Discretization

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In this lecture, we will put last week's theory on operator approximations into practise. Since we were dealing with integral equations

i) first kind: $f(x) = \int_{\partial D} K(x,y)\,\varphi(y)\,dy$

ii) second kind: $f(x) = \varphi(x) - \int_{\partial D} K(x,y)\,\varphi(y)\,dy$

we need a way to evaluate integral operators

$$A\varphi(x) = \int_{\partial D} K(x,y)\,\varphi(y)\,dy$$

where we assume ∂D to be compact and K smooth. Since we were dealing with integrals, it is natural to approximate these operators by quadrature

$$A_n\varphi(x) := \sum \alpha_k^n\, K(x, x_k^n)\,\varphi(x_k^n),$$

where α_k^n, x_k^n are the quadrature weights and nodes. This is called the Nyström method. Here we denote $(\varphi_n)_i = \varphi(x_i^n)$, $(f_n)_i = f(x_i^n)$ and $(K_n)_{ij} = K(x_i^n, x_j^n)$, then the integral equations have the nice form

$$K_n\varphi_n = f_n \qquad \text{and} \qquad (\mathrm{Id} - K_n)\varphi_n = f_n$$

Assuming that $f_n \to f$ in the L^∞ norm, we now study the convergence of these schemes. Do we get pointwise/uniform convergence?

Before we can prove anything, we need the following classical result

Theorem (Arzela-Ascoli): Let K be a compact metric space and $\mathcal{F} \subset K$ bounded. Assume that $\mathcal{F}$ is equicontinuous, i.e.

$$\forall \varepsilon > 0 : \exists \delta > 0 : \forall x_1, x_2 \in K, f \in \mathcal{F} : |x_1 - x_2| < \delta \rightarrow |f(x_1) - f(x_2)| < \varepsilon$$

Then $\overline{\mathcal{F}}$ is compact in $C(K)$.

We now can prove the following result.

Theorem: Assume that the quadrature rule is convergent and f continuous. Then the sequence $\{A_n\}$ is collectively compact and pointwise convergent.

Proof: Since the quadrature rule is convergent, one can show that there exists a constant C s.t.

$$\infty > C := \sup_n \sum_{i=1}^{n} \alpha_i^n$$

It therefore holds that

$$\| A_n \varphi \|_\infty \leq C \, \| K \|_\infty \, \| \varphi \|_\infty$$

Next, let $x_1, x_2 \in \partial\Omega$, then

$$| A_n \varphi(x_1) - A_n \varphi(x_2) | \leq C \, \| K(x_1, \cdot) - K(x_2, \cdot) \|_\infty \, \| \varphi \|_\infty$$

hence $A_n \varphi$ is continuous. If $U \subset C(\partial\Omega)$ is bounded, the Arzela-Ascoli Theorem hence implies that $A_n(U)$ is compact. Therefore $\{A_n\}$ is collectively compact.
Pointwise convergence is a consequence of the quadrature rule's convergence.

We have already seen that pointwise convergence need not imply uniform convergence, so what's the use here?

Proposition: The sequence A_n is not norm convergent.

Proof: Fix n and choose $\varepsilon < \min_{i \neq j} |x_i^n - x_j^n|$. Let $0 \leq \varphi_\varepsilon(x) \leq 1$ satisfy

$$\varphi_\varepsilon(x) = \begin{cases} 1 & x = x_i \\ 0 & \min_i |x_i - x| \geq \varepsilon \end{cases}$$

We then have

$$\|A\varphi_\varepsilon\varphi - A\varphi\| \leq \|K\|_\infty \|\varphi_\infty\| \int_{\partial\Omega} |1 - \varphi_\varepsilon| \, ds$$

which tends to 0. On the other hand, $A_n \varphi_\varepsilon \varphi = 0$. Hence

$$\|A - A_n\|_\infty = \sup_{\|\varphi\|_\infty = 1} \|(A - A_n)\varphi\|$$

$$\geq \sup_{\|\varphi_\infty\| = 1} \sup_\varepsilon \|A\varphi_\varepsilon\varphi\|$$

$$= \|A\|_\infty$$

Fortunately, for integral operators of the second kind we are in a better position

