M397C

Fast algorithms in scientific computing – theory & practice

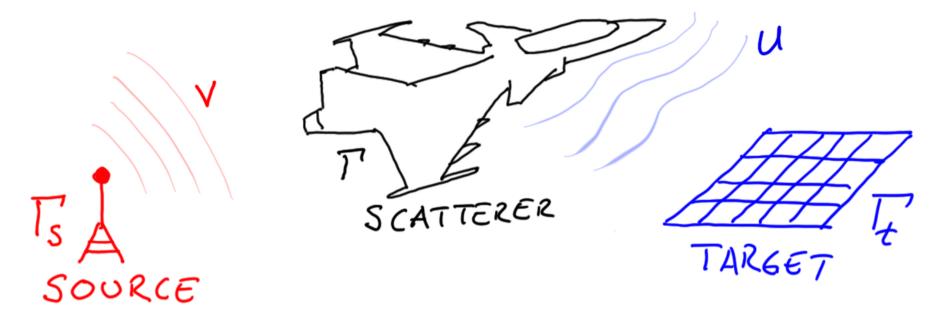
Lecture 26: Boundary Integral Equations

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Archetypical example — scattering off a finite body (here acoustic scattering):



The "sound-soft" acoustic scattering problem is to find a field *u* that satisfies

(1)
$$\begin{cases} -\Delta u(\mathbf{x}) - \kappa^2 u(\mathbf{x}) = 0 & \mathbf{x} \in \Omega^c, \\ u(\mathbf{x}) = -v(\mathbf{x}) & \mathbf{x} \in \Gamma, \\ \frac{\partial u(\mathbf{x})}{\partial |\mathbf{x}|} - i\kappa u(\mathbf{x}) = O(1/|\mathbf{x}|) & |\mathbf{x}| \to \infty, \end{cases}$$

given an "incoming field" v. One can show that (1) is "equivalent" to the equation

(2)
$$\frac{1}{2}\sigma(\boldsymbol{x}) + \int_{\Gamma} G_{\kappa}(\boldsymbol{x}, \boldsymbol{x}') \, \sigma(\boldsymbol{x}') \, dA(\boldsymbol{x}') = -v(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma.$$

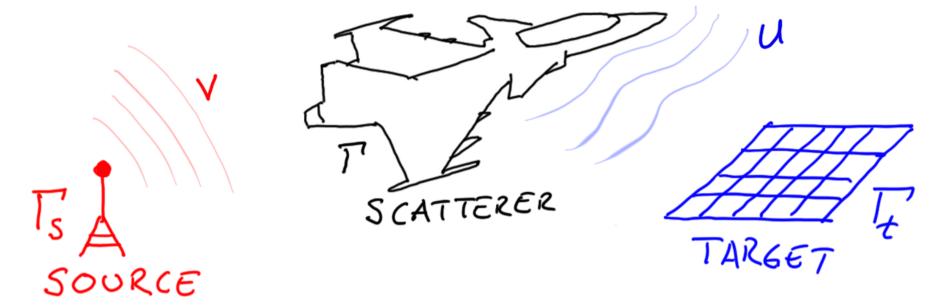
where

$$G_{\kappa}(\mathbf{x}, \mathbf{x}') = \frac{\partial \phi_{\kappa}(\mathbf{x}, \mathbf{x}')}{\partial \mathbf{n}(\mathbf{x}')} + i\kappa \,\phi_{\kappa}(\mathbf{x}, \mathbf{x}') \quad \text{and} \quad \phi_{\kappa}(\mathbf{x}, \mathbf{x}') = \frac{e^{i\kappa|\mathbf{x} - \mathbf{x}'|}}{4\pi|\mathbf{x} - \mathbf{x}'|}.$$

Obvious advantages of (2): Lower dimensionality, radiation condition satisfied exactly.

Obvious disadvantage of (2): *global* operator leads to *dense* linear system.

