Boundary integral equation methods for elliptic problems - part 2

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Last lecture...

- We saw that Laplace’s equation in Ω could be reformulated as an integral equation on the boundary ∂Ω of the domain in several ways.
- We derived Green’s representation formula and noted that it could be used to solve Laplace’s equation.
- Opting for simplicity we instead picked the double layer representation

\[
U(x_0) = \frac{1}{2\pi} \int_{\partial\Omega} \mu(x) \frac{\partial}{\partial n} \log(|x_0 - x|) \, dl(x)
\]

of the solution in Ω
- Using the jump relations we got the following integral equation for the density μ on ∂Ω:

\[
\frac{1}{2} \mu(x_0) + \frac{1}{2\pi} \int_{\partial\Omega} \mu(x) \frac{\partial}{\partial n} \log(|x_0 - x|) \, dl(x) = f(x_0)
\]
Last lecture...

- I decided that the equivalent complex representation was easier to handle (which it is). The double layer representation in complex variables is

\[ U(z_0) = \frac{1}{2\pi} \int_{\partial \Omega} \mu(z) \text{Im} \left\{ \frac{dz}{z-z_0} \right\}. \]

and using the jump relations we get the integral equation

\[ \frac{1}{2} \mu(z_0) + \frac{1}{2\pi} \int_{\partial \Omega} \mu(z) \text{Im} \left\{ \frac{dz}{z-z_0} \right\} = f(z_0), \]

for \( \mu \) on the boundary.
Compact integral operators

- We can write

\[
\frac{1}{2} \mu(z_0) + \frac{1}{2\pi} \int_{\partial \Omega} \mu(z) \text{Im} \left\{ \frac{dz}{z - z_0} \right\} = f(z_0),
\]

symbolically as

\[
\left( \frac{1}{2} \mathcal{I} + \mathcal{K} \right) \mu = f.
\]

- Here, we call \( \mathcal{I} \) the identity operator and \( \mathcal{K} \) is an integral operator with kernel

\[
K(z, z_0) = \frac{1}{2\pi} \text{Im} \left\{ \frac{dz}{z - z_0} \right\}.
\]

- Integral operators are in general infinite dimensional, but there is a special kind of integral operator that is ”almost finite dimensional”.

- We call such operators compact integral operators.
Compact integral operators

- We will need some terminology.
- A linear space is a collection of objects on which the operations addition and multiplication by scalar are defined, obeying the common rules such as commutativity, etc.
- A normed linear space $\mathcal{S}$, also has a norm $\| \cdot \|$ defined on it for which it should hold for $x, y \in \mathcal{S}$ that
  - $\|x\| = 0$ then $x = 0$,
  - $\|ax\| = |a|\|x\|$ for scalars $a$,
  - $\|x + y\| \leq \|x\| + \|y\|$
- There are many examples of normed linear spaces. For example $\mathbb{R}^n$ equipped with various norms.
- We will discuss spaces of functions here. Popular examples of such are
  - $C([a, b])$, the space of continuous functions over $[a, b]$ with norm $\|f\| = \sup_{x \in [a, b]} f(x)$,
  - $L^2([a, b])$, the space of square integrable functions over $[a, b]$ with norm $\|f\| = \sqrt{\int_a^b |f(x)|^2 dx}$.
Compact integral operators

- An open ball of radius $r$ centered at $x_0$ consists of all $x$ such that $\|x - x_0\| < r$.

- A sequence is an ordered list $x_1, x_2, \ldots$ of elements and a Cauchy sequence is a sequence where elements get closer and closer. That is for any $\varepsilon > 0$, $\|x_n - x_k\| < \varepsilon$ for some $N$ such that $n > N, k > N$.

- A sequence converges to $x$ if $\|x - x_n\| \rightarrow 0$ as $n \rightarrow \infty$.

- A space for which all Cauchy sequences converge is called a Banach space.

- The closure of a set $\mathcal{X}$ is $\mathcal{X}$ but with the limit points added. For example, the closure of the interval $(a, b)$ on the real line is $[a, b]$. 
Compact integral operators

- We first need the concept of a compact set.