Theorem: Suppose $(Id - A)$ is invertible. For f continuous, the Nyström method converges uniformly

Proof: Follows from last lecture

Neumann-Poincaré operator

In practise, the integral kernels we work with, are not going to be smooth. As a particular example, we are going to examine the Neumann-Poincaré operator. To this end, let

$$K_D^0 : L^2(\partial D) \longrightarrow L^2(\partial D)$$
$$\varphi \longmapsto K_D^0[\varphi](x) := \frac{1}{\omega_d}\, \text{p.v.} \int_{\partial D} \frac{\langle y-x, n(y)\rangle}{|x-y|^d}\, \varphi(y)\, dy$$

The Neumann-Poincaré operator is then defined as the adjoint of K_D^0. An explicit calculation yields

$$(K_D^0)^* : H^{-1/2}(\partial D) \longrightarrow H^{-1/2}(\partial D)$$
$$\varphi \longmapsto (K_D^0)^*[\varphi](x) = \frac{1}{\omega_d}\, \text{p.v.} \int_{\partial D} \frac{\langle x-y, n(x)\rangle}{|x-y|^d}\, \varphi(y)\, dy$$

One can show that if D is of class $C^{1,\alpha}$ for some $\alpha > 0$, then it is compact.

Example: Lets take $d=2$ and $D = B_1(0)$. Then the integral kernel has the explicit form

$$\frac{\langle x-y,\, x\rangle}{|x-y|^2} \cdot \frac{1}{2-2\langle y, x\rangle} = \frac{1}{2}$$

and hence

$$(K_D^0)^*[\varphi](x) = K_D^0[\varphi](x) = \frac{1}{4\pi} \int_{\partial D} \varphi(y)\, dy$$

Unfortunately, this example is a bit misleading, since in general, the NP-operator is not self-adjoint. This actually makes it quite troublesome to handle - both analytically and numerically. Fortunately, we can remedy this through **symmetrisation**.

Let $D \subset \mathbb{R}^3$ sufficiently smooth, then the single layer potential operator is unitary from $H^{-1/2}(\partial D)$ to $H^{1/2}(\partial D)$. Calderon's identity then

yields

$$S_0^0 \circ (K_0^0)^* = K_0^0 \circ S_0^0$$

We can use this to define a Hilbert space where $(K_0^0)^*$ is self-adjoint. Denote $\mathcal{H} = H^{-1/2}$ equipped with the scalar product

$$\langle f, g \rangle_{\mathcal{H}} = \langle S_0^0[g], f \rangle_{1/2,-1/2}$$

We then have

$$\begin{aligned}
\langle (K_0^0)' f, g \rangle_{\mathcal{H}} &= \langle S_0^0[g], (K_0^0)'[f] \rangle_{1/2,-1/2} \\
&= \langle K_0^0 \circ S_0^0[g], f \rangle_{1/2,-1/2} \\
&= \langle S_0^0 \circ (K_0^0)^*[g], f \rangle_{1/2,-1/2} \\
&= \langle f, (K_0^0)^*[g] \rangle_{\mathcal{H}}
\end{aligned}$$

To make this work in two dimensions, some more care is needed as the single layer potential might fail to be invertible.

