BOUNDARY INTEGRAL METHODS

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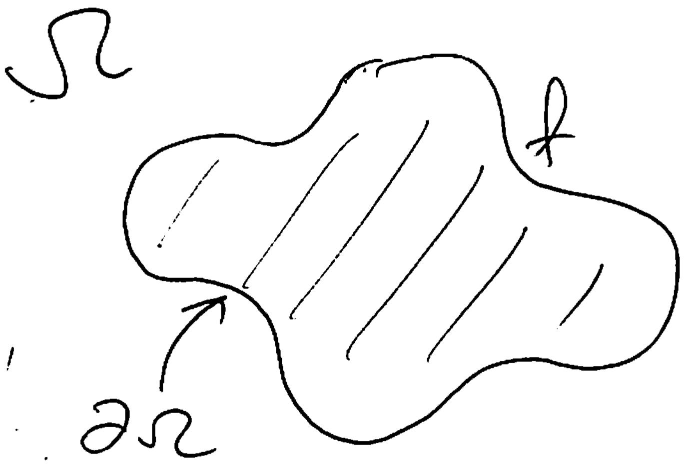
(based on notes by Mike O'Neil & Alex Barnett)

Let's consider now solving constant coeff. homogeneous elliptic PDEs in 2D with non-trivial BCs in complex domains – take Poisson eq. as an example but biharmonic, Helmholtz, Stokes and others can be handled also.

Simple linear PDE (known Green's function) + Complex domains

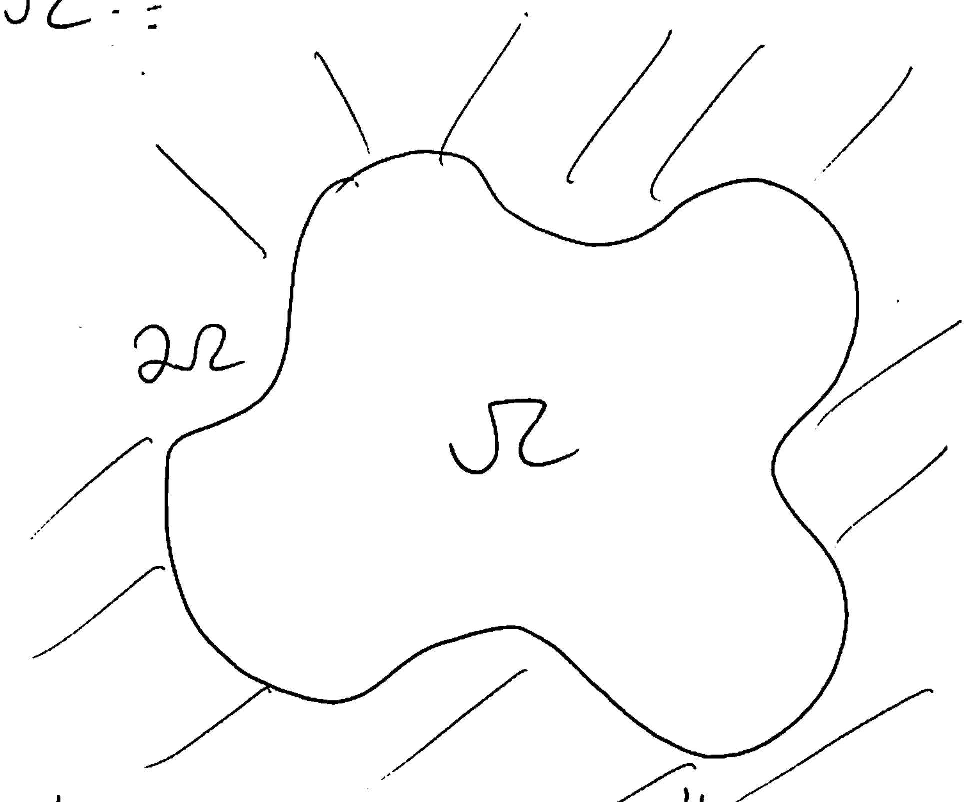
e.g. $\nabla^2 u = 0$ in Ω (homogeneous!)

$u = f$ on $\partial\Omega$



"Exterior" problem

$u \to$ const at "infinity".