Archetypical example — scattering off a finite body (here acoustic scattering):



	PDE	Integral equation
Computational domain is:	infinite	finite
Computational domain is:	three dimensional	two dimensional
Radiation condition is satisfied:	approximately (hopefully)	exactly
Mathematical operator is:	unbounded	bounded (often 2 nd kind Fredholm)
Resulting linear system is:	sparse	dense

Example — **BIE for Laplace:** Consider our standard example of a BVP:

(3)
$$\begin{cases} -\Delta u(\boldsymbol{x}) = 0, & \boldsymbol{x} \in \Omega, \\ u(\boldsymbol{x}) = h(\boldsymbol{x}), & \boldsymbol{x} \in \Gamma. \end{cases}$$

Recall from the intro lecture that the exact solution operator takes the form

$$u(\mathbf{x}) = \int_{\Gamma} H(\mathbf{x}, \mathbf{y}) h(\mathbf{y}) dS(\mathbf{y}), \qquad \mathbf{x} \in \Omega,$$

where H is the *Green's function* of (3). For some simple domains, H is known analytically. For instance, if $\Omega = \{ \boldsymbol{x} \in \mathbb{R}^2 : |\boldsymbol{x}| \leq 1 \}$, then

$$H(r,\theta,\theta')=(2\pi)^{-1}\sum_{n=-\infty}^{\infty}r^{|n|}e^{in(\theta-\theta')}.$$

For a general domain, H is typically not known. We look for a solution of the form

(4)
$$u(\mathbf{x}) = \int_{\Gamma} \phi(\mathbf{x} - \mathbf{y}) \, \sigma(\mathbf{y}) \, d\mathbf{s}(\mathbf{y}).$$

Note that we now use a known kernel function — the free space fundamental solution $\phi(\mathbf{x} - \mathbf{y}) = -\frac{1}{2\pi} \log |\mathbf{x} - \mathbf{y}|$. The price we have to pay is that now the function σ is not known. But the boundary condition immediately provides an equation for σ — simply insert a point $\mathbf{x} \in \Gamma$ in (4):

(5)
$$h(\mathbf{x}) = \int_{\Gamma} \phi(\mathbf{x} - \mathbf{y}) \, \sigma(\mathbf{y}) \, d\mathbf{s}(\mathbf{y}), \qquad \mathbf{x} \in \Gamma.$$

(Note that a function of the form (4) satisfies $-\Delta u = 0$ for any σ .)

The PDE (3) and the BIE (5) are mathematical formulations of the same problem.

We can do better than merely achieving dimension reduction. Consider again the BVP

(6)
$$\begin{cases} -\Delta u(\boldsymbol{x}) = 0, & \boldsymbol{x} \in \Omega, \\ u(\boldsymbol{x}) = h(\boldsymbol{x}), & \boldsymbol{x} \in \Gamma. \end{cases}$$

Now look for a solution in the form of a double layer potential:

(7)
$$u(\mathbf{x}) = \int_{\Gamma} \frac{\mathbf{n}(\mathbf{y}) \cdot (\mathbf{x} - \mathbf{y})}{2\pi |\mathbf{x} - \mathbf{y}|^2} \, \sigma(\mathbf{y}) \, d\mathbf{s}(\mathbf{y}),$$

where n(y) is the unit length outwards pointing normal to Γ at $y \in \Gamma$.

The function u defined by (7) is discontinuous across Γ and for $\mathbf{x} \in \Gamma$ we get

(8)
$$\frac{1}{2}\sigma(\mathbf{x}) + \underbrace{\int_{\Gamma} \frac{\mathbf{n}(\mathbf{y}) \cdot (\mathbf{x} - \mathbf{y})}{2\pi |\mathbf{x} - \mathbf{y}|^2} \sigma(\mathbf{y}) \, d\mathbf{s}(\mathbf{y})}_{\text{Compact operator!}} = h(\mathbf{x}), \quad \mathbf{x} \in \Gamma.$$

The point here is that (8) is a *second kind Fredholm equation*.