Numerical implementation

We now turn to the numerical implementation of the BEP-operator. To keep matters simple, let $D \subset \mathbb{R}^2$ sufficiently smooth and $\gamma : [0, 2\pi] \longrightarrow \mathbb{R}^2$ a parametrisation of ∂D.
If we choose the naivest quadrature rule, our discrete kernels are

$$(K_n)_{ij} = \begin{cases} \dfrac{\langle x_i - x_j, n(x_i) \rangle}{|x_i - x_j|^2} \cdot \dfrac{|\partial D|}{n} & i \neq j \\ 0 & i = j \end{cases}$$

where $T(x_i)$ is the tangent vector at x_i. Now, how do we take care of the singularity on the main diagonal? Let t_0

$$\gamma(t_0) = x_i$$

Then

$$\begin{aligned}\gamma(t_0+h) &= \gamma(t_0) + h\dot{\gamma}(t_0) + \frac{h^2}{2}\ddot{\gamma}(t_0) \\ &= x_i + hT(t_0) + \frac{h^2}{2}a(t_0)\end{aligned}$$

where T is the tangent vector and a the acceleration vector. We then have

$$\frac{\langle x_i - \gamma(t_0+h), n(x_i)\rangle}{|x_i - \gamma(t_0+h)|^2} = \frac{\langle a(t_0), n(x_i)\rangle}{2|T|^2} + O(h)$$

Thus we have found an appropriate expression!

Muller's method

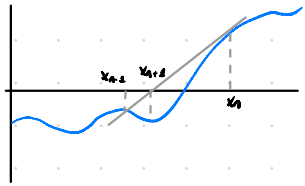
We are now in a position where we can implement the boundary layer integrals numerically. Therefore, we can also attempt to find resonances numerically. To do this, we have to find the characteristic values of $A_n(\zeta, \delta)$. It is not difficult to see that this is equivalent to finding the roots (ζ in k) of

$$\det A_n(k, \delta) = 0$$

What options do we have? Some examples are

i) Newton's method: Fast, stable but requires evaluating the derivative
ii) Secant Method: Struggles with finding complex roots

... but they are not ideal for our purposes. Instead, we will make use of Muller's Method. We begin with a quick recap of the secant method, as they are conceptually similar.

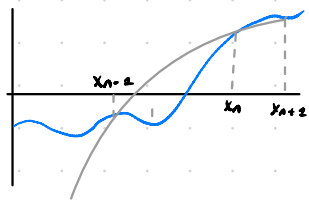


Given $(x_{n-1}, f(x_{n-1}))$, $(x_n, f(x_{n+1}))$

let $f(x) = \frac{(x_n - x)}{x_n - x_{n-2}} f(x_{n-1}) - \frac{(x_{n-2} - x)}{x_n - x_{n-1}} f(x_n)$

x_{n+1} = solution of $f(x_{n+1}) = 0$

In Muller's method, we instead use a quadratic interpolation polynomial



That is, given $(x_0, f(x_0))$, $(x_1, f(x_1))$, $(x_2, f(x_2))$, we let

$$Q(x) := a(x - x_2)^2 + b(x - x_2) + c$$

where a, b, c are choosen such that

$$Q(x_i) = f(x_i)$$

That is

$$\begin{aligned} f(x_0) &= a(x_0 - x_2)^2 + b(x_0 - x_2) + c \\ f(x_1) &= a(x_1 - x_2)^2 + b(x_1 - x_2) + c \\ f(x_2) &= c \end{aligned}$$

which then yields for a and b

$$a = \frac{(x_1 - x_2)(f(x_0) - f(x_2)) - (x_0 - x_2)(f(x_1) - f(x_2))}{(x_0 - x_1)(x_0 - x_2)(x_1 - x_2)}$$

$$b = \frac{(x_0 - x_2)^2(f(x_1) - f(x_2)) - (x_1 - x_2)^2(f(x_0) - f(x_2))}{(x_0 - x_1)(x_0 - x_2)(x_1 - x_2)}$$

By defining $\tilde{x} = x - x_2$, we find that the roots of $l(\tilde{x})$ are

$$\tilde{x} = \frac{-2c}{b \pm \sqrt{b^2 - 4ac}} = x - x_2$$

trick $\frac{-2c}{b \mp \sqrt{\ }} \cdot \frac{b \pm \sqrt{\ }}{b \pm \sqrt{\ }} = \frac{b \pm \sqrt{\ }}{2a}$

choose the sign s.t. the denominator is maximised. Then,

$$x_3 = x_2 + \tilde{x} = x_2 + \frac{-2c}{\max(b \pm \sqrt{b^2 - 4ac})}.$$

The large denominator is choosen to ensure convergence of the sequence. For sufficiently good starting values, it then follows from the standard estimates in polynomial interpolation that this sequence converges to a root of f.