"Interior" problem

A physical example is

<u>electrostatics</u> : $u \equiv \varphi$ is potential

$$\begin{cases} \nabla^2 \varphi = \rho = \text{charge density} \\ u = u_0 \text{ on } \partial\Omega \text{ for a conductor} \end{cases}$$

<u>Integral formulation</u>

in FREE SPACE (<u>non-local</u>)

PDE is local so works with any BCs!

$$\varphi(\underline{r}) = \int \rho(\underline{r}') \, G(\underline{r}, \underline{r}') \, dr'$$

Green's function

$$l = \| \underline{r} - \underline{r}' \|_2$$

$$G(\underline{r}, \underline{r}') = G(\underline{r} - \underline{r}') = G(l)$$

<u>ISOTROPIC</u> TENSOR

$$G(r) = \frac{1}{4\pi r} \quad \text{in } 3D$$ (4)

$$G(r) = -\frac{1}{2\pi} \ln(r) \quad \text{in } 2D$$

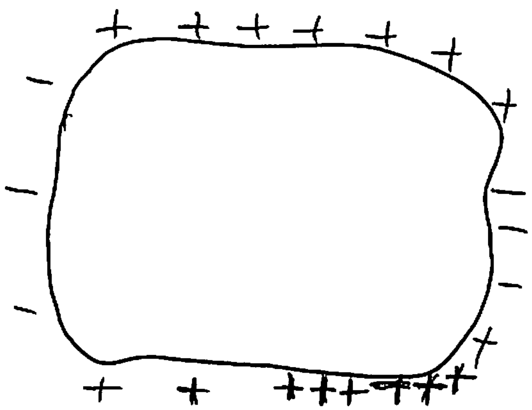
$\Big\{$ Observe $G(r)$ decays <u>slowly</u> in 3D and does not actually decay in 2D

$\Big\{$ Observe: $G(\underline{r})$ is a solution of $\nabla^2\varphi = 0$ away from zero, and is the potential due to a <u>point charge</u>, $\nabla^2 G = \delta(0)$.

$\Big[$ $\partial G/\partial \underline{n} = (\nabla_r G)\cdot\underline{n}$ is also a solution and is the potential of a <u>dipole</u>

Consider now a surface $\partial\Omega$ (5)
with a surface bound charge
density $\varsigma(r \in \partial\Omega)$. The
potential created by it is

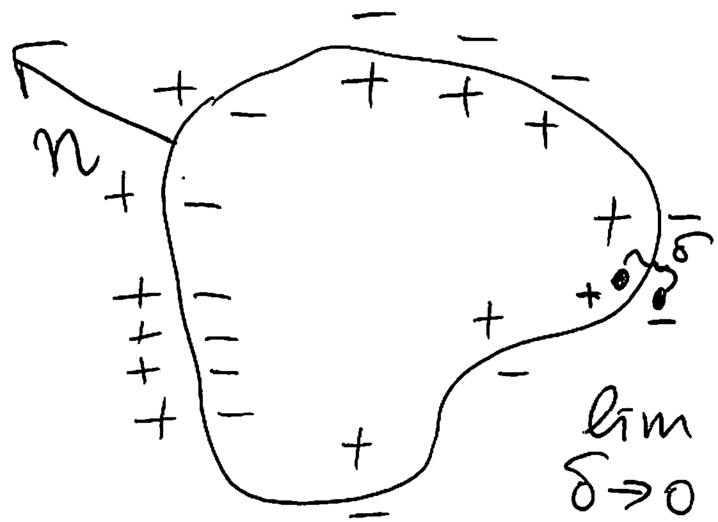
$$\boxed{\varphi(r) = \int_{\partial\Omega} \varsigma(r')\, G(r,r')\, dS(r')}$$



$$\boxed{\varphi(r) = S[\varsigma(\partial\Omega)]}$$

this is called the
"single layer potential"

Now consider a surface with a given density of <u>dipoles</u>



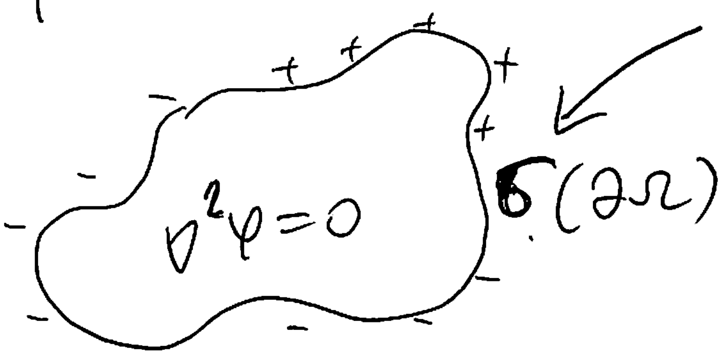
$$\varphi(r) = \int_{\partial\Omega} \rho(r')\, ds(r') \cdot \lim_{\delta \to 0} \left[\frac{G(r,r') - G(r, r' + n(r')\delta)}{\delta} \right]$$

$$\Rightarrow \boxed{\varphi(r) = \int_{\partial\Omega} \rho(r') \frac{\partial G(r,r')}{\partial n(r')}\, ds(r') \equiv D[\rho(\cdot)]}$$