**Definition**

A set $X$ in a Banach space is called compact if and only if every sequence $x_1, x_2, x_3, ...$ of elements in $X$ contains a converging subsequence.

If a set $X$ can be covered by a finite number of balls of radius $\varepsilon$ for each $\varepsilon > 0$ then the closure of $X$ is compact.

- These definitions are equivalent and they both hint that compact sets are in some sense small.
- Heine-Borel’s theorem says that any closed and bounded subset of $\mathbb{R}^n$ is compact.
- So $[a, b]$ is compact for any finite $a$ and $b$ but the whole real line $\mathbb{R}$ is not.
Compact integral operators

Definition

An integral operator $K$ taking inputs from $X$ and producing outputs in $Y$ is called a compact integral operator if and only if every bounded subset of $X$ is mapped into a subset of $Y$ whose closure is compact.

- We could say that a compact integral operator takes inputs from a potentially large set and produces outputs in a smaller set.
- So what are the conditions for an integral operator to be compact?
- Well, it depends on what space we are dealing with. For our purposes we can limit ourselves to the space of square integrable functions on the interval $[a, b]$. Then

Theorem

An integral operator from $L^2([a, b])$ to $L^2([a, b])$ is compact if its kernel $K(x, x_0)$ obeys

$$\int_a^b \int_a^b |K(x, x_0)|^2 dx_0 dx < \infty.$$
Compact integral operators

- Let us check how our integral operator

\[ \mathcal{K}_\mu(z_0) = \int_{\partial \Omega} \mu(z) \text{Im} \left\{ \frac{dz}{z - z_0} \right\} \]

does.

- Introduce a parameterization \( z(t), t \in [0, 2\pi] \) of the boundary. We then get

\[ \mathcal{K}_\mu(z_0) = \int_0^{2\pi} \mu(z) \text{Im} \left\{ \frac{z'(t)}{z(t) - z_0} \right\} \, dt, \]

and using the same parameterization for \( z_0 \) we write the kernel as

\[ K(t, s) = \text{Im} \left\{ \frac{z'(t)}{z(t) - z(s)} \right\}. \]

- Is \( K(t, s) \) square integrable? Yes, for smooth boundaries it is, even though the denominator looks problematic for \( t = s \). It is in fact continuous, which you will show in the homework.
Compact integral operators

- Great, so our integral operator is compact. What does that buy us?
- First off, we have the following theorem

**Theorem**

*If $\mathcal{K}$ is a compact operator then its spectrum consists of either a finite number of eigenvalues, or a denumerable set of eigenvalues accumulating only at the origin.*

- This basically says that either $\mathcal{K}$ has a finite number of eigenvalues, in which case $\mathcal{K}$ is finite dimensional, or
- $\mathcal{K}$ has infinitely many eigenvalues, but they tend toward zero. $\mathcal{K}$ is ”almost finite dimensional”.
- In either case, making $\mathcal{K}$ finite dimensional by discretizing it should not remove too much information.
- These spectral properties will also be very advantageous later when we discuss iterative solvers for solving the discretized linear systems of equations.
Compact integral operators

- Knowing that $\mathcal{K}$ is compact gives us the opportunity to use another theorem

**Theorem**

**Fredholm’s alternative.** If the integral operator $\mathcal{K}$ is compact, then either the homogenous integral equation $(\mathcal{I} + \mathcal{K})\mu = 0$ has a non-trivial solution ($\mu$ not identically zero), or $(\mathcal{I} + \mathcal{K})\mu = f$ has a unique solution for every $f$.

- Compare this to the finite dimensional case: either the linear system of equations $Ax = 0$ has a non-trivial solution, or $Ax = f$ has a unique solution for every $f$

- One can show that $(\mathcal{I} + \mathcal{K})\mu = 0$ for our integral operator has only the solution $\mu = 0$, thereby showing by Fredholm’s alternative that $(\mathcal{I} + \mathcal{K})\mu = f$ is uniquely solvable for any $f$. This requires quite a lot of analytic function theory so we will skip that here.
Recap and what now?