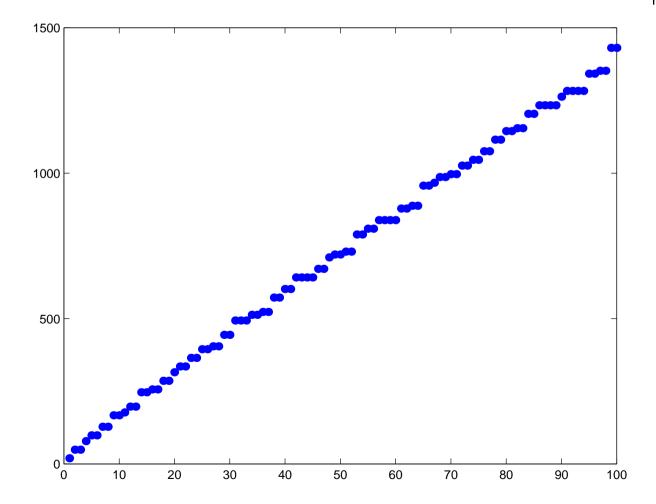
- Discretizing (8) leads to well-conditioned linear systems.
- Iterative solvers converge very fast. (Double precision in, say, 10–20 iterations is not uncommon.)

Partial Differential Equation

$$\begin{cases} -\Delta u = 0 & \text{on } \Omega \\ u = h & \text{on } \Gamma \end{cases}$$

 $-\Delta$ is an unbounded operator.

Typical spectrum of $-\Delta$:

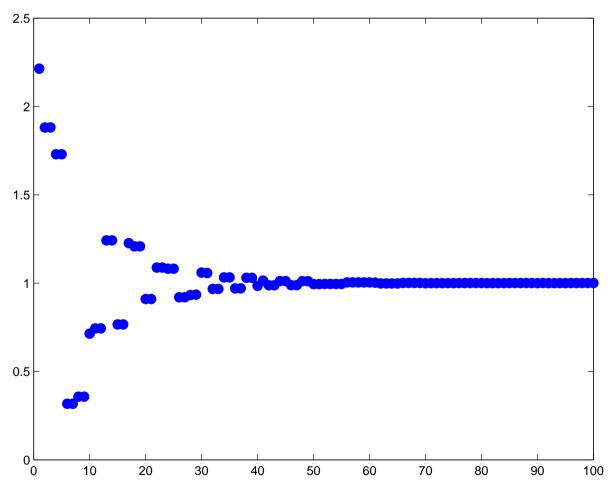


Second kind Fredholm Eqn.

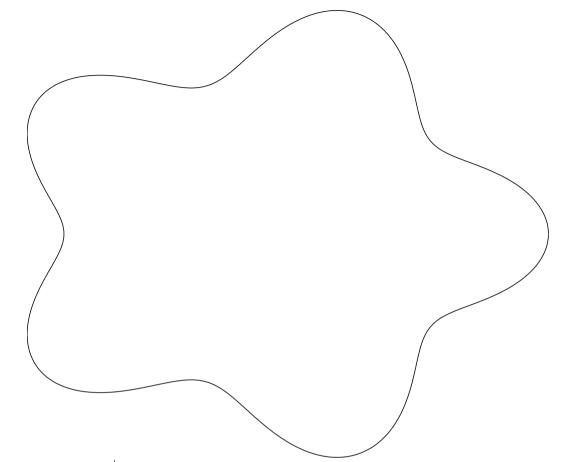
$$(I+K)q=h$$
 on Γ

K is a compact operator.(It is "almost finite-dimensional.")

Typical spectrum of I + K:



The condition numbers of the *discretized* operators.



h	Cond. nr. of discretized BIE		
0.2	8.546837835256035	(N = 25)	
0.1	7.053618952378199	(N = 50)	
0.05	6.993154106860152	(N = 100)	
0.025	6.993012937976997	(N = 200)	
0.0125	6.993012936936591	(N = 400)	
0.00625	6.993012936936595	(N = 800)	

Rewriting the BVP as a BIE can be viewed as analytic pre-conditioning.