$\nabla_{r'} G(r,r') \cdot n(r')$ "double layer potential"

Now consider a conducting closed surface (wire in 2D):

$\nabla^2 \varphi = 0$



induced surface charge density $\sigma(\partial\Omega)$

Some BC at infinity, e.g., applied electric field

$\nabla \varphi \to -\vec{E}_0$ at infinity

If we can find $\sigma(\partial\Omega)$ then

$\varphi(r) = S[\sigma(\cdot)]$

everywhere in R^2

The single-layer potential is <u>continuous across $\partial\Omega$</u>:

$$\lim_{h\to 0^{\pm}} (S\sigma)(x+nh) = S\sigma(x\in\partial\Omega)$$

For a conductor, we have

$$(S\sigma)(x\in\partial\Omega) = \varphi_0 = \text{const}$$

$$\Rightarrow \boxed{\int_{\partial\Omega} G(r,r')\,\sigma(r')\,dS(r') = \varphi_0}$$

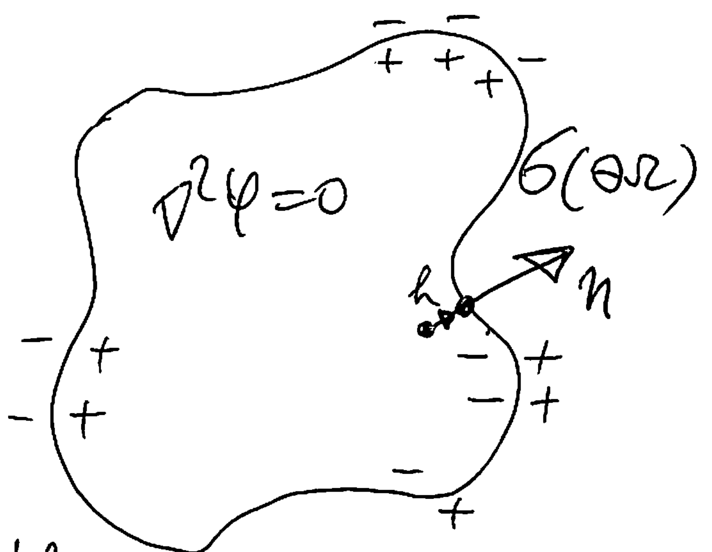
integral equation of the first kind

The variable $\sigma(\partial\Omega)$ has a clear physical interpretation (charge density on $\partial\Omega$) but this integral equation is not well-posed and discretizations of it will lead to very ill-conditioned matrices.

But this illustrates the key idea:

Solve an integral equation for densities on $\partial\Omega$ instead of a PDE in Ω : BOUNDARY INTEGRAL METHODS

We can get a well-conditioned integral equation by using an unphysical "density" as our variable: double-layer or dipole density:



$\varphi = f$ on $\partial\Omega$
(Dirichlet BC)

<u>Ansatz</u>:

$$\varphi = D[\sigma(\partial\Omega)]$$

in Ω

B.C. for $r \in \partial\Omega$:

$$\lim_{h \to 0^+} D\sigma(r - nh) = f(r)$$

11

The double layer potential is <u>NOT</u> continuous across $\partial\Omega$, it has a jump. It can be shown that:

$$\boxed{\lim_{h\to 0^+} D\sigma(r \pm nh) = \pm\frac{1}{2}\sigma(r\in\partial\Omega) + \tilde{D}\sigma(r\in\partial\Omega)}$$

where $\tilde{D}$ is the principal value of the double layer evaluated at a point on the boundary.