- To recap, compactness of our integral operator gave us
  - a way to show existence and uniqueness of solutions to the integral equation,
  - that the integral operator is almost finite dimensional, it should discretize nicely, and
  - once discretized, the linear system of equations can be solved rapidly using iterative solvers (but more on that later).

- So, let us discretize the integral equation. We will need to evaluate integrals, and we will do this using the good old trapezoidal rule.

- As it turns out, the trapezoidal rule is astoundingly good for evaluating the integrals we will encounter.
Trapezoidal rule error

- The standard error estimate for the trapezoidal rule says that the error decays as $h^2$.
- This is a massive overestimation of the error when
  1. the integrand is smooth, many times continuously differentiable,
  2. the integrand is periodic.
- For periodic functions the trapezoidal rule becomes the midpoint rule, but this does not explain the higher order. Why would the error be much lower?
- A first ”hand waving” explanation might be that because of periodicity, the over and underestimations cancel over one period.
Trapezoidal rule error

- More precisely we have the following:

**Theorem**

Let \( m \geq 0, \ N \geq 1 \), and define \( h = \frac{2\pi}{N}, x_j = jh \) for \( j = 0, 1, \ldots, N - 1 \). Further assume that \( f(x) \) is \( 2m + 2 \) times continuously differentiable on \([0, 2\pi]\) for some \( m \geq 0 \). Then, for the error in the trapezoidal rule

\[
\int_{0}^{2\pi} f(x)dx - T_N(f) = - \sum_{k=1}^{m} \frac{B_{2k}}{(2k)!} h^{2k} \left( f^{(2k-1)}(2\pi) - f^{(2k-1)}(0) \right)
\]

\[
-2\pi h^{2m+2} \frac{B_{2m+2}}{(2m + 2)!} f^{(2m+2)}(\xi)
\]

for some \( \xi \) in \([0, 2\pi]\). The \( B_k \) are the Bernoulli numbers, and \( T_N(f) \) denotes the \( N \)-point trapezoidal rule applied to \( f \).

- For smooth \((m \text{ large}),\) periodic \((f^{(n)}(0) = f^{(n)}(2\pi))\) functions we get very high order, ”spectral accuracy”.

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Nyström discretization

- Given a periodic parameterization $z(t), t \in [0, 2\pi]$ we would like to discretize our integral equation so that we can solve it.

- Introducing the parameterization in our equation we get

$$\frac{1}{2}\mu(z(s)) + \frac{1}{2\pi} \int_{\partial\Omega} \mu(z(t)) \text{Im} \left\{ \frac{z'(t)}{z(t) - z(s)} \right\} \, dt = f(z(s)).$$

for $s \in [0, 2\pi]$.

- Let us pick $N$ equidistant points $t_j = 2\pi j/N, j = 0, ..., N - 1$. The distance between them is $h = 2\pi/N$. Evaluating the integral with the trapezoidal rule we get

$$\frac{1}{2}\mu(z(s)) + \frac{h}{2\pi} \sum_{j=0}^{N-1} \mu(z(t_j)) \text{Im} \left\{ \frac{z'(t_j)}{z(t_j) - z(s)} \right\} = f(z(s)).$$

- We are halfway there. We can now compute this for every $s \in [0, 2\pi]$, but there are an infinite number of values of $s$. We need to pick a finite number of them.
Nyström discretization

- The idea in Nyström discretization is to pick the quadrature nodes as the points at which we require the integral equation to hold. We get

\[
\frac{1}{2} \mu(z(t_i)) + \frac{h}{2\pi} \sum_{j=0}^{N-1} \mu(z(t_j)) \operatorname{Im}\left\{ \frac{z'(t_j)}{z(t_j) - z(t_i)} \right\} = f(z(t_i)),
\]

for \( i = 0, 1, \ldots, N - 1 \).