Body loads: Now consider a BVP with a body load

(9)
$$\begin{cases} -\Delta u(\mathbf{x}) = g(\mathbf{x}), & \mathbf{x} \in \Omega, \\ u(\mathbf{x}) = h(\mathbf{x}), & \mathbf{x} \in \Gamma. \end{cases}$$

First construct a function v such that $-\Delta v = g$, disregarding boundary conditions. This is easy:

(10)
$$v(\mathbf{x}) = \int_{\Omega} \phi(\mathbf{x} - \mathbf{y}) f(\mathbf{y}) d\mathbf{y}, \qquad \mathbf{x} \in \Omega.$$

Now look for a solution to (9) of the form u = v + w. Then w must satisfy

$$\begin{cases} -\Delta w(\mathbf{x}) = 0, & \mathbf{x} \in \Omega, \\ w(\mathbf{x}) = g(\mathbf{x}) - v(\mathbf{x}), & \mathbf{x} \in \Gamma. \end{cases}$$

The solution w is found by solving $\frac{1}{2}\sigma(x) + \int_{\Gamma} \frac{n(y) \cdot (x - y)}{2\pi |x - y|^2} \sigma(y) ds(y) = g(x) - v(x)$,

for
$$\sigma$$
, and then setting $w(\mathbf{x}) = \int_{\Gamma} \frac{\mathbf{n}(\mathbf{y}) \cdot (\mathbf{x} - \mathbf{y})}{2\pi |\mathbf{x} - \mathbf{y}|^2} \sigma(\mathbf{y}) ds(\mathbf{y}).$

Note: In practice, this strategy is not entirely trivial to implement. In particular, finding high-order accurate quadratures for evaluating (10) is a bit tricky for a general domain Ω (note that ϕ is weakly singular). Then you need an FMM for evaluation, etc.

For a given BVP, there are usually different choices of BIE:

Example: Recall that the BVP

$$\begin{cases} -\Delta u(\mathbf{x}) = 0, & \mathbf{x} \in \Omega, \\ u(\mathbf{x}) = h(\mathbf{x}), & \mathbf{x} \in \Gamma. \end{cases}$$

can be rewritten either using a single layer formulation

(11)
$$\int_{\Gamma} \frac{-1}{2\pi} \log |\mathbf{x} - \mathbf{y}| \, \sigma(\mathbf{y}) \, ds(\mathbf{y}) = h(\mathbf{x}), \qquad \mathbf{x} \in \Gamma,$$

or a double layer formulation

(12)
$$\frac{1}{2}\sigma(\mathbf{x}) + \int_{\Gamma} \frac{\mathbf{n}(\mathbf{y}) \cdot (\mathbf{x} - \mathbf{y})}{2\pi |\mathbf{x} - \mathbf{y}|^2} \sigma(\mathbf{y}) \, d\mathbf{s}(\mathbf{y}) = h(\mathbf{x}), \qquad \mathbf{x} \in \Gamma.$$

The formulation (12) is a second kind Fredholm equation, which is much "nicer" than (11). (It also involves a C^{∞} kernel, which is *very* nice, but this is unusual.)

This situation is very typical — there are usually several different ways of formulating a physical problem as an integral equation. Choosing the best one is important.

BIEs for the Helmholtz equation — brief notes: Consider the equation

(13)
$$\begin{cases} -\Delta u(\mathbf{x}) - \kappa^2 u(\mathbf{x}) = 0, & \mathbf{x} \in \Omega, \\ u(\mathbf{x}) = h(\mathbf{x}), & \mathbf{x} \in \Gamma. \end{cases}$$

Introduce boundary operators

$$[S_{\kappa}\sigma](\mathbf{x}) = \int_{\Gamma} \phi_{\kappa}(\mathbf{x} - \mathbf{y}) \, \sigma(\mathbf{y}) \, dS(\mathbf{y}), \qquad [D_{\kappa}\sigma](\mathbf{x}) = \int_{\Gamma} [\partial_{\mathbf{n}(\mathbf{y})}\phi_{\kappa}](\mathbf{x} - \mathbf{y}) \, \sigma(\mathbf{y}) \, dS(\mathbf{y}).$$

where ϕ_{κ} is the free space fundamental solution $(\phi_{\kappa}(\mathbf{x}) = \frac{i}{4}H_0^{(1)}(\kappa|\mathbf{x}|)$ in 2D and $\phi_{\kappa}(\mathbf{x}) = \frac{e^{i\kappa|\mathbf{x}|}}{4\pi|\mathbf{x}|}$ in 3D). Then we can proceed as we did for Laplace, and rewrite (13) as

$$\frac{1}{2}\sigma(\boldsymbol{x})+[D_{\kappa}\sigma](\boldsymbol{x})=h(\boldsymbol{x}), \qquad \boldsymbol{x}\in\Gamma.$$

However, there are problems with so called *spurious resonances*. The standard fix is to look for a solution of the form

$$u(\mathbf{x}) = \int_{\Gamma} G_{\kappa}(\mathbf{x}, \mathbf{y}) \, \sigma(\mathbf{y}) \, dS(\mathbf{y}),$$

where

$$G_{\kappa}(\mathbf{x},\mathbf{x}') = \frac{\partial \phi_{\kappa}(\mathbf{x},\mathbf{x}')}{\partial \mathbf{n}(\mathbf{x}')} \pm i\kappa \,\phi_{\kappa}(\mathbf{x},\mathbf{x}').$$

Then (13) can be written as a combined field BIE, (without spurious resonances),

$$\frac{1}{2}\sigma(\boldsymbol{x}) + \int_{\Gamma} G_{\kappa}(\boldsymbol{x}, \boldsymbol{x}') \, \sigma(\boldsymbol{x}') \, dA(\boldsymbol{x}') = -v(\boldsymbol{x}), \quad \boldsymbol{x} \in \Gamma.$$

Integral equation formulations of other elliptic PDEs — brief notes

Time-harmonic Maxwell: Similar to Helmholtz problem, but vector-valued, and substantially more subtle. Finding formulations without artificial resonances is a subject of current research (see, e.g., Greengard-Epstein).

The equations of linear elasticity: Similar to Laplace mathematically, but messier in practice. The fundamental solutions are tensor valued, for instance.

Singular kernels: Most BIE formulations involve singular kernels. Discretizing these to high accuracy requires some deftness. For weakly singular kernels, it is quite manageable. Strongly singular, and hyper-singular, kernels can be challenging.

Domains with corners/edges: At points where the boundary is not smooth, the layer potentials typically develop singularities \rightarrow loss of accuracy unless special care is taken.

Mixed boundary conditions: Most standard formulations are derived for either pure Dirichlet, or pure Helmholtz problems. Situations where different conditions apply to different parts of the domain are more challenging.

Active area of research! The ideal would be to automate this process ...

Nyström discretization of BIEs with smooth kernel functions

At this point, we have rephrased our problem as the task of solving the BIE

(14)
$$\alpha q(\mathbf{x}) + \int_{\Gamma} k(\mathbf{x}, \mathbf{y}) q(\mathbf{y}) dS(\mathbf{y}) = f(\mathbf{x}), \qquad \mathbf{x} \in \Gamma,$$

where Γ is a contour in \mathbb{R}^2 or a surface in \mathbb{R}^3 .

Suppose first that the kernel function k is smooth, such as, e.g., the double layer kernel associated with the Laplace equation in 2D:

$$k(\mathbf{x},\mathbf{y}) = \frac{\mathbf{n}(\mathbf{y}) \cdot (\mathbf{x} - \mathbf{y})}{2\pi |\mathbf{x} - \mathbf{y}|^2}.$$

(Note: Smooth kernels are *very* unusual! We will consider the general case shortly.) Suppose that we are given a quadrature rule for smooth functions on Γ . In other words, suppose that we are given *nodes* $\{x_i\}_{i=1}^N \subset \Gamma$ and *weights* $\{w_i\}_{i=1}^N \subset [0,\infty)$ such that

(15)
$$\int_{\Gamma} \varphi(\mathbf{y}) dS(\mathbf{y}) \approx \sum_{j=1}^{N} w_{j} \varphi(\mathbf{x}_{j}), \quad \text{for } \varphi \text{ smooth..}$$

In order to discretize (14), we first collocate the equation at the quadrature nodes:

(16)
$$\alpha q(\mathbf{x}_i) + \int_{\Gamma} k(\mathbf{x}_i, \mathbf{y}) q(\mathbf{y}) dS(\mathbf{y}) = f(\mathbf{x}), \qquad i = 1, 2, 3, ..., N.$$

Then insert (15) in to (17) to approximate the integral:

(17)
$$\alpha q(\mathbf{x}_i) + \sum_{j=1}^{N} k(\mathbf{x}_i, \mathbf{x}_j) w_j q(\mathbf{x}_j) = f(\mathbf{x}_i), \qquad i = 1, 2, 3, \ldots, N.$$

Examples of convenient quadrature rules (review from A. Barnett lecture):

Trapezoidal rule: Simple to use and extremely accurate for smooth simple contours in 2D.

Gaussian quadrature on "panels": Quite simple to use. Allows for local refinement. Good for domains with corners and edges. Slight drawback in that points cluster near the edges.

Curtis-Clenshaw quadrature: Panel based, just like Gaussian quadrature. Theoretically, it is much less accurate (with p points per panel of "size" h, the error in C-C is of order h^p , while the error in Gaussian quadrature is h^{2p-1}). In practice, it is indeed a bit less accurate than Gaussian quadrature, but still very good. Useful when you want nodes at the panel interfaces.

Nyström discretization of BIEs with weakly singular kernel functions

Now consider a more realistic situation of a BIE

$$\alpha q(\mathbf{x}) + \int_{\Gamma} k(\mathbf{x}, \mathbf{y}) q(\mathbf{y}) dS(\mathbf{y}) = f(\mathbf{x}), \qquad \mathbf{x} \in \Gamma,$$

where $k(\boldsymbol{x}, \boldsymbol{y})$ is smooth for $\boldsymbol{x} \neq \boldsymbol{y}$, and $k(\boldsymbol{x}, \boldsymbol{y}) \sim \log |\boldsymbol{x} - \boldsymbol{y}|$ as $\boldsymbol{y} \rightarrow \boldsymbol{x}$.

Assume for now that Γ and f are smooth.

We again start with a quadrature rule $\{x_i, w_i\}_{i=1}^N$ designed for smooth functions

$$\int_{\Gamma} \varphi(\mathbf{y}) dS(\mathbf{y}) \approx \sum_{i=1}^{N} w_i \varphi(\mathbf{x}_i), \quad \text{for } \varphi \text{ smooth..}$$

Collocating at the quadrature nodes, we get the equation

$$\alpha q(\mathbf{x}_i) + \int_{\Gamma} k(\mathbf{x}_i, \mathbf{y}) q(\mathbf{y}) dS(\mathbf{y}) = f(\mathbf{x}), \qquad i = 1, 2, 3, ..., N.$$

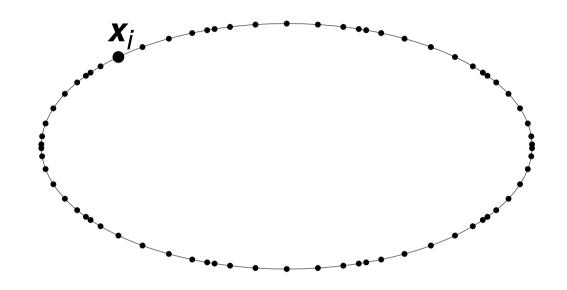
The trick is now to construct an $N \times N$ matrix **A** such that

$$\sum_{j=1}^{N} \mathbf{A}(i,j) \, q(\mathbf{x}_j) \approx \int_{\Gamma} k(\mathbf{x}_i,\mathbf{y}) \, q(\mathbf{y}) \, dS(\mathbf{y}), \qquad i=1,\,2,\,3,\,\ldots,\,N.$$

Key observation: The unknown q is smooth, even though k is not.