Error $\sim \frac{(x_n - x_0)^{k+1}}{k+1!} \max f^{(k+1)}$

Theorem: Suppose f is C^3 and let x^* be a root of f. Assume additionally that f' is non zero in a neighbourhood of x^*. If the initial guesses x_1, x_2, x_3 are sufficiently close to x^*, then Mullers method converges to x^* and

$$|x^* - x_n| \leq C \cdot |x^* - x_{n-1}|^\nu,$$

where $\nu = 1.839$ is the Tribonacci constant.

Part II: Implementations

i) Muller's Method

We begin with an example for the Muller's method. Consider the function

$$f(x) := \sin(x) + 5$$

We deviate slightly from the tutorial notes here.

The exact roots are

$$x_1 = 2\pi n - \sin^{-1}(5)$$
$$x_2 = 2\pi n + \pi + \sin^{-1}(5)$$

We first try the secant method and note that only with complex valued initial guesses we find a correct solution.

Muller's method on the other hand also works for real-valued starting points!

ii) Neumann-Poincare Operator

Next, we take a look at the numerical implementation of the Neumann-Poincare operator.

Quick Recap: The NP-operator is

$$(K_D^w)^* : L^2(\partial D) \longrightarrow L^2(\partial D), \quad \varphi \longrightarrow \int_{\partial D} \frac{\partial G^w}{\partial n_x}(x,y)\,\varphi(y)\,d\sigma(y)$$

To realise it numerically, we discretised ∂D using a set of points $\{x_i\}_{i=1}^{nr} \subset \partial D$ to write

$$K\varphi := \begin{pmatrix} K_{11} & \cdots & K_{1nr} \\ \vdots & \ddots & \vdots \\ K_{nr1} & \cdots & K_{nrnr} \end{pmatrix} \begin{pmatrix} \varphi(x_1) \\ \vdots \\ \varphi(x_{nr}) \end{pmatrix}$$

where

$$K_{ij} := \begin{cases} \frac{\partial}{\partial n} G^k(x_i, x_j) & i \neq j \\ \text{some approximation} & i = j \end{cases}$$

We look at three examples

Ellipse: Here the exact eigenvalues admit an exact representation:

$$\lambda_j = \begin{cases} 1/2 & j = 0 \\ \pm 1/2 \left(\frac{a-b}{a+b}\right)^j \end{cases}$$

where a, b are the semi-axes

Theoretical	Numerical
0.5000	0.5000
0.4091	0.4091
−0.4091	−0.4091
0.3347	0.3347
−0.3347	−0.3347
0.2739	0.2739
−0.2739	−0.2739
0.2241	0.2241

Two disks: Suppose this time D consists of two separated disks $D = D_1 \cup D_2$ where each disk has radius r and the distance between them is ε. Then

$$\lambda^{\pm}_{\varepsilon,j} = 1/2 \pm \exp(-2|j|\gamma_0)$$

where $\gamma_0 = \sinh^{-1}\left(\sqrt{\varepsilon(r+\varepsilon/4)}\, r^{-1}\right)$.

