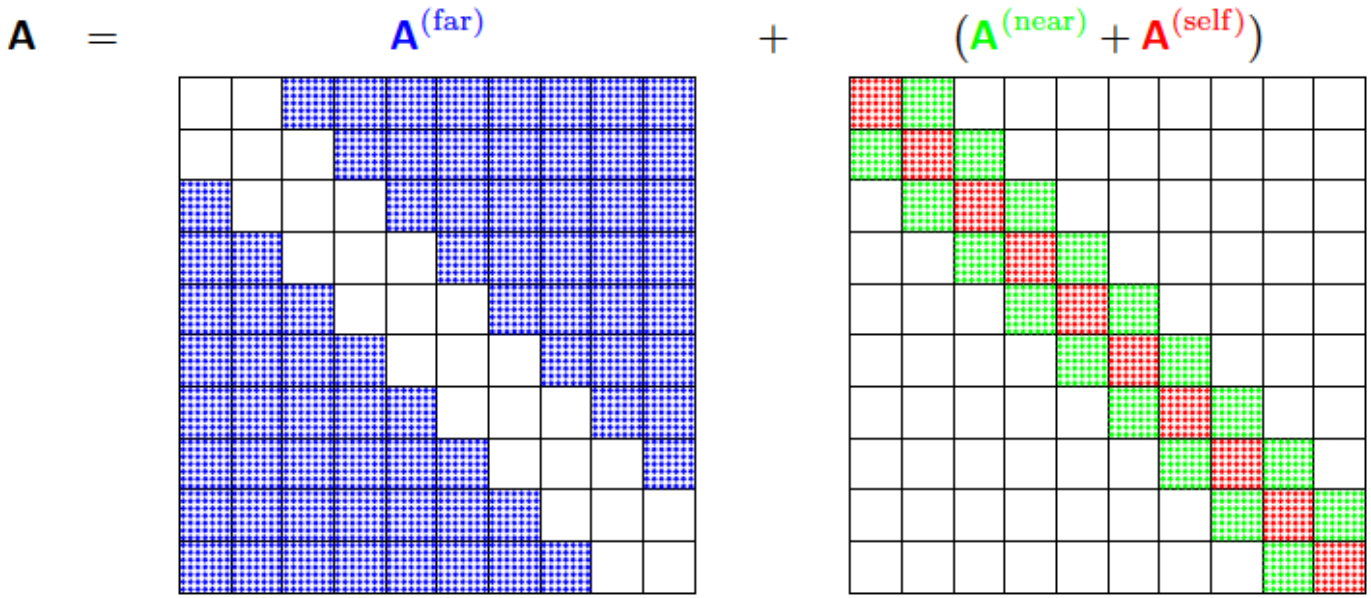
$$\int_{\Gamma} k(\mathbf{x}_i, \mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y}) = \int_{\Gamma_{self}} k(\mathbf{x}_i, \mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y}) + \\ + \int_{\Gamma_{near}} k(\mathbf{x}_i, \mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y}) + \int_{\Gamma_{far}} k(\mathbf{x}_i, \mathbf{y})\sigma(\mathbf{y})ds(\mathbf{y})$$

1. Γ_{far} : Integrand is smooth and matrix entries determined analytically by $\mathbf{A}(i,j) = k(\mathbf{x}_i, \mathbf{x}_j)w_j$.
2. Γ_{self} : Integrand has singularity within panel and matrix entries determined numerically.
3. Γ_{near} : Integrand is smooth but Gauss quadrature not accurate due to large derivative magnitudes, hence computed numerically.