- If we write \( z_j = z(t_j) \), \( z'_j = z'(t_j) \), \( \mu_j = \mu(z(t_j)) \), \( f_j = f(z(t_j)) \) we get

\[
\frac{1}{2} \mu_i + \frac{h}{2\pi} \sum_{j=0}^{N-1} \mu_j \operatorname{Im}\left\{ \frac{z_j'}{z_j - z_i} \right\} = f_i.
\]

- This is an \( N \times N \) equation system with \( \mu_j \) as unknowns. We can write it as

\[
\left( \frac{1}{2} I + K \right) \mu = f
\]
Nyström discretization

- Once we have solved 
  \[
  \left( \frac{1}{2}I + K \right) \mu = f
  \]
  for \( \mu \) we know the value of the density \( \mu(z) \) at the quadrature nodes.

- We may then directly use 
  \[
  U(z_0) = \frac{1}{2\pi} \int_{\partial \Omega} \mu(z) \text{Im} \left\{ \frac{dz}{z - z_0} \right\},
  \]
  discretized in the same way to compute the solution \( U(z_0) \) at any point \( z_0 \) in the domain.

- This is a natural and simple idea, and there are other upshots as well.
Nyström discretization

- For the error in Nyström discretization we have

**Theorem**

If \( K_N \) is \( K \) but with its integral evaluated numerically by the \( N \) point trapezoidal rule, and \( x \) and \( x_N \) obeys \((I + K)x = f\) and \((I + K_N)x_N = f\) then

\[
\|x - x_N\| \leq C \max_s \left| \int K(t, s)x(t)dt - h \sum_{j=0}^{N-1} K(t_j, s)x(t_j) \right|
\]

- It turns out that Nyström discretization preserves the order of the underlying quadrature rule.
- This is very good for us, since the trapezoidal rule has very high order.
Solving the system

- The matrix $K$ with elements

$$K_{ij} = \frac{h}{2\pi} \text{Im} \left\{ \frac{z_j'}{z_j - z_i} \right\}$$

is not sparse.

- This means that solving

$$\left( \frac{1}{2} I + K \right) \mu = f$$

using Gaussian elimination costs $O(N^3)$ operations for $N$ discretization points. This is too expensive for larger problems.

- We need iterative solvers, but our choice is limited by the fact that the matrix $\frac{1}{2} I + K$ is neither symmetric nor positive definite. These are properties often exploited by iterative solvers.
GMRES

- Let’s say we wish to solve $Ax = b$ (with $A$ invertible).
- Iterative solvers in general work by computing the matrix-vector products $A\mathbf{y}_n$ for some $\mathbf{y}_n$ and using the information to construct an approximate solution.
- Each matrix-vector multiplication costs $O(N^2)$ operations for an $N \times N$ matrix, so if we need much less than $N$ such multiplications we gain something.
- The iterative solver that best suits our problem is GMRES (Generalized Minimum RESidual).
- GMRES belongs to the class of Krylov subspace methods, along with for example the conjugate gradient method.
- Unlike the conjugate gradient method it works on general matrices, but as we will see, this is not the only reason for choosing GMRES.
GMRES

- When solving the system $Ax = b$, the main idea of GMRES is to look for approximate solutions in the successive Krylov subspaces

$$S_k = \text{span}\left\{b, Ab, A^2b, \ldots, A^{k-1}b\right\}.$$ 

- For an invertible $N \times N$ matrix, the solution $x$ can be written as a linear combination of the columns in $S_N$. But we hope to be able to find an accurate solution for $k$ much less than $N$.

- At step $k$, we look for the vector $x_k$ in $S_k$ that minimizes the Euclidean norm of the residual

$$r_k = b - Ax_k.$$ 

- There are many technical details involved here, but we are mainly interested in the convergence properties of GMRES.
The convergence theory for Krylov subspace methods is complicated, but for GMRES we can at least say that if the spectrum of the matrix $A$ is clustered away from the origin, then GMRES converges quickly.

We can roughly say that the convergence depends on the size of the cluster of eigenvalues.

Remember that for compact operators the spectrum tends to the origin.

But we have $\frac{1}{2}I + K$ with $K$ compact so the spectrum tends to $\frac{1}{2}$. The same holds for the discrete version $\frac{1}{2}I + K$.

Because of this, as we increase the size of the system the additional eigenvalues will be very close to $\frac{1}{2}$ and will not increase the size of the cluster of eigenvalues. GMRES will converge as rapidly as before.