Theoretical	Numerical
0.5000	0.5000
0.5000	0.5000
−0.2315	−0.2315
−0.2315	−0.2315
0.2315	0.2315
0.2315	0.2315
−0.1072	−0.1072
−0.1072	−0.1072

Conductivity Problem: Let $D \subset \mathbb{R}^d$ be a bounded Lipschitz domain, h a harmonic function and for $0 < k < \infty$, $k \neq 1$ define $\lambda(k) := (k+1)/(2(k-1))$. We consider the transmission problem

$$\begin{cases} \nabla \cdot \left((1 + (k-1)\chi_D) \nabla u_k \right) = 0 \\ u_k(x) - h(x) = O(|x|^{1-d}) \end{cases}$$

This has various physical interpretations. Essentially, if we think of u_k as a potential and $\sigma(x) := 1 + (k-1)\chi_D(x)$ as a piecewise constant material parameter, then

$j := \sigma \nabla u_n$ can be interpreted as flux of some soot and hence the first line is conservation of flux. The second condition then states that as $|x| \to \infty$, u_n should approach some background field.

Continuity of the flux then requires

$$\frac{\partial u_n}{\partial n}\Big|_+ = k \frac{\partial u_n}{\partial n}\Big|_-$$

If we make the ansatz

$$u_n(x) = h(x) + S_D^0[\phi](x)$$

This yields

$$\frac{\partial h}{\partial n} + \tfrac{1}{2}\phi + (K_D^0)'[\phi] = k\left(\frac{\partial h}{\partial n} - \tfrac{1}{2}\phi + (K_D^0)'[\phi]\right)$$

$$\Leftrightarrow \quad \left(\lambda(k)\,\mathrm{Id} - (K_D^0)'\right)[\phi] = \frac{\partial h}{\partial n}$$

and the problem reduces to inverting $\lambda(k)\,\mathrm{Id} - (K_D^0)'$. This is possible if $\lambda(k)$ is not in the spectrum of $(K_D^0)'$.

We now choose the following set of parameters: Let $D \subset \mathbb{R}^2$ be a disk of radius 5, $k = 3$ and $h(x) = x_1$. The solution then admits an exact representation.
$\longrightarrow$ Our numerical approximation is very good.

iii) Minnaert Resonances

Finally, we are going to put everything we've seen together and compute the Minnaert resonances.
That is, we consider a spherical bubble embedded in a liquid extending to infinity in all directions.
Denote by ρ_b and k_b denote the density and bulk modulus of the bubble and ρ, k that of the background liquid.
The governing set of equations is

$$\begin{cases} \left(\frac{1}{\rho_b}\Delta + \frac{\omega^2}{\kappa_b}\right) u = 0 & \text{in } B \\ \left(\frac{1}{\rho}\Delta + \frac{\omega^2}{\kappa}\right) u = 0 & \text{in } \mathbb{R}^2 \setminus B \\ u_+ = u_- \\ \frac{1}{\rho}\frac{\partial u}{\partial n}\Big|_+ = \frac{1}{\rho_b}\frac{\partial u}{\partial n}\Big|_- \\ \text{Sommerfeld radiation condition} \end{cases}$$

As we already know, the problem of finding the values of ω^2 for which the above has a nontrivial solution is equivalent to finding the characteristic values of

$$A(\omega, \delta) := \begin{pmatrix} S_D^{\kappa_b} & -S_D^{\kappa} \\ -\tfrac{1}{2}\mathrm{Id} + (K_D^{\kappa_b})' & -\tfrac{1}{2}\delta(\mathrm{Id} + (K_D^{\kappa})') \end{pmatrix}$$

where $\delta = \rho_b/\rho$ and $\kappa_b = \sqrt{\frac{\rho}{\kappa_b}}\,\omega$.
To solve this, we ...

i) need to approximate the layer potential
ii) discretise the boundary integral formulation
iii) solve for complex roots using Muller's method

Further reading & sources

i) Tutorial notes, Chapter 1.
ii) Haim Brezis, Functional Analysis, Sobolev Spaces and PDEs.
iii) Convergence ball and error analysis of Muller's method; Qingbiao Wu, Yaoming Ren, Weihong Bi; Applied Mathematics and Computation, 2007
iv) An Introduction to Numerical Analysis, Kendall E. Atkinson, 1989
v) Spectra and Pseudospectra, N. Trefethen