Recall: We seek to build a matrix **A** such that $\sum_{j=1}^{N} \mathbf{A}(i,j) \, q(\mathbf{x}_j) \approx \int_{\Gamma} k(\mathbf{x}_i,\mathbf{y}) \, q(\mathbf{y}) \, dS(\mathbf{y}).$

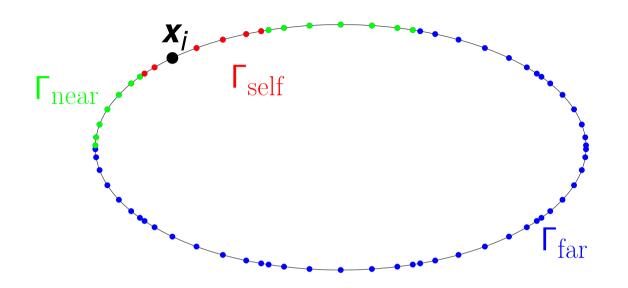
Consider the a 2D smooth contour Γ , and a composite Gaussian "base" quadrature:



Fix a point x_i . We seek to determine the row A(i, :).

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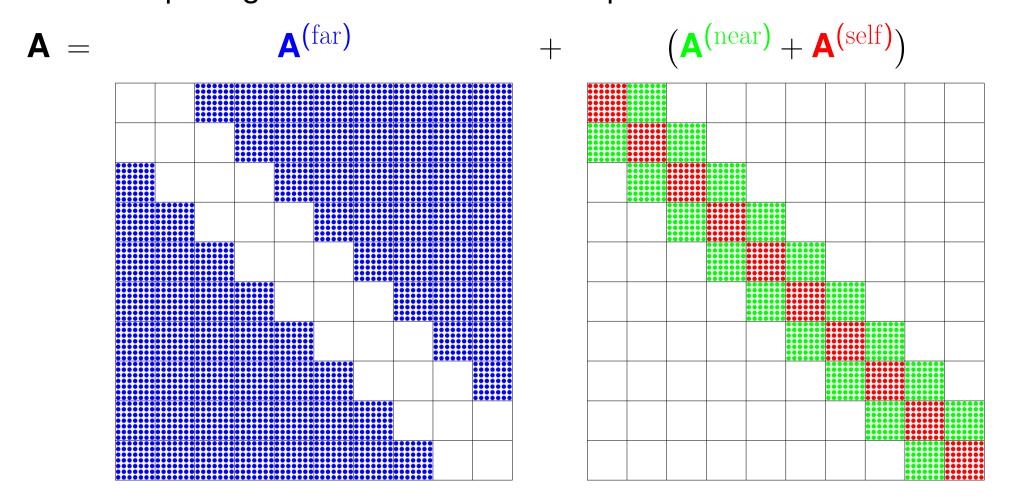
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Partition $\Gamma = \Gamma_{\text{far}} \cup \Gamma_{\text{self}} \cup \Gamma_{\text{near}}$. Then

$$\int_{\Gamma} k(\boldsymbol{x}_{i},\boldsymbol{y}) \, q(\boldsymbol{y}) \, dS(\boldsymbol{y}) = \int_{\Gamma_{\text{far}}} k(\boldsymbol{x}_{i},\boldsymbol{y}) \, q(\boldsymbol{y}) \, dS(\boldsymbol{y}) + \int_{\Gamma_{\text{near}}} k(\boldsymbol{x}_{i},\boldsymbol{y}) \, q(\boldsymbol{y}) \, dS(\boldsymbol{y}) + \int_{\Gamma_{\text{self}}} k(\boldsymbol{x}_{i},\boldsymbol{y}) \, q(\boldsymbol{y}) \, dS(\boldsymbol{y}).$$

In $\Gamma_{\rm far}$ (which contains essentially all points), just use the plain quadrature rule. In $\Gamma_{\rm near}$ and $\Gamma_{\rm self}$ we have to numerically build the relevant matrix blocks.