We say that the number of GMRES steps is bounded as the system size grows for these kinds of matrices.
Each matrix-vector multiply costs $O(N^2)$ operations.

Since the number of iterations is bounded for a given problem, we have decreased the work required by an order of magnitude, from $O(N^3)$ to $O(N^2)$. Not bad.

However, we need to set up the matrix $K$ which requires $N^2$ memory storage. For complicated boundaries, the number of discretization points required can easily exceed $10^5$, which translates into 80 Gb of memory.

We can actually do better, both in terms of operation count and memory. The structure of the matrices arising from boundary integral equation methods is a special one.

The solution is the fast multipole method.
The fast multipole method

- The elements of our matrix are

\[ K_{ij} = \frac{\hbar}{2\pi} \text{Im} \left\{ \frac{z_j'}{z_j - z_i} \right\}. \]

- Ignoring the imaginary part for the moment and setting \( q_j = \frac{\hbar}{2\pi} z_j' \)

we have

\[ K_{ij} = \frac{q_j}{z_j - z_i}. \]

- So multiplying the matrix \( K \) with a real vector \( x \) amounts to evaluating

\[ \sum_{j=0}^{N-1} \frac{q_j x_j}{z_j - z_i} \]

for all \( i \) and then taking the imaginary part.

- This is basically an \( n \)-body problem.
The fast multipole method

- Basic idea - gravity
- Consider two clusters of $n/2$ particles each.
- Classic evaluation costs $\sim n^2$.
- Instead compute an equivalent center of mass for each cluster.
- Cost drops to $\sim n^2/2$.
- By subdividing the clusters this could drop further.
The fast multipole method

- Some details need to be addressed:
  - What is the error?
  - Higher order "centers of mass"?
  - How to turn this into an efficient algorithm?

- The Fast Multipole Method (FMM) handles this.
  - Rigorous error estimates.
  - Uses multipole expansions for higher order approximations.
  - Uses a tree structure to handle interactions on several scales.
The fast multipole method

- Our goal is to compute

\[ \phi(z) = \sum_{j=0}^{N-1} \frac{q_j}{z - z_j}, \]

for many points \( z \).

- We would like to separate the sources \( z_j \) from the target \( z \).

- To this end we use the identity

\[ \frac{1}{z - z_j} = \frac{1}{z} \frac{1}{1 - \frac{z_j}{z}} = \frac{1}{z} \sum_{k=0}^{\infty} \left( \frac{z_j}{z} \right)^k, \]

which is valid for \(|z| > |z_j|\).

- Putting these two together gives us the multipole expansion.
The fast multipole method

The multipole expansion.
Suppose that \( N \) sources with strengths \( q_k \) are located at points \( z_k \), with \( |z_k| < r \). Then for any \( z \) with \( |z| > r \) we have

\[
\phi(z) = \sum_{k=0}^{\infty} \frac{a_k}{z^{k+1}},
\]

where

\[
a_k = \sum_{j=0}^{N-1} q_j z_j^k.
\]

For a truncated sum with only \( p \) terms, we have the error bound

\[
\left| \phi(z) - \sum_{k=0}^{p} \frac{a_k}{z^k} \right| \leq C \left| \frac{r}{z} \right|^p
\]
The fast multipole method

- So how do we turn this into an algorithm?
- Divide the computational domain into successively finer square grids.
- Do this until the number of particles in each box is small enough for multipole evaluation not to pay off.
- Evaluate multipole expansions whenever the source box is far enough away.
The fast multipole method

- We have to take care not to evaluate interactions more than once.
- Only treat particles in the *interaction list* of each box.
- At the finest level we use direct summation.

\[
\begin{array}{c|c|c}
\text{Box 1} & \text{Box 2} & \text{Box 3} \\
\hline
\text{Particle A} & \text{Particle B} & \text{Particle C} \\
\hline
\text{Particle D} & \text{Particle E} & \text{Particle F} \\
\end{array}
\]
The fast multipole method

- The algorithm described here is $O(N \log N)$, and technically not the FMM per se.
- For the $O(N)$ algorithm, the FMM, further machinery is needed.
- See *A short course on fast multipole methods* by Beatson and Greengard if you are curious.