Thus the matrix $\mathbf{A}$ is decomposed as:

$$\mathbf{A} = \mathbf{A}^{(far)} + \mathbf{A}^{(near)} + \mathbf{A}^{(self)}$$

Modified panel-based quadrature rules for singular kernels



To determine $\mathbf{A}^{(self)}$: We first choose a panel τ and then index it on domain and range as (I_τ, Γ_τ). We can find that and numerically estimate:

$$\mathbf{A}^{(self)}(i,j) = \int_0^1 k(\mathbf{x}_i, \mathbf{G}_\tau(t)) l_{j'}(t) |\mathbf{G}'_\tau(t))| dt$$

where $(i,j) \in I_\tau$, $\mathbf{G}_\tau$ is parameter with respect to Γ_τ and $l_{j'}$ is interpolating Legendre polynomial on $[0,1]$ around $\mathbf{x}_j$. We can use local refinement in each panel too. $\mathbf{A}^{(near)}$ is found analogously.

Extension to 3D

1. Though conceptually similar, extending from $\mathbb{R}^2 \to \mathbb{R}^3$ practically is harder.
2. Ex: Replace the domain $[0, 1]$ in panel based method to a triangular domain T, then use local maps $\mathbf{G}_j$ to make them curved triangles to wrap a surface $\Gamma \in \mathbb{R}^3$.
3. Such wraps may not be "watertight".
4. 3D will have far more points for a given discretization order than the $[0, 1]$ case.
5. Weakly singular easier than more singular kernels for $\mathbb{R}^3$ case. So usually one uses simple triangulations on surface with piecewise linear approximations, rather than higher order discretizations.

Extension to 3D

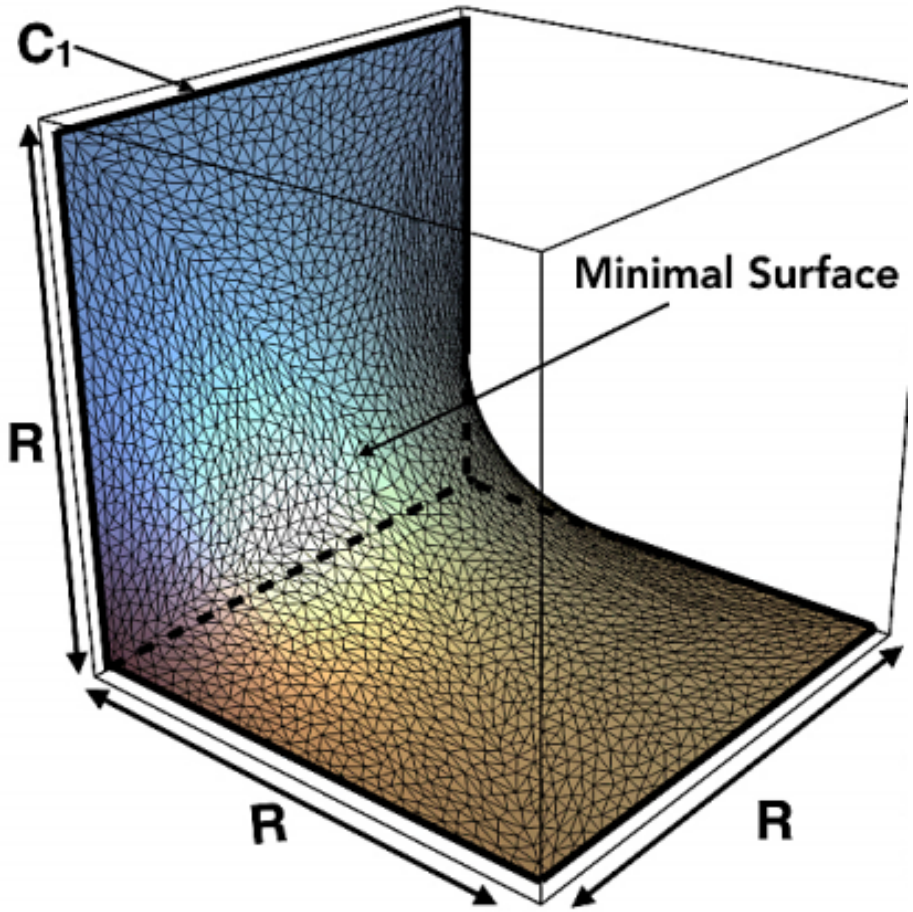


Figure: Minimal surface triangulation (**arXiv:2007.06723v1**)