The end result is a splitting of the matrix into three parts:



All entries in $\mathbf{A}^{(\text{far})}$ take the form $\mathbf{A}(i,j) = k(\mathbf{x}_i, \mathbf{x}_j) w_j$. Analogous modifications also exist for surfaces in 3D.

Remark: Observe that in practice, the adjudication of whether a point is "near" is done in physical space, not in parameter space.

Weighting of elements in building the coefficient matrix

Suppose we are given a BIE with a smooth kernel

(18)
$$\alpha q(\mathbf{x}) + \int_{\Gamma} k(\mathbf{x}, \mathbf{y}) q(\mathbf{y}) dS(\mathbf{y}) = f(\mathbf{x}), \qquad \mathbf{x} \in \Gamma.$$

Then given a quadrature rule $\{x_i, w_i\}_{i=1}^N$ for Γ , the Nyström discretization of (18) is

(19)
$$\alpha q(\mathbf{x}_i) + \sum_{j=1}^{N} w_i k(\mathbf{x}_i, \mathbf{x}_j) q(\mathbf{x}_j) = f(\mathbf{x}_i), \qquad i = 1, 2, 3, \ldots, N.$$

To write (19) as a matrix equation, we now define vectors $\mathbf{q}, \mathbf{f} \in \mathbb{R}^N$ via

$$\mathbf{f}(i) = \sqrt{w_i} f(\mathbf{x}_i)$$
 given data $\mathbf{q}(i) \approx \sqrt{w_i} q(\mathbf{x}_i)$ sought data

Then define an $N \times N$ matrix **A** via

$$\mathbf{A}(i,j) = \sqrt{\mathbf{w}_i} \, k(\mathbf{x}_i, \mathbf{x}_j) \, \sqrt{\mathbf{w}_j} + \alpha \, \delta_{i,j}$$

and (19) can be written

$$\mathbf{A}\,\mathbf{q}=\mathbf{f}.$$

The purpose of the weighting scheme is to have $\|\mathbf{q}\|_{\ell^2} \approx \|\mathbf{q}\|_{L^2(\Gamma)}$ and $\|\mathbf{f}\|_{\ell^2} \approx \|f\|_{L^2(\Gamma)}$. Then the singular values of \mathbf{A} approximate the singular values of $A: L^2(\Gamma) \to L^2(\Gamma)$. Moreover, this avoids giving undue weight to regions where the mesh is *refined*.

Summary:

- Many physical problems that are commonly modeled using PDEs, can advantageously be modeled using integral equations. Advantages include:
 - Reduction of dimensionality either a PDE in 3D or a BIE on a 2D surface.
 - Bounded (often compact) operators instead of unbounded operators.
 - Second kind Fredholm formulations are often possible excellent conditioning.
 - Radiation conditions on infinite domains enforced automatically.
- Discretization of an integral equation leads to a dense linear system.
 Linear complexity algorithms are still possible, but more memory per degree of freedom is usually required. (But you typically need much fewer degrees of freedom!)
- There often exist many different integral equation formulations for a given problem. Choosing the right one is tremendously helpeful!
- The integral equation framework is slightly less flexible than FEM. Handling novel equations, multi-physics, non-linearities, etc, is cumbersome (at best...).
- Nyström discretization is very convenient. Often leads to a system matrix

$$\mathbf{A} = \mathbf{A}^{\text{(far)}} + \mathbf{A}^{\text{(close)}},$$

where $\mathbf{A}^{(\mathrm{close})}$ is very sparse. All elements in $\mathbf{A}^{(\mathrm{far})}$ take a simple form, such as,

$$\mathbf{A}^{(\mathrm{far})}(i,j) = k(\mathbf{x}_i,\mathbf{x}_j) w_j, \qquad \text{or} \qquad \mathbf{A}^{(\mathrm{far})}(i,j) = \sqrt{w_i} k(\mathbf{x}_i,\mathbf{x}_j) \sqrt{w_j}.$$