In 2D, explicitly

$$D[\sigma](r \notin \partial\Omega) = \int_{\partial\Omega} \sigma(r') \, ds(r') \cdot \underbrace{\frac{n(r')\cdot(r-r')}{2\pi \|r-r'\|^2}}_{K(r,r')}$$

← Double layer **kernel** or "dipole kernel"

$$D[\sigma](r \notin \partial\Omega) = \int K(r,r')\,\sigma(r')\,ds(r')$$

$$D[\sigma](r \in \partial\Omega) =$$

$$\lim_{\varepsilon \to 0} \lim_{h \to 0^+} \underbrace{\int_{\partial\Omega \cap \underset{\substack{\uparrow \\ \text{ball}}}{B}(r,\varepsilon)} K(r \pm h\hat{n}, r')\, \sigma(r')\, ds(r')}_{\pm \frac{1}{2}\sigma(r)}$$

$$+ \lim_{\varepsilon \to 0} \underbrace{\int_{\partial\Omega \setminus B} K(r,r')\, \sigma(r')\, ds(r')}_{\tilde{D}\sigma(r)}$$

Another important result is that (14)

$$\lim_{r \to r'} K(r, r') = \frac{\kappa(r)}{4\pi}$$

signed curvature of $\partial\Omega$

This miracle, that the kernel is continuous at $r = r'$, only works for smooth 2D curves & some simple equations like Poisson & Stokes — in general the kernels (single/double) are (hyper) singular

Let's go back to the interior Dirichlet Poisson problem

Anzatz: $\varphi = D[\sigma(\partial\Omega)]$

B.C.s $\varphi(r \in \partial\Omega) = -\frac{\sigma(r)}{2} + \tilde{D}\sigma = f(r)$

$$\Rightarrow \boxed{-\frac{\sigma(r)}{2} + \int K(r,r')\,\sigma(r')\,ds(r') = f(r) \quad \forall r \in \partial\Omega} \quad (*)$$

This is a Fredholm integral equation of the SECOND KIND

There is a well-developed <u>Fredholm theory</u> of integral equations that proves $(*)$ is well posed: It has a <u>unique solution</u> for any $f \in L^2(\partial\Omega)$.

Since $\varphi = D\sigma$ satisfies $\nabla^2\varphi = 0$ in Ω and satisfies the BCs, it <u>must</u> be the unique solution of the PDE!

Summary of <u>boundary integral</u> method for interior Poisson : (17)

(1) Solve the integral equation for $\sigma(\partial\Omega)$ (surface <u>only</u> not volume !)

$$\boxed{-\frac{\sigma}{2}+\tilde{D}\sigma=f} \quad (\partial\Omega)$$

(2) Solution in Ω (volume not surface) is $\varphi = D\sigma$ if you need it

To make this into a numerical method we need to figure out

#1 how to solve integral equation

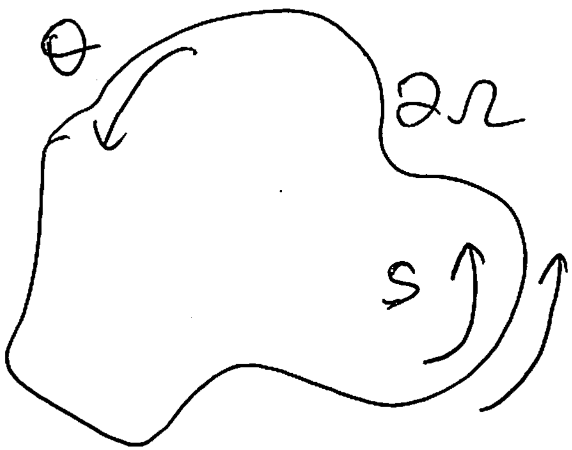
#2 how to evaluate solution in interior/exterior

First thing we need is a way to discretize integrals over curves in 2D or surfaces in 3D, involving potentially singular kernels

$\Rightarrow$ Hard in 2D, <u>really</u> hard in 3D

19

But we are in luck for Poisson in 2D – the double layer integral has a continuous kernel, so <u>quadrature</u> is easy: <u>trapezoidal rule</u>



Parametrize $\partial\Omega$ by an arc length parameter

$\underline{X}(s) \in \partial\Omega$

Now convert to a parameter $\theta \in [0, 2\pi)$ for convenience (not crucial)

$X : \mathbb{R} \to \mathbb{R}^2$ s.t.

$X([0, 2\pi)) = \partial\Omega$

← Lagrangian coordinate

Now take an integral over $\partial\Omega$:

$$I = \int_{\partial\Omega} f(r)\, dl(r) =$$

$$\int_0^{2\pi} f(X(\theta))\, |X'(\theta)|\, d\theta$$

$$\simeq \sum_{j=1}^{N} f(\underset{\substack{||| \\ X_j}}{X(\theta_j)})\, |X'(\theta_j)|\, w_j$$

quadrature weight

Here we can use any 1D quadrature over $[0, 2\pi)$ but recall that the trapezoidal rule is spectrally accurate for analytic integrands on a periodic interval! (lecture #2)

$$I \simeq \sum_{j=1}^{N} f(X(\theta_j)) \, |X'(\theta_j)| \, \frac{2\pi}{N}$$

equal weights

(one can use also Gauss quadrature)

the simplest and most common discretization of an integral equation

$$\int_0^{2\pi} \tilde{K}(t,\theta)\sigma(\theta)\,d\theta + \sigma(t) = f(t) \quad \forall t \in [0,2\pi)$$

is the Nyström method

$$\sum_{j=1}^{N} \tilde{K}(\theta_i,\theta_j)\, w_j\, \sigma(s_j) + \sigma(s_i) = f(\theta_i)$$

This is like a finite-difference discretization

Note: there are also FEM-like "Galerkin" & "collocation" methods.

This gives us the linear system:

$$\sigma_i + \sum_{j=1}^{N} \tilde{K}_{ij}\, \sigma_j w_j = f_i \quad , \quad i=1,\dots,N$$

$$\boxed{(I + A)\sigma = f}$$

$$A_{ij} = \tilde{K}(\theta_i, \theta_j) w_j = -2K(x_i, x_j)|x_j'| w_j$$

for Poisson

A common transformation is to make

$$\tilde{\sigma}_j = |X'(\theta_j)|\, w_j\, \sigma_j$$

the unknown so that

$$A\sigma = \mathbb{K}\tilde{\sigma}$$

where

$$\boxed{\mathbb{K}_{ij} = K(x_i, x_j)}$$

$$\boxed{(\mathrm{Diag} + \mathbb{K})\tilde{\sigma} = f} \quad (**)$$

Observations (follow from Fredholm theory) / notes:

1. The conditioning number of (**) is bounded by a "small" constant <u>independent</u> of the number of points on the curve $\partial\Omega$

$\Rightarrow$ Often a dozen <u>GMRES</u> iterations enough to get 9-12 digits

2. The matrix-vector product $\mathbb{K}\tilde{\sigma}$ can be computed in $O(N \log N)$ time using FAST MULTIPOLE METHODS

So instead of discretizing a PDE with FEM to get many volume elements & huge ILL-CONDITIONED linear systems, we can only discretize the boundary to get a smaller & well-conditioned system that we can solve in near linear time!

Sounds too good to be true?

It is amazing "when it works"

Now the problems / issues :

1. Only worked for linear homogeneous constant-coefficient problems with known Green's functions
(but note we can handle "exterior" problems in <u>unbounded domains</u> which FEM cannot).

2. Discretizing surfaces in <u>3D</u> is much harder than discretizing curves in 2D $\Rightarrow$ not easy or impossible to get spectral accuracy

3 (Biggest issue IMHO)
Kernels of interest in 3D are (hyper) singular, and even in 2D single-layer is singular.
Singular quadrature rules are needed and these are specific to both the kernel / singularity & to the discretization of the boundary.
Methods exist but very complicated & often expensive (QBX)

If we had used a single layer formulation, i.e. anzatz

$$\varphi = S[\sigma] \quad \text{in 2D}$$

we would need to use special quadratures like Alpert (see notes by Alex Barnett)

$$S[\sigma] = \int G(r,r')\sigma(r')\,ds(r') \to \overleftrightarrow{\mathbb{G}}\,\vec{\sigma}$$

$$\mathbb{G}_{ij} = \begin{cases} G(x_i, x_j) & \text{if } |i-j| > p \\ \text{BANDED correction for singularity} & \text{otherwise} \end{cases}$$

These Alpert quadratures are not spectrally-accurate but they can be high order (e.g. 8th)

But note that the linear system

$$\mathbb{G}\,\sigma = f$$

would be ill-conditioned so one would have to use <u>direct methods</u>, not GMRES.

This is OK if not too many points <u>per curve</u>.

Finally, note that in practice (31)
sometimes a mix of first & second-kind formulations is used,

$$\varphi = S\sigma_1 + D\sigma_2 \qquad \text{(anzatz)}$$

with some conditions to make the solution unique for both σ_1 & σ_2.
this is sometimes needed for good conditioning number.

Experts @ Courant: L. Greengard & M. O'Neil
Users: A. Cerfon, A. Donev