Math 126 Winter 2012: Rough lecture notes

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March 1, 2012

1 Introduction

Numerical mathematics is at the intersection of analysis (devising and proving theorems), computation (devising algorithms, coding efficiently), and addressing application areas (e.g. PDE problems in engineering, science, technology).

This course will focus on the first two: analysis, and coding/testing computer algorithms. What is numerical analysis? Trefethen [1] gives an inspiring answer: it is not merely the study of rounding errors in computations, rather, it is the study of algorithms for the problems of continuous mathematics. We should also remind ourselves that carelessness over rounding errors, and over convergence issues, in numerical algorithms has caused loss of life and equipment destruction with losses of $\$10^8$ (see Arnold disasters website). Our goal is to understand the mathematics behind our algorithms, and be able to code them reliably and invent new ones.

Our topic is the solution of PDEs via integral equations (IEs). Along the way we touch upon rounding error, quadrature, numerical linear algegra, convergence, etc.

Paradigm PDE: Let $\Omega \subset \mathbb{R}^2$ be an open connected domain. (All of this works in higher dimensions too.) The interior BVP for Laplace's equation is

$$\Delta u = 0 \text{ in } \Omega \quad (1)$$

$$u = f \text{ on } \partial\Omega \quad (2)$$

where $\partial\Omega$ denotes the boundary of the set Ω, i.e. the set of points that are both limit points of sequences in Ω and in $\mathbb{R}^2$
Omega. The 'boundary data' is the given function f on $\partial\Omega$. Applications include electrostatics (u represents electric potential), steady-state heat distribution (u is temperature), complex analysis (u is the real part of an analytic function), and Brownian motion or diffusion (u is probability density).

Paradigm IE: Let $[0, 1]$ be an interval, and we are given $f \in C([0, 1])$, and $k \in C([0, 1]^2)$ i.e. a continuous function on the unit square. Then find a function u satistfying the integral equation

$$u(t) + \int_0^1 k(t,s)u(s)ds = f(t) \qquad \text{for all } t \in (0,1) \quad (3)$$

This is a Fredholm equation, and since u itself is present on the LHS, is called '2nd kind'.

To give an idea of the intimate connection between the above BVP and IE, consider that uniqueness for the BVP is easy to prove: Let u and v be solutions, then $w = u - v$ satisfies $\Delta w = 0$ in Ω, and $w = 0$ on $\partial\Omega$. But by the maximum principle, the maximum of w over Ω cannot exceed the maximum on $\partial\Omega$, which is zero. The same holds for $-w$, so $w \equiv 0$, and we have uniqueness. In contrast, *existence* of a solution to the BVP is much harder. It was first proved by transformation of the BVP to an IE, in 1900 by Fredholm, and, along with Hilbert's work that decade, became the foundation of modern functional analysis. Here the identification is made between the 1D sets $\partial\Omega$ and $[0, 1]$. Thus the IE becomes a *boundary integral equation* or BIE.

The beautiful thing is that this method of proof leads to an efficient numerical method for solving the BVP. Crudely speaking, the efficiency stems from the reduction in dimensionality from u being an unknown function in 2D in the BVP to only in 1D in the IE.

Waves: As well as Laplace, we will also study the Helmholtz equation

$$(\Delta + \omega^2)u = 0 \tag{4}$$

where $\omega > 0$ is a frequency. What do solutions of this look like? The 1D analog is the ODE $u'' + \omega^2 u = 0$ which has solutions such as $\sin \omega x$ or $e^{i\omega x}$ which oscillate with wavelength $2\pi/\omega$. Similar things happen in higher dimensions, except that waves may travel in all directions. See picture

Notice that Laplace and Helmholtz are both *elliptic* PDE since the signs of the 2nd derivatives are the same. The contrasts with the wave equation,

$$\tilde{u}_{xx} + \tilde{u}_{yy} - \tilde{u}_{tt} = 0 \tag{5}$$

for the time-dependent field $\tilde{u}(x, y, t)$, which could represent acoustic pressure, for example. The wave equation is *hyperbolic* since its has mixed signs of 2nd derivatives. The mnemonic is to convert derivatives to powers of the coordinate (this is actually called the 'symbol' of a differential operator; see pseudodifferential operators):

$$\begin{array}{lclcl} u_{xx} + u_{yy} = 0 & \leftrightarrow & x^2 + y^2 = \text{const} & \leftrightarrow & \text{ellipse (here happens to be a circle)} \\ u_{xx} - u_{yy} = 0 & \leftrightarrow & x^2 - y^2 = \text{const} & \leftrightarrow & \text{hyperbola} \end{array}$$

Equations such as the heat equation have no 2nd-derivative in one of the variables, and are thus parabolic. Given even rough boundary data, elliptic PDEs lead to very smooth (even sometimes analytic) solutions; on the other hand, with hyperbolic PDEs rough initial data is carried along characteristics and remains nonsmooth. The picture for the wave equation is of the light cone disturbance produced by point-like initial data at the origin at $t = 0$.

The Helmholtz equation follows from the wave equation when the assumption of motion in time at a single frequency is made, e.g. if I were to sing in this room with a pure tone at a single frequency, the pressure field would settle into one with 'harmonic' time-dependence

$$\tilde{u}(x, y, t) = u(x, y)e^{-i\omega t}$$

Substitution of this into (5) and canceling exponential factors gives (4).

When waves traveling in free space hit an obstacle this is a scattering problem. One then needs to solve an exterior problem, with (4) holding in the unbounded domain $\mathbb{R}\ \overline{\Omega}$, with given boundary data as before, and a so-called 'radiation condition'.

What BIE methods are good for: Piecewise-homogeneous media, i.e. the coefficients of the PDE are constant in chunks of space touching on lower-dimensional boundaries. BIEs are excellent especially for exterior problems, finite element methods cannot easily handle the infinite extent of the domain. Also, BIE are excellent for high frequencies $\omega \gg 1$, since then there are many wavelengths across the domain, and the lower dimensionality of BIE vs FEM is a huge advantage.

What BIE methods are not good for: Variable-coefficient PDEs, or nonlinear PDEs. Note that there are IE methods for some of these, namely, volume-integral based methods such as Lippman-Schwinger.

2 Numerical Linear Algebra: Stability and Conditioning

Well, now we go over to scanned paper lectures...

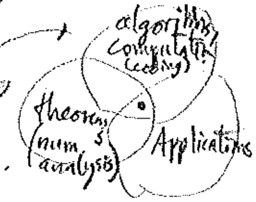
(One day I will TEX up the whole thing)

References

[1] L. Trefethen. The definition of numerical analysis. *SIAM News*, November 1992. `http://people.maths.ox.ac.uk/trefethen/essays.html`.

M126 (Lec 1)   welcome - info slips.   • slips • LNT article. • HW1.   ① 1/5/12

Numerical math:



Focus on these two.

⇒ your HW is mix of theory & coding numerical methods & experiments. ← practical skills for any math/scientist

Topic: solution of PDEs via integral equations (IEs)

eg. interior BVP: given domain $\Omega \subset \mathbb{R}^2$, cont. func f on $\partial\Omega$ (bdry of Ω). Find func $u(x,y)$

$$\begin{cases} \text{st. } \Delta u = 0 \text{ in } \Omega, \text{ Laplace's eqn.} \\ \text{ask? } \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \text{ in } \mathbb{R}^2. \\ \& \quad u = f \text{ on } \partial\Omega \quad \text{boundary data.} \end{cases}$$

App: electrostatics (show website), heat steady state, diffusion chemicals.
We will develop some PDE & IE theory along the way.

→ given $f \in C([0,1])$ ← ask? cont.
$k \in C([0,1]^2)$ ← ask? func on the square.

Then find func u solving
$$u(t) + \underbrace{\int_0^1 k(t,s)\,u(s)\,ds}_{\text{func of } t\text{: operator acting on } u} = f(t) \quad \forall t \in [0,1].$$
Fredholm IE "2nd kind".

Eg
• uniqueness of BVP is simple. (← max. principle — anyone heard of?)
• but existence is hard: first proven using IEs (100 yrs ago: Fredholm, Hilbert).

The link between BVPs & IEs: instead of [0,1], use the boundary $\partial\Omega$.
Beautiful mathematics & gives efficient num alg! since reduction from 2d to 1d prob! BIE.

We will need other key numerical areas such as rounding errors, quadrature, lin. algebra, convergence...
What is num anal? LNT essay: not just errors, (read from essay). → { • impact of computation huge: 3rd branch of sci. • NA disasters both. Math, Algs key. • goal: understand math behind algs, code your own.

30 mins. Syll. (show online). HW → post online, do in Latex. project (hence HW1 due 11 days).
X-hrs — coding. eg. meet Wed 3-3:50 do Matlab exercises (please install & go through intro codes).
Languages - doesn't have to be Matlab.
books; we draw from several. Take notes.

Waves? different PDE: $(\Delta + \omega^2)u = 0$ Helmholtz: acoustics, also Maxwell (light, radar) in certain cases.
ω = freq. of waves.
solns. oscillate in space. Why? 1d version $u'' + \omega^2 u = 0$
eg show pic on website top. is ODE w/ solns: $\begin{cases}\sin \omega x \\ \cos \omega x\end{cases}$ ← repeats when $\omega x = 2\pi$ ie $x = \frac{2\pi}{\omega}$ wavelength.

Comes from wave eqn. for $\tilde{u}(x,y,t)$: $\tilde{u}_{xx} + \tilde{u}_{yy} - \tilde{u}_{tt} = 0$ WE (wave speed = 1).
assume const. freq. $\tilde{u}(x,y,t) = u(x,y)\,e^{-i\omega t}$ sub into WE: $\tilde{u}_{tt} \to (-i\omega)^2 \tilde{u}$
cancel $e^{-i\omega t}$ since holds $\forall t$ ⇒ Helmholtz.
Note Laplace & Helm are elliptic PDE (same sign in 2nd derivs), but WE is hyperbolic (1 different sign) → { elliptic: smooth solns; hyperbolic: char.
• Scattering: send in a solution to Helm in $\mathbb{R}^2$ (eg. plane wave), but which 'hits' obstacle Ω.

solve exterior BVP
$$\begin{cases} (\Delta + \omega^2) u = 0 & \text{in } \underbrace{\mathbb{R}^2 \setminus \bar{\Omega}} \\ u = f & \text{on } \partial\Omega. \\ \text{'radiation condition'}. \end{cases}$$

② 1/5/12

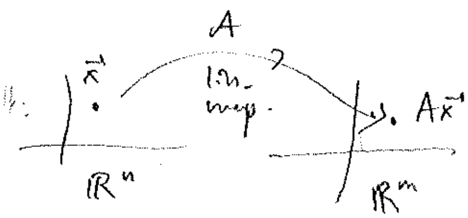
? who's seen?
Ω = open set
$\bar{\Omega}$ = closure.
so $\mathbb{R}^2 \setminus \bar{\Omega}$ excludes $\partial\Omega$.

50 mins. break?

Num. Lin. Alg.

(Tref + Bau book).

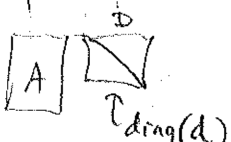
solve $A\vec{x} = \vec{b}$ $\quad A \in \mathbb{C}^{m \times n}$ matrix



Review.
mat-vec mult: $A\vec{x}$ is lin. combo of cols of A w/ coeffs $x_1 \cdots x_n$.

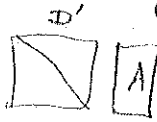
col $\vec{a}_1$ $\quad$ col $\vec{a}_n$

Rescaling columns: what mult A by if want col $\vec{a}_j$ to become $d_j \vec{a}_j$ where $\vec{d} \in \mathbb{C}^n$ given?



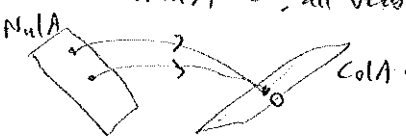
postmultiply A by D.

what does



do? rescale rows.

Spaces $\quad \text{Col} A = \text{Span}\{\vec{a}_j\} \subset ? \mathbb{R}^m$
$\text{Nul} A = ?$ all vects which A kills $= \{\vec{x} : A\vec{x} = \vec{0}\} \subset \mathbb{R}^n$



dim Col$A$ called? rank(A) = # pivots $\le \min(m,n)$

Say A 'tall' $m > n$: when is A (map) one-to-one?

each $\vec{y} = A\vec{x}$ must be unique lin combo of $\{\vec{a}_j\}$ $\Rightarrow$ cols lin. indep $\Rightarrow$ dim Col$A = n$
Converse also

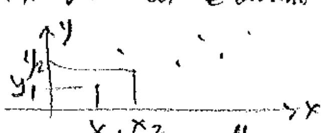
$\Rightarrow$ Thm $(m \ge n)$: A full rank $\Leftrightarrow$ map 1-1 (soln to $Ax = b$ unique, if exists).

Square case $m = n$, (lin. alg). full rank $\Leftrightarrow$ A^{-1} exists (nonsingular) st $A^{-1}A = AA^{-1} = I$. $\Leftrightarrow$ soln $x = A^{-1}b$ exists, unique, for all b.

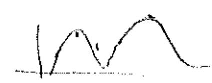
App: polynomial approx.

let $\{x_j\}_{j=1}^n$ be distinct set of reals
Claim: $n \times n$ matrix A w/ element $a_{ij} = x_i^{j-1}$ $\; i,j = 1 \cdots n$ is nonsingular.

How A arise? data $(x_j, y_j)_{j=1}^n$ pts in plane.



What is $n-1$ th degree poly passing exactly thru data?



$\vec{c}$ = coeffs, $= \{c_0, \cdots c_{n-1}\}$ $\quad p_{\vec{c}}(x) = c_0 + c_1 x + c_2 x^2 + \cdots c_{n-1} x^{n-1}$

match at each pt:
Lin. eqns: $p(x_j) = y_j$ ③ 1/?/12

ie
$$\left\{\begin{array}{l} c_0 + c_1 x_1 + \cdots c_{n-1} x_1^{n-1} = y_1 \\ \vdots \\ c_0 + c_1 x_n \cdots c_{n-1} x_n^{n-1} = y_n \end{array}\right\} \quad A\vec{c} = \vec{y}$$

Vandermonde matrix.

Supp. $\vec{c} \neq \vec{c}'$ were two such solns,

Then $p_{\vec{c}}(x) - p_{\vec{c}'}(x)$ is nontriv. degree-$(n-1)$ poly vanishing at each x_j, ie have n distinct roots $\Rightarrow$ impossible. $\Rightarrow \vec{c}$ unique $\Rightarrow A$ full rank. $\square$

Matlab interlude: (proj)

$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$ rank(A) = 2. change $\begin{bmatrix} 1 & 2 \\ 3 & 6 \\ 5 & 10 \end{bmatrix}$ rank = 1. null(A) = $\begin{bmatrix} 2/\sqrt{5} \\ -1/\sqrt{5} \end{bmatrix}$.

n = 10;

~~x = -1 : 0.1 : 1~~ linspace(-1, 1, n)

A = vander(x); A = A(:, end:-1:1) ← reverse order of cols.

A ⟶ hard to see #s by eye ⟶ ways to view: imagesc(A), spy(A), plot(A) ← graphs each col.

rank(A) = 10 as Thm says. ~~but solve~~.

ok try n = 30, 40, 100 : rank(A) never > 36. why?

numerical rank ≠ Theor. rank

n = 10; size of soln x ~ 10^2

n = 20 " ~ grows!

→ 10^{16} when size 40 same place!

need singular values of A.

M126 lec 2 — SVD, Conditioning, Stability. ACMS @ 4pm here. · ellipse.m, WS (→ laptop). ① 1/10/12

Orthogonality (review lin. alg.)

A matrix, A^* hermitian transpose : $(A^*)_{ij} = \overline{A_{ji}}$ c.c.

$A = A^*$ symm?..

Ex. prove $(AB)^* = B^*A^*$, $(A^{-1})^* = (A^*)^{-1}$

x col. vec, x^* row vec.

$x, y \in \mathbb{C}^m$, $x^*y = ?$ inner prod $[\rightarrow]\begin{bmatrix}\downarrow\end{bmatrix} = \sum_{i=1}^m \bar{x}_i y_i$ 2-norm $\|x\|_2 := \sqrt{x^*x}$ won't always write.

Defn of a norm? i) $\|\alpha x\| = |\alpha|\,\|x\|$ α scalar
ii) $\|x\| = 0 \Rightarrow x = 0 \leftarrow$ vector.
iii) $\|x+y\| \le \|x\| + \|y\|$ tri

2-norm also has. $|x^*y| \le \|x\|\,\|y\|$ Cauchy–Schwarz

$x^*y = 0$? x, y orthog.

Thm: mutually orthog. set of vectors are lin. indep. (pf: Ex).

$\Rightarrow$ m orthog. vecs in $\mathbb{C}^m$ form basis; if unit length, o.n.b.

Say $\vec{q}_1, \dots \vec{q}_m \in \mathbb{C}^m$ o.n.b., can stack into cols. of Q, then $(Q^*Q)_{ij} = i[\rightarrow]\,\overset{j}{[\downarrow]} = q_i^* q_j = \delta_{ij}$ i,j^{th} entry.

so $Q^*Q = I$ i.e. $Q^{-1} = Q^*$ $\boxed{\text{cols o.n.b.} \Leftrightarrow \text{unitary}}$

so Q^*b is coeffs of expansion of b in o.n.b $\{q_i\}$

$\|Qx\| = \sqrt{(Qx)^*Qx} \overset{?}{=} \sqrt{x^*\cancel{Q^*Q}x} = \|x\|$. preserves lengths. (rotation, poss w/ reflectn)

Matrix 2-norm: $\|A\|$ ← 2 implied, smallest # c st. $\|Ax\| \le c\|x\|$ $\forall x \in \mathbb{C}^m$

"max growth factor"

or $\|A\| := \sup_{x \ne 0} \frac{\|Ax\|}{\|x\|} = \sup_{\|x\|=1} \|Ax\|$

Eg i) 2-norm of diag matrix? Its largest-magnitude entry.

ii) 2-norm of $A = uv^*$? (rank-1). $\|u\underbrace{v^*x}_{\text{scalar}}\| = \underbrace{|v^*x|\,\|u\|}_{\text{C-S}} \le \underbrace{\|v\|\,\|u\|}_{=\|A\|}\|x\|$

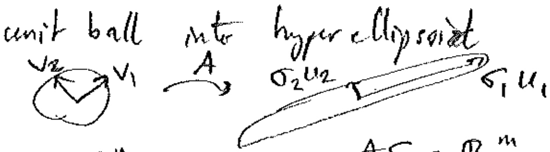
2-norm submultiplicative: $\|ABx\| \underset{\text{why?}}{\le} \|A\|\,\|Bx\| \le \|A\|\,\|B\|\,\|x\|$

So $\|AB\| \le \|A\|\,\|B\|$.

Ex. show QA & AQ have same 2-norm as A. (Thm 3-1)

Singular Value Decomposition (SVD) — as important as spectral decomp.

Geom fact: every $A \in \mathbb{C}^{m\times n}$ maps unit ball into hyperellipsoid



$S \subset \mathbb{R}^n$ $\qquad$ $AS \subset \mathbb{R}^m$

($\mathbb{C}^n$ harder to plot!) $\qquad$ show ellipse.m. 2×2 case.

'tall' case $m \geq n$ & full rank ($=n$): left sing. vecs $u_1 \cdots u_n$ unit orthog.
sing. vals. $\sigma_1 \geq \sigma_2 \geq \cdots \sigma_n > 0$ semiaxes.
so what is $\|A\|$? $= \sigma_1$
right sing. vecs v_j $j=1\cdots n$, unit preimages of $\sigma_j u_j$ also orthog amazingly! $\Rightarrow$ o.n.b. for $\mathbb{C}^n$.

rank $r<n$ then $\sigma_1, \cdots \sigma_r > 0$ while $\sigma_{r+1} = \cdots \sigma_n = 0$.

So $Av_j = \sigma_j u_j$ $\quad j = 1 \cdots n$.

$$A \underbrace{\begin{bmatrix} v_1 & \cdots & v_n \end{bmatrix}}_{V} = \underbrace{\begin{bmatrix} u_1 & \cdots & u_n \end{bmatrix}}_{\hat U} \underbrace{\begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_n \end{bmatrix}}_{\hat\Sigma}$$

(postmult by V^*) so $A = \underset{m\times n}{\hat U}\ \underset{n\times n}{\hat \Sigma}\ \underset{n\times n}{V^*}$ reduced SVD.

May complete $\underset{m\times n}{\hat U}$ to $\underset{m\times m}{U}$ o.n.b. for $\mathbb{C}^m$.
& pad $\underset{n\times n}{\hat\Sigma}$ to $\underset{m\times n}{\Sigma}$

then $A = \underset{m\times m}{U}\ \underset{m\times n}{\Sigma}\ \underset{n \times n}{V}$ $\qquad$ (analogous if $m<n$)

Thm (eg. 4.1 in NLA): every $A \in \mathbb{C}^{m\times n}$ has SVD, $\{\sigma_j\}$ unique,
& if σ_j simple, u_j & v_j unique up to phase.

Every matrix is rotation (w/ refl.) $\to$ coord stretch $\to$ rot. (w. refl.) even nonsymm or nonsquare ones. (cf. spectral decomp may not exist.)

or: every matrix is diag in correct bases for $\mathbb{C}^n$ & $\mathbb{C}^m$ (V^* projects to coeffs of onb)

If A square invertible, $A^{-1} = (U\Sigma V^*)^{-1} \overset{?}{=} V\Sigma^{-1}U^*$ is the SVD of A^{-1} (if reorder Σ^{-1}!)
$\Sigma^{-1} = \operatorname{diag}\{\sigma_j^{-1}\}$ $\quad$ What is $\|A^{-1}\|$? largest sing val of A^{-1} $= \sigma_n^{-1}$ smallest sing val of A.

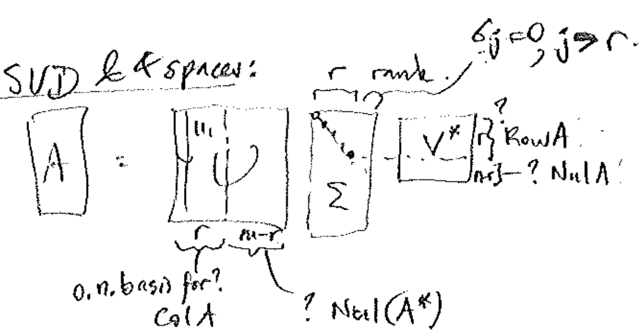
$\to$ WS (PTO). $\qquad$ needed for WS.

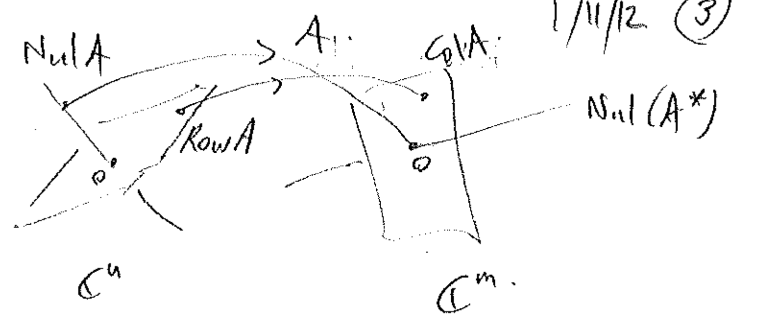
break

Notes on SVD: existence pf either by induction (NLA Ch. 4 — beautiful proof: grad studs read)
or A^*A has eigvals $\{\sigma_j^2\}$ & complete eigvecs v_j o.n.b. $\quad$ why? A^*A symm.
AA^* " " " u_j "
eigvals $\lambda_j \geq 0$ & then define $\sigma_j = \sqrt{\lambda_j}$.

1/11/12 ③

Anatomy: SVD & 4 spaces:





rank $r := \#\{j : \sigma_j > 0\}$

numerical rank $r_\varepsilon := \#\{j : \sigma_j > \varepsilon\}$ $\quad \varepsilon \sim \sigma_1 \varepsilon_{mach}$ (machine precision! $\sim 10^{-16}$)

Qu: what do think σ_j's of Vandermonde did? Shot down to ε when $m \sim 40$.

Conditioning (§12 NLA) : property of a math problem (vs. Stability: property of alg. used to solve it).

problem is map $f : X \to Y$ (X: problem input space, Y: space of sol'ns) $\quad$ eg. $f(x)$ could return $\begin{cases} \cdot\ 2x & \text{the easy "doubling prob"} \\ \cdot \text{ vector of roots of poly given } x = \text{vec. of poly coeffs.} \end{cases}$

f well-cond if infinitesimal pert δx (one symbol!) n x causes 'small' pert $\delta f := f(x+\delta x) - f(x)$ in soln.

Abs. cond. # $\hat{\kappa} = \hat{\kappa}(x) := \lim_{\delta \to 0} \sup_{\|\delta x\| \le \delta} \frac{\|\delta f\|}{\|\delta x\|} \overset{\text{abbrev}}{=} \sup_{\delta x} \frac{\|\delta f\|}{\|\delta x\|}$ (2-norms)

if x, f vectors, ($\mathbb{C}^n$, $\mathbb{C}^m$) $\quad \frac{\partial f_i}{\partial x_j} = J_{ij}(x)$ is Jacobean matrix $J \in \mathbb{C}^{m \times n}$

As $\|\delta x\| \to 0$ have $\delta f \approx J(x)\,\delta x$ so $\hat{\kappa}(x) = \|J(x)\|$ matrix 2-norm.

more useful is:

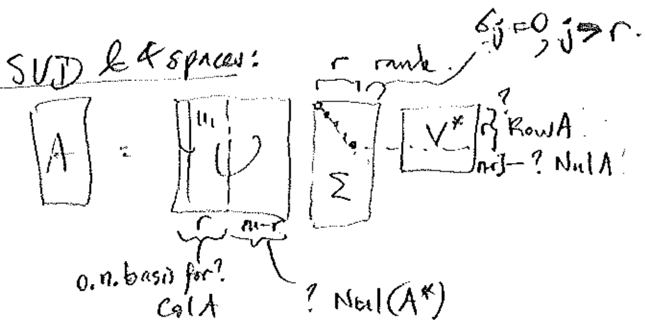
Rel. cond # $\kappa := \sup_{\delta x} \frac{\|\delta f\| / \|f\|}{\|\delta x\| / \|x\|} = \frac{\|J(x)\|_2}{\|f\| / \|x\|}$ $\quad$ important since compute brings in relative errors.

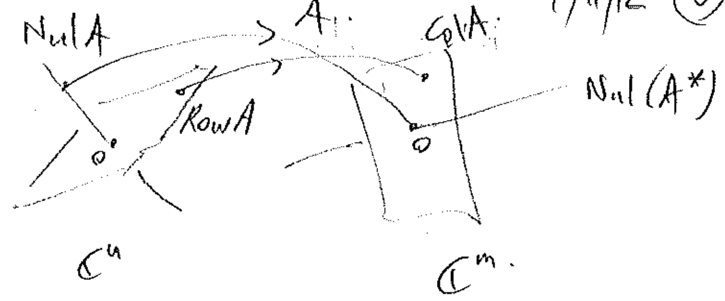
$\kappa < 10^3$ 'well cond'
$\gg 10^3$ ill-cond

Basic ops:
- $f(x) = x/2$ $\ (m=n=1)$ $\ J = f' = 1/2$ so $\kappa = \frac{|1/2|}{1/2} = 1$.
- $f(x) = x^\alpha$ $\quad J = f' = \alpha x^{\alpha-1}$ $\quad \kappa = \frac{|\alpha x^{\alpha-1}|}{x^\alpha / x} = |\alpha|$. $\ll 10^3$ well-cond for reasonable powers.
- $f(x_1, x_2) = x_1 - x_2$ subtraction $(n=2, m=1)$. $\quad J = [1\ -1]$ $\quad \|J\| = \sqrt{2}$
  $\kappa = \frac{\sqrt{2}\sqrt{x_1^2 + x_2^2}}{|x_1 - x_2|} \to \infty$ as $x_1 \to x_2 \neq 0$. can be ill-cond.
- $f(x) = \sin x$, for $x \approx 10^{100}$ say: $\|J\| \le 1$ but $\kappa = \frac{\|J\|\,|x|}{|\sin x|} \ge |x| = $ huge. (but abs cond # ≤ 1).
- finding poly roots ill-cond
- eigvals of nonsymm matrices: eg $A = \begin{bmatrix} 1 & 10^3 \\ & 1 \end{bmatrix}$ vs $\begin{bmatrix} 1 & 10^3 \\ 10^{-3} & 1 \end{bmatrix}$ $\quad \|\delta x\| = 10^{-3}$
  $\lambda = \{1, 1\}$ $\quad \lambda = \{0, 2\}$ $\quad \|\delta f\| \sim 1$
  $\hat{\kappa} \sim 10^3,\ \kappa \sim 10^6$

but symm, $\hat{\kappa} \approx 1$.

Anatomy: SVD & 4 spaces: 1/11/12 (3)





rank $r := \#\{j : \sigma_j > 0\}$

numerical rank $r_\varepsilon := \#\{j : \sigma_j > \varepsilon\}$ $\qquad \varepsilon \sim \sigma_1 \varepsilon_{mach}$ (machine precision! $\sim 10^{?} \leftarrow -16$

Qu: what do think σ_j's of Vandermonde did? Shot down to ε when $m \sim 40$.

Lec 3

Conditioning (§12 NLA) : property of a math problem (vs. Stability: property of alg. used to solve it).

problem is map $f : \underset{\text{problem input space}}{X} \longrightarrow \underset{\text{space of solns.}}{Y}$ $\qquad$ eg. $f(x)$ could return $\begin{cases} \cdot\ 2x & \text{the easy "doubling prob"!} \\ \cdot\ \text{vector of roots of poly given } x = \text{vec. of poly coeffs.} \end{cases}$

f well-cond if infinitesimal pert δx (one symbol!) in x causes 'small' pert $\delta f := f(x+\delta x) - f(x)$ in soln.

<u>Abs.</u> cond. # $\hat{\kappa} = \hat{\kappa}(x) := \lim_{\delta \to 0} \sup_{\|\delta x\| \leq \delta} \dfrac{\|\delta f\|}{\|\delta x\|} \overset{\text{abbrev}}{=} \sup_{\delta x} \dfrac{\|\delta f\|}{\|\delta x\|}$

2-norms

if x, f vectors ($\mathbb{C}^n$, $\mathbb{C}^m$), $\dfrac{\partial f_i}{\partial x_j} = J_{ij}(x)$ is Jacobean. matrix $J \in \mathbb{C}^{m \times n}$

As $\|\delta x\| \to 0$ have $\delta f \approx J(x)\,\delta x$ so $\hat{\kappa}(x) = \|J(x)\|$ matrix 2-norm.

more useful is:

<u>Rel</u>. cond # $\kappa := \sup_{\delta x} \dfrac{\|\delta f\| / \|f\|}{\|\delta x\| / \|x\|} = \dfrac{\|J(x)\|_2}{\|f\| / \|x\|}$ $\qquad$ important since computer brings in <u>relative</u> errors.

$\kappa < 10^3$ 'well cond'
$\quad \gg 10^3$ ill-cond

Basic ops: $\cdot\ f(x) = x/2 \quad (m=n=1) \quad J = f' = 1/2 \quad$ so $\kappa = \dfrac{|1/2|}{1/2} = 1$.

do as W/S:

- $f(x) = x^\alpha \qquad J = f' = \alpha x^{\alpha-1} \qquad \kappa = \dfrac{|\alpha x^{\alpha-1}|}{x^\alpha / x} = |\alpha|$. $\ll 10^3$ well-cond for reasonable powers.
- $f(x_1, x_2) = x_1 - x_2$ subtraction $(n=2, m=1)$. $J = [1\ \ -1] \quad \|J\| = \sqrt{2}$
  $\kappa = \dfrac{\sqrt{2}\sqrt{x_1^2 + x_2^2}}{|x_1 - x_2|} \to \infty$ as $x_1 \to x_2 \neq 0$. can be ill-cond.
- $f(x) = \sin x$, for $x \approx 10^{100}$ say: $\|J\| \leq 1$ but $\kappa = \dfrac{\|J\|\,|x|}{|\sin x|} \geq |x| = $ huge. (but abs cond # ≤ 1).

- finding poly roots ill-cond
- eigvals of <u>nonsymm</u> matrices: eg $A = \begin{bmatrix} 1 & 10^3 \\ & 1 \end{bmatrix}$ vs $\begin{bmatrix} 1 & 10^3 \\ 10^{-3} & 1 \end{bmatrix}$ $\qquad \|\delta x\| = 10^{-3}$
  $\lambda = \{1, 1\}$ $\qquad \lambda = \{0, 2\}$ $\qquad \|\delta f\| \sim 1$
  $\hat{\kappa} \sim 10^3,\ \kappa \sim 10^6$

but <u>symm</u>, $\hat{\kappa} \approx 1$.

Mat-vec mult? $f(x) = \underset{m\times m}{A}x \xrightarrow{J=?A} \kappa = \|A\| \dfrac{\|x\|}{\|Ax\|}$ → if A nonsing., $\le \|A^{-1}\|$, why? ② 1/11/12

pf: $\|x\| = \|A^{-1}Ax\| \le \|A^{-1}\|\,\|Ax\|$ ← defn of 2-norm

with equality if $x = v_m$. so, tight. ← Ex: check.

so $\kappa \le \|A\|\,\|A^{-1}\|$

Solving lin sys? $Ax = b$ so soln is $f(b) = A^{-1}b$ replace A by A^{-1} in above, get again $\kappa \le \|A^{-1}\|\|A\|$.

w/ equality if $b = u_1$

call $\|A\|\|A^{-1}\| =: \kappa(A)$ cond # of matrix A $= \dfrac{\sigma_1}{\sigma_m}$ = eccentricity of hyperellipse. ← Ex: check.

What if A perturbed instead, in solving lin sys? input is A, output x (b held const).

consider infinitesimal changes: δA causing δx

$(A + \delta A)(x + \delta x) = b$

so $\underbrace{\cancel{Ax}}_{\text{cancels } b} + \delta A x + A\delta x + \cancel{\delta A \delta x} = \cancel{b}$ ignore to 1st order

so $\delta x = -A^{-1}\delta A x$, $\dfrac{\|\delta x\|}{\|x\|} \le \|A^{-1}\|\,\|\delta A\|$

rel. cond #:

⇒ Thm (12.2): $\dfrac{\|\delta x\|/\|x\|}{\|\delta A\|/\|A\|} \le \|A^{-1}\|\|A\| = \kappa(A)$ again.

- since A, b stored to 16 digits, expect to get x to $16 - \log_{10}\kappa$ digits acc.

Floating Point

$x \in \mathbb{R}$ digital rep: finite # bits ⇒ finite subset F of $\mathbb{R}$ ⇒ must be { lowest & highest $\pm 10^{308}$ ← in IEEE 'double prec' system. gaps!

eg $[1,2]$ rep by set $\{\underbrace{1,\ 1+2^{-52}},\ 1+2\cdot 2^{-52}, \dots 2\}$

$[2,4]$ is twice these (larger gaps!). relative gap 2.2×10^{-16} never exceeded.

(but a poor algorithm can cause this to dominate).

Formally, base $= \beta = 2$, precision $= t = 53$

set is $F = \{0, \pm \dfrac{m}{\beta^t}\beta^e, \overbrace{\pm \mathrm{Inf},\ \mathrm{NaN}}\}$ special codes, rather than members of $\mathbb{R}$.

$\beta^{t-1} \le m \le \beta^t$

so $\dfrac{m}{\beta^t} \in [\frac{1}{\beta}, 1]$

$e \in \mathbb{Z}$ exponent (we ignore over/underflow: that there is in fact a largest $|e|$).

Note $\beta F = F$, self-similar.

$\varepsilon_{mach} = \frac{1}{2}\beta^{1-t}$ is largest relative error: ie $\forall x \in \mathbb{R}, \exists x' \in F$ s.t. $|x' - x| \le \varepsilon_{mach}|x|$

β^{1-t}: largest rel. gap.

let such an x' be called $fl(x)$

Then $\forall x \in \mathbb{R}, \exists \varepsilon, |\varepsilon| \le \varepsilon_{mach}$ s.t. $fl(x) = (1+\varepsilon)x$ bounded rel. err.

IEEE double precision $\varepsilon_{mach} = 2^{-53} \approx 1.1\times 10^{-16}$

③ 1/12/12

Arithmetic let $\oplus\ \ominus\ \otimes\ \oslash$ be analogs of $+ - \times \div$ except done by machine.

let $\circledast$ be any of 4: could require $x \circledast y = fl(x * y)$, ie gives the unique rounding of answer.

But only need weaker: Fund Axiom of Floating pt:

$$\forall x, y \in F \quad \exists \varepsilon \text{ w/ } |\varepsilon| \le \varepsilon_{mach} \text{ s.t. } x \circledast y = (1+\varepsilon)(x * y)$$

ie rel. err bnded by ε_{mach}.

For $\mathbb{C}$ instead of $\mathbb{R}$, turns out to be $2^{3/2}\varepsilon_{mach}$, similar.

Stability (§14 NLA) alg getting 'right' ans. even if not exact.

fix: { problem $f: X \to Y$ eg $y = \sin x$ or y is soln to $Ay = b$ (here 'x' data is A, b).
fl. pt. sys
algorithm for f, also a map $\tilde{f}: X \to Y$

Steps in alg: $\underset{\text{input}}{\overset{\text{data}}{x}} \xrightarrow{\text{round}} fl(x) \xrightarrow[\text{alg}]{\text{machine}} \tilde{f}(x)$

Defn relative error of computation $\dfrac{\|\tilde{f}(x) - f(x)\|}{\|f(x)\|}$ ← alg. certainly good if this is $O(\varepsilon_{mach})$
'of the order of',

Formally: $O(\varepsilon_{mach})$ means $\le C\varepsilon_{mach}$ as $\varepsilon_{mach} \to 0$
ie a family of floating pt sys, for some const C, uniformly over all data $x \in X$.

Practically: $< 10^3 \varepsilon_{mach}$ ok, $> 10^8 \varepsilon_{mach}$ not ok.

But if problem f ill-cond, unreasonable to demand this! Why? rounding on input changes $x \to fl(x)$ & if κ v. high, change gets blown up by κ so even if alg. exact, cannot have $O(\varepsilon_{mach})$ rel. err in output.

Instead: defn

Alg Stable if $\forall x \in X$, $\dfrac{\|\tilde{f}(x) - f(\tilde{x})\|}{\|f(\tilde{x})\|} = O(\varepsilon_{mach})$ for some $\tilde{x}$ s.t. $\dfrac{\|\tilde{x} - x\|}{\|x\|} = O(\varepsilon_{mach})$

"nearly right answer to nearly right question"

stronger: Backward stable: $\forall x \in X$, $\tilde{f}(x) = f(\tilde{x})$ for some $\tilde{x}$ s.t. $\dfrac{\|\tilde{x} - x\|}{\|x\|} = O(\varepsilon_{mach})$

"exactly right ans. to nearly right question".

Eg [§15] is $\ominus$ bkw stable? prob is $f(x_1, x_2) = x_1 - x_2$
alg. is $\tilde{f}(x_1, x_2) = fl(x_1) \ominus fl(x_2)$

$$= [x_1(1+\varepsilon_1) - x_2(1+\varepsilon_2)](1+\varepsilon_3) \overset{\text{set}}{=} x_1(1+\varepsilon_4) - x_2(1+\varepsilon_5) = f(\tilde{x}_1, \tilde{x}_2)$$

for $|\varepsilon_i| \le \varepsilon_{mach}$ $i = 1,2,3$.

$|\varepsilon_4|, |\varepsilon_5| \le 2\varepsilon_{mach} + O(\varepsilon_{mach}^2)$

exact for some data rel. close to x_1, x_2.

[lec 4. cont]

(4) 1/12/12

Is $f(x) = x \ominus 1$ bkw st? $\tilde{f}(x) = [x(1+\varepsilon_1) - 1](1+\varepsilon_2) \overset{\text{set}}{=} x(1+\varepsilon_3) - 1 =: f(\tilde{x})$.

how big is ε_3? $x\varepsilon_3 = x(\varepsilon_1+\varepsilon_2+O(\varepsilon^2)) - \varepsilon_2$

so $\varepsilon_3 = \varepsilon_1+\varepsilon_2 - \frac{\varepsilon_2}{x} = O(\varepsilon_{mach}) + \frac{1}{x}O(\varepsilon_{mach})$

So as $x \to 0$, not bkw stable. But, is stable.

Some algs unst! (eg. poly roots)

meaning: computed soln $\tilde{y}$ sat. $(A+\delta A)\tilde{y} = b$ exactly for some δA with $\|\delta A\|/\|A\| = O(\varepsilon_{mach})$

Take-home msg: algs (in Matlab, LAPACK, etc) for solving $Ay=b$ are bkw stable (A is data 'x', y is answer '$f(x)$')

$m=n$ (nonsing. square): QR is (Thm 16.2 NLA)

Gaussian elim. w/ partial pivoting is Ch. 22. (if avoid incredibly rare pathological matrices)

$m>n$: least-squares soln, ie find x st. $\|Ax-b\|$ minimized.

is bkw stable via SVD (Thm 19.4)

How do? $A \backslash b$ mldivide does it.

~~of~~ or, explicitly, $A = U\Sigma V^*$ so $x = \underbrace{V^*\Sigma^{-1}U}_{\text{pseudoinverse}}b =: A^+b$

Reminder: $\frac{\|\tilde{y}-y\|}{\|y\|}$ may not be small, ie y itself inaccurate! What is only cause of this in bkw.-stable alg? κ v. large.

But in this case, such is bkw st: as good as one could hope for!

How accurate is $\tilde{y}$, ie $\tilde{f}(x)$? For any bkw-stable alg: $x \to f(x)$

Thm (15.1): if cond # is $\kappa(x)$ for problem $f(x)$, alg is bkw st, and computer obeys floating pt axioms, then rel. err. satisfies

$$\frac{\|\tilde{f}(x) - f(x)\|}{\|f(x)\|} = O(\kappa(x)\,\varepsilon_{mach})$$

- Ie, error is κ times worse. If $\kappa > 10^{16}$ you lose all digits of $f(x)$, or of y. But it still holds that $(A+O(\varepsilon_{mach}))\tilde{y} = b$ exactly!
- Pf easy: by defn. $\tilde{f}(x) = f(\tilde{x})$ (a) for some $\frac{\|\tilde{x}-x\|}{\|x\|} = O(\varepsilon_{mach})$ (b)

Defn. of κ: $\frac{\|f(\tilde{x}) - f(x)\|}{\|f(x)\|} \le (\kappa + o(1))\frac{\|\tilde{x}-x\|}{\|x\|}$ & sub in (a) & (b). QED.

since not infinitesimal.

Stability & rounding done.

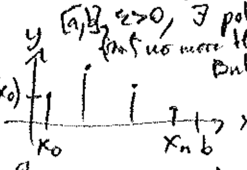
Lec 4 part 2. ① 1/17/12

Interpolation [from Kress NA §8.1]

Approx func f on $[a,b]$ by degree-n poly $p(x) = \sum_{k=0}^{n} a_k x^k$ ← monomials

why good idea? Weierstrass: for each $[a,b]$, $\varepsilon > 0$, $\exists$ poly differing from f no more than ε. But degree unknown (finite?).

If choose $n+1$ distinct pts ('nodes') to make f & p match, we've already solved this:



$x_j \in [a,b]$.

$$p(x_j) = y_j \qquad j = 0, \dots n.$$

so
$$\underbrace{\begin{bmatrix} 1 & x_0 & x_0^2 & \cdots \\ 1 & x_1 & x_1^2 & \\ \vdots & & & \\ 1 & x_n & & \end{bmatrix}}_{M} \begin{bmatrix} a_0 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} f(x_0) \\ \vdots \\ f(x_n) \end{bmatrix}$$

proved $\det M \neq 0$ in lec 1 $\Rightarrow$ soln exists, unique.

Let $\ell_k(x) = \prod_{\substack{j=0 \\ j \neq k}}^{n} \frac{x - x_j}{x_k - x_j}$ $\quad k = 0, \dots n$ called Lagrange basis (1794)

Prop: unique interp. poly $p = \sum_{k=0}^{n} y_k \ell_k$ why? pf: $\ell_k(x_i) = \begin{cases} \prod_{j \neq k} \frac{x_k - x_j}{x_k - x_j} = 1, & i = k \\ 0 & i \neq k \text{ since one factor is } x_i - x_i \end{cases} = \delta_{ik}$

so $p(x_i) = \sum y_k \delta_{ki} = y_i \quad \forall i$ is a solution & unique.

Note:
- n large (>30) may cause stability probs since $\sup_{x \in [a,b]} |\ell_k(x)|$ exp. large
- Newton 1676 realised more practical method 'divided differences' we don't need.
- map $f \to$ its unique interp poly p through $\{x_j\}$ is linear: $p = L_n f$ $\quad L_n : C[a,b] \to \mathbb{P}_n$ ← space of degree-n poly's.

  for any $p \in \mathbb{P}_n$, $L_n p = p$ so what kind of op. is L_n? projection: $L_n^2 = L_n$.

Error of interp. $L_n f - f$ is a func.

recall $C^k[a,b]$ space of k-times cont. diff'ble funcs, ie k^{th} deriv is cont.

Thm (8.10) Let $f \in C^{n+1}[a,b]$, then for each $x \in [a,b]$ there exists $\xi \in [a,b]$ st.

$$f(x) - L_n f(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{j=0}^{n} (x - x_j)$$

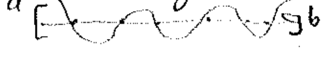
- So if you know $|f^{(n+1)}(x)| \le C$ in $x \in [a,b]$ you get an error estimate ← in math 'estimate' means rigorous bound!

pf: trivial if $x = x_j$

Fix $x \neq x_j$ & define $g(y) := f(y) - L_n f(y) - \prod_{j=0}^{n} (y - x_j) \frac{f(x) - L_n f(x)}{\prod_{j=0}^{n} (x - x_j)} \qquad y \in [a,b]$

set $y = x_j$: $\underbrace{f(y) - L_n f(y)}_{0}$, $\underbrace{\prod (y-x_j)}_{0}$ $\Rightarrow g(x_j) = 0 \quad j = 0, \dots n$

$y = x$: $g(x) = 0$ too! (that was why constructed), so g has $n+2$ zeros in $[a,b]$



By Rolle's thm. g' has $\ge n+1$ zeros.

etc. ... $g^{(n+1)}$ has ≥ 1 zero, call it ξ

Set $y = \xi$ & eval $g^{(n+1)}(\xi)$: $\quad 0 = f^{(n+1)}(\xi) - 0$ ← since degree n $\; - (n+1)! \frac{f(x) - L_n f(x)}{\prod_{j=0}^{n} (x - x_j)}$ QED sneaky!

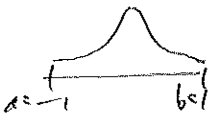
lec. 5 . M126.

· WS
· Runge applet.
· demos: charges — potential, etc

① 1/19/12

Write top of WS on board.?)
WS on n=1 Lagrange.

Equispaced nodes bad: Demo applet on smooth func. $f(x) = \frac{1}{1+25x^2}$ (C^∞, ie all derivs. cont.)



$x_j = -1 + \frac{2j}{n}$ in $[-1,1]$ (show Runge applet). → interpolant $L_n f$ { converges as $n\to\infty$ in central part, blows up in outer regions of $[-1,1]$ as $n\to\infty$. ! why?

But if cluster pts near ends,
e.g. $x_j = -\cos\frac{j\pi}{n}$ 'Chebyshev nodes', uniformly convergent, ie $\max_{x\in[-1,1]} |f - L_n f| \to 0$ as $n\to\infty$.
why?

$\| f - L_n f\|_\infty$ "L^∞ bound".

If assume nothing about nodes, product $\left|\prod_{j=0}^{n}(x-x_n)\right| \le (b-a)^{n+1} =: H^{n+1}$ (length of interval.)

& then $\| f - L_n f\|_\infty \le \frac{\|f^{(n+1)}\|_\infty}{(n+1)!} H^{n+1}$

We want small! — max Taylor coeff of f expanded at any point in (a,b)

How big are high Taylor coeffs of a func?

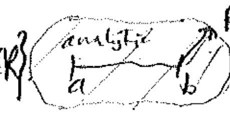
Recall Taylor series (about 0) $f(z) = \sum_{n=0}^{\infty} a_n z^n$, $a_n = \frac{f^{(n)}(0)}{n!}$:

std result: If f analytic at 0, $\exists \rho>0$ st series converges absolutely $\forall z$ in disc $|z|<\rho$ & diverges $\forall z$ outside, $|z|>\rho$, & f analytic in $|z|<\rho$.

abs. conv. ⇒ for $|z| = \rho-\varepsilon$, $\forall \varepsilon>0$: terms decreasing as $n\to\infty$ certainly ⇒ $|a_n|(\rho-\varepsilon)^n \le C$

ie $|a_n| \le \frac{C}{(\rho-\varepsilon)^n}$

Let's say f analytic in open domain containing 'stadium' $\{z\in\mathbb{C} \mid \text{dist}(z,[a,b])\le R\}$

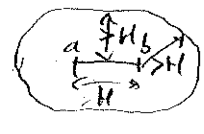


, then Taylor coeffs. $|a_n| \le \frac{C}{R^n}$ unif. wrt. expansion center in $[a,b]$

then $\| f - L_n f\|_\infty \le \frac{C}{R^n} H^{n+1} \le C\left(\frac{H}{R}\right)^n \to 0$

if $R>H$, exponentially fast as $n\to\infty$.

So if f analytic in



get good uniform convergence regardless of nodes.

(analytic: much stronger than merely C^∞)

But if f analytic in neighborhood of $[a,b]$, but singularities are H or closer, may fail to converge. (Runge).

I leave for you to say where poles of $\frac{1}{1+25x^2}$ are! $[a \;\; b]$ · pole.

The bad news: if construct sq. of interp. operators (L_n) each with $\{x_j^{(n)}\}_{j=0}^{n}$ nodes,

Thm (8.17) (Faber): for each such seq. $\exists f\in C[a,b]$ st. $L_n f \not\to f$ unif. on $[a,b]$.

The good news: Thm (8.16, Marcinkiewicz) For each $f\in C[a,b]$, $\exists$ sq of nodes st. $L_n f \to f$ unif on $[a,b]$

Why best to cluster nodes at ends of $[-1,1]$? [skip]? (Trefethen, Spec. Meth §5) ② 1/18/12

$$\frac{1}{n+1} \ln \Big| \underbrace{\prod_{j=0}^{n}(z-x_j)}_{=: q_{n+1}(z)} \Big| = -\frac{1}{n+1}\sum_{j=0}^{n} \ln\frac{1}{|z-x_j|}$$ = electrostatic potential in $\mathbb{R}^2 = \mathbb{C}$ due to $n+1$ charges strength $\frac{-1}{n+1}$ at nodes. $=: \phi_{n+1}(z)$

so $|q_{n+1}(z)| = e^{(n+1)\phi(z)}$

Say as $n\to\infty$, nodes tend to fixed density func $\rho(x)>0$ on $[-1,1]$, then $\phi_{n+1} \to$

normalized $\int_{-1}^{1}\rho(x)dx = 1$. $\quad \phi(z) = -\int_{-1}^{1}\rho(x)\ln\frac{1}{|z-x|}dx$

Uniform case $\rho = 1/2$ so $\phi(z) = \frac{1}{2}\int_{-1}^{1}\ln|z-x|dx$: $\to$ you can eval.

& check $\phi(0) = -1$ but $\phi(\pm 1) = -1+\ln 2$ larger at ends.

so $|q_{n+1}|$ is $\approx e^{(n+1)\ln 2} = 2^{n+1}$ times bigger at ends

- Show charges_potential.m.

$\nwarrow$ this same applies to $l_k(x)$: for $k \approx n/2$ in middle. exp. large at ends $\Rightarrow$ unstable.

Is there a ρ density that gives ϕ, hence $|q_{n+1}|$, const on $[-1,1]$?

- show charges_equilibrate.m

Can show via complex analysis (map from exterior of disc to line); $\rho(x) = \frac{1}{\pi\sqrt{1-x^2}}$ Chebyshev density.

This is density that $x_j = -\cos\frac{\pi j}{n}$ approach

Gives smallest poss $\max_{z\in[-1,1]} \phi(z)$ hence smallest $|q_{n+1}|$, best interp. convergence.

Can show singularities of f (analytic on $[a,b]$) can be arb. close to $[a,b]$ & still get exponential conv.

$\hookrightarrow$ 'Spectral method'.

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§9.1 Quadrature.

want to approximate $Q(f) := \int_a^b f(x)dx$

use $Q_n(f) := \sum_{k=0}^{n} \underset{\text{weights}}{w_k} f(\underset{\text{nodes in } [a,b]}{x_k})$

$\Big\}$ $Q, Q_n : C[a,b] \to \mathbb{R}$, linear functionals.

Given nodes, what are good weights? Pick s.t. $Q_n(f) = \int_a^b (L_nf)(x)dx$ ie integrate the interpolation poly exactly $\Rightarrow$ 'interpolatory' quad.

$$= \sum_{k=0}^{n} \underbrace{\int_a^b l_k(x)\,dx}_{\text{fixed } w_k} \; f(x_k)$$

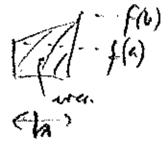
Thm (9.2) given distinct nodes $\{x_j\}_{j=0}^{n}$, the above $\{w_j\}_{j=0}^{n}$ are the unique set which integrates all $p\in\mathbb{P}_n$ exactly.

Pf: $Q_n(p) = \int_a^b (L_np)(x)dx = \int_a^b p(x)dx$ exact. Unique since $\sum w_k f(x_k) = \sum w_k (L_nf)(x_k) \overset{\text{exact}}{=} \int (L_nf)(x)dx$ (since $f = L_nf$ @ nodes.) $\Rightarrow$ interpolatory

so interp $\Leftrightarrow$ exact.

So exact integration up to degree n can be taken as defining feature: called Newton-Cotes (1600's) (sometimes used to mean equispaced)

(Eg n=1) $w_0 = \int_a^b l_0(x)\,dx = \int_a^b \frac{x-b}{a-b}\,dx = \frac{1}{2}(b-a) = \frac{h}{2}$, w_1 = same (3) 1/19/12

so $Q_1(f) = \frac{h}{2}(f(a)+f(b)) =$  trapezoid rule.

Error anal? Thm 9.4 Let $f \in C^2[a,b]$, then $\underbrace{\int_a^b f(x)\,dx - Q_1(f)}_{E_1(f)} = -\frac{h^3}{12} f''(\xi)$ for some $\xi \in [a,b]$

pf. $E_1(f) = \int_a^b f(x) - L_1 f(x)\,dx = \int_a^b \underbrace{(x-a)(x-b)}_{\le 0} \underbrace{\frac{f(x)-L_1 f(x)}{(x-a)(x-b)}}_{\text{cont. by l'Hopital at endpoints.}} dx$

MVT for integrals: if $g \geq 0$, $f \in C$, then $\int_a^b g f\,dx = g(z)\int_a^b f\,dx$ for some z in (a,b)

so $E_1(f) = \frac{f(z)-L_1 f(z)}{(z-a)(z-b)} \underbrace{\int_a^b (x-a)(x-b)\,dx}_{= -\frac{1}{6}h^3}$

by Thm 8.10 last time

$= \frac{f''(\xi)}{2!}$ some ξ.

Lec 6. M126 · guess n=2 WS. ① 1/24/12

HW2. for log plots, easiest to use semilogy, loglog, etc, rather than take log of data. $\log$ is $\ln$ not $\log_{10}$.

$\downarrow$ demo importance of Chebychev vs equally-spaced nodes!

recall Quadr $Q_n(f) = \sum_{j=0}^{n} w_j f(x_j)$ $\quad \exists$ unique $\{w_j\}$ st. Q_n exact $\forall f \in \mathbb{P}_n$.

last time: Interpolatory quad on a — b, $n=1$, ie $n+1 = 2$ nodes, choose $x_0 = a$, $x_1 = b$, get $Q_1(f) = h\frac{f(a)+f(b)}{2}$ trapezoid rule.

Thm (9.4): Let $f \in C^2[a,b]$, then $\left|\int_a^b f(x)dx - Q_1(f)\right| \le \frac{1}{12}\|f''\|_\infty h^3$

Pf [Thm 12.1 LIE]: Peano kernel $K(x) = \frac{1}{2}(x-a)(b-x) \ge 0$ on $[a,b]$, $\quad K'' = -1$ on (a,b). $\quad K' = \frac{b-a}{2}$, $K' = \frac{a-b}{2}$

$\int_a^b K(x) f''(x)dx = -\int K' f' dx + \underbrace{[Kf']_a^b}_{0} = \int K'' f\, dx - [K'f]_a^b = -\int_a^b f(x)dx + \frac{h}{2}(f(a)+f(b))$

magnitude $\le \underbrace{\int_a^b K(x)\,dx}_{\frac{h^3}{6}} \cdot \|f''\|_\infty$ $\quad$ QED.

May split interval into smaller & apply above to each: a |h|h| ... |h| b "composite trapezoid rule"

error $\le \frac{1}{12}\|f''\|_\infty h^3 \cdot \underbrace{\frac{b-a}{h}}_{\#\text{ intervals}}$ $\quad Q_{ctr}(f) = h\left(\frac{1}{2}f(a) + f(a+h) + \cdots + f(b-h) + \frac{1}{2}f(b)\right)$

$= \frac{b-a}{12}\|f''\|_\infty h^2 = O(h^2)$ convergence algebraic, order = # of nodes $(n+1)$

$\uparrow$ low-order.

Can increase n: more points on single interval, eg. $n=2$ Simpsons' (1743)

Say choose w/ equispaced pts. a $\overset{0 \cdots n}{\vdash}$ b $\leftarrow$ single interval. h $\quad$ Guesses for w_j as $n \to \infty$? w_j are $\int_a^b \ell_j(x)dx$

$\Rightarrow$ exp. large & oscillatory $\to$ bad for roundoff.

Another way in which negative weights bad: Convergence. (§9.2)

Consider seq. $(Q_n)_{n=0}^{\infty}$ of schemes $\quad Q_n(f) := \sum_{j=0}^{n} w_j^{(n)} f(x_j^{(n)})$

Defn (Q_n) conv. if $Q_n(f) \to Q(f)$ as $n \to \infty$, $\forall f \in C[a,b]$ $\quad$ nice property! (but could be slow). (Recall impossible for interp! L_∞ error)

• Thm (Szegö) (Q_n) conv. $\iff$ (Q_n) conv. for all poly's & $\exists C$ st. $\sum_{j=0}^{n}|w_j^{(n)}| \le C, \forall n$

note: this means if weights blow up as $n \to \infty$, cannot be conv! (eg: equispaced)

Facts 1) $\mathbb{P}$ = poly's 'dense' in $C[a,b]$, meaning: $\forall f \in C[a,b]$ & $\forall \varepsilon > 0$, $\exists p \in \mathbb{P}$ st. $\|f-p\|_\infty \le \varepsilon$

Weierstrass.

$\uparrow$ if need intuition: like $\mathbb{Q} \subset \mathbb{R}$, but metric space is $C[a,b]$ w/ sup norm.

2) each Q_n is lin. op: $C[a,b] \to \mathbb{R}$ w/ $|Q_n(f)| \le \|f\|_\infty \sum_{j=0}^{n}|w_j^{(n)}| \le C\|f\|_\infty$.

sum. $\quad$ so in our norm, this is $\|Q_n\|_\infty$ operator norm.

Pf: use facts 1 & 2 w/ Banach-Steinhaus thm:

let (Q_n) be seq. of bnd lin. ops, & Q bnd lin. op, $X = C[a,b]$ Banach space.

pointwise convergence $\iff$ (Q_n) uniformly bnded & convergent on some dense subset

$\forall f \in X, \lim_{n\to\infty}\|Q_n f - Qf\| = 0$ $\qquad$ $\|Q_n\| \le C, \forall n$ $\qquad$ $\exists U \subset X$ dense st. $\forall f \in U$, $\lim_{n\to\infty}\|Q_n f - Qf\| = 0$.

Banach–Steinhaus is a variant of 'Principle of Uniform Boundedness'? both std. in func. anal. ② 1/24/12
This is pretty abstract, ← the $\boxed{\Rightarrow}$ in B-S.
so let's prove the non-P.U.B. part, the $\boxed{\Leftarrow}$ in thm: [ptwise conv. ⇐ dense & unif bnd conv.]

For any $\varepsilon>0$,

$$Q_nf - Qf = Q_nf - Q_np + Q_np - Qp + Qp - Qf$$

our '$\mathcal{U}$' ↓ can find $p \in \mathbb{P}$ st. $\|p-f\|_\infty \le \varepsilon$

Take abs val & use tri ineq:

$$|Q_nf - Qf| \le \underbrace{|Q_nf - Q_np|}_{\substack{\le C\|f-p\|_\infty \\ = C\varepsilon}} + \underbrace{|Q_np - Qp|}_{\substack{\le \varepsilon \\ \forall n>N \text{ for some } N \text{ suff. large.}}} + \underbrace{|Qp - Qf|}_{\le (b-a)\varepsilon}$$

← if you like, $\|Q\|$.

$$\le \underbrace{(C+1+b-a)}_{\text{fixed const.}}\varepsilon$$

So for each $\delta>0$, choose $\varepsilon = \frac{\delta}{C+1+b-a}$ & $\exists N$ st. $\forall n>N$, $|Q_nf - Qf| < \delta$. QED.

"up & over"

$$\begin{tikzcd} Q_np \arrow[r] & Qp \arrow[d] \\ Q_nf \arrow[u] \arrow[r, dotted] & Qf \end{tikzcd}$$

bound by $\le$ sum of 3 dists.

· Also called "$\varepsilon/3$" argument, common in func. anal.

Positive weights is enough:

Corollary (9.11, Steklov): if (Q_n) conv for all polys, & $w_j^{(n)} \ge 0$, then (Q_n) conv.

pf: $\|Q_n\|_\infty = \sum_{j=0}^{n} |w_j^{(n)}| \underset{\text{nonneg.}}{=} \sum_{j=0}^{n} w_j^{(n)} = Q_n(1) \xrightarrow[\text{1 is a poly}]{} Q(1) = \int_a^b 1\,dx = b-a$

so $\exists C$ st. $\|Q_n\|_\infty \le C$ $\forall n$, use Szegö.

◦ Also minimal round-off error since sizes of weights as small as poss.

◦ Eg: composite trap. conv. (+ve w's, conv. ∀poly's since each has $\|p''\|_\infty < \infty$). , But equispaced

Now improved quadr. schemes on $[a,b]$ ... w/ positive weights ...

Gaussian Quadrature (§9.3)

: optimal choice of nodes → queen of quadratures. on $[a,b]$

→ w's. straight in.

↳ get $n=2$ degree 5 exact, generally can do degree $2n+1$ exact, compared to only n for Newton-Cotes w/ general nodes.
↳ defines a Gaussian quad w/ $n+1$ nodes.

Let's show why:

◦ orthogonality for funcs. $f \perp g \iff 0 = (f,g) := \int_a^b f(x)g(x)\,dx$

Lemma (9.13) Let $x_0, \dots x_n$ be distinct nodes of a Gaussian quadr.

Then $q_{n+1}(x) := \prod_{j=0}^{n}(x-x_j) \perp p \quad \forall p \in \mathbb{P}_n$

q_{n+1}: a x_0 ... x_n b

pf: $q_{n+1}p \in \mathbb{P}_{2n+1}$ so $\int_a^b q_{n+1}(x)p(x)\,dx \overset{\text{by Gauss.}}{=} \sum_{k=0}^{n} w_k \underbrace{q_{n+1}(x_k)}_{\text{vanish at nodes.}} p(x_k) = 0$ QED.

Lec. 7. · projector · ① 1/26/12

HW2 debrief:

$\boxed{\text{finish Gauss } n=2 \text{ WS.} \quad \text{Do §9.3 from ②-③ 1/24/12.}}$ → $2\beta\alpha^2 = \int_{-1}^{1} x^2 dx = 2/3$, $2\beta\alpha^4 = \int_{-1}^{1} x^4 dx = 2/5$ $\quad \alpha = \sqrt{3/5}$, $\beta = 5/9$, $w_1 = 2 - 2\beta = 8/9$

$\mathbb{P}_5$ exact.

Claim $2n+1$ is highest poss. degree for $(n+1)$-node quadr.

Pf: $p = \prod_{j=0}^{n} (x - x_j)^2 \in \mathbb{P}_{2n+2}$ has $Q_n(p) = 0$ but $Q(p) > 0$.

Thm: (9.18) Gauss weights non-negative. Pf $l_k(x_j) = \delta_{jk}$ so $l_k^2(x_j) = \delta_{jk}$ so

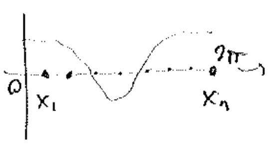
$$\forall k: \quad \underset{\text{nonneg.}}{0 <} \int_a^b l_k^2(x)\,dx \underset{\substack{\text{exact}\\ \text{since } l_k^2 \in \mathbb{P}_{2n}}}{=} \sum_{j=0}^{n} w_j l_k^2(x_j) = w_k.$$

Cor: Gaussian quadr. convergent (last time).

There are error bnds for Gauss quadr, eg order-n rule err $\le \dfrac{\|f^{(2n+2)}\|_\infty}{(2n+2)!} \cdot \overbrace{\int_a^b q_{n+1}^2(x)\,dx}^{\text{gets exp. small as } n\to\infty}$.

May generalize to weighted quadr. $Q(f) = \int_{-1}^{1} f(x) W(x)\,dx$, has some uses.

Periodic Quadrature §9.4.



$f(x + 2\pi) = f(x)\ \forall x$. $\quad Q(f) = \int_0^{2\pi} f(x)\,dx$

$$Q_n(f) = \underbrace{\frac{2\pi}{n}}_{w_j \text{ equal.}} \sum_{j=1}^{n} f\Big(\underbrace{\frac{2\pi j}{n}}_{\text{equally spaced nodes.}}\Big)$$

Thm (9.27) Let $f \in C^{2m+1}(\mathbb{R})$ be 2π-periodic, $m \ge 1$, then $\underbrace{|Q_n(f) - Q(f)|}_{\text{error}} \le \underbrace{c_m}_{\text{const indep. of } f.} \int_0^{2\pi} |f^{(2m+1)}(x)|\,dx \cdot \frac{1}{n^{2m+1}}$

Pf: see [NA], Euler-Maclaurin.

Ie, smoother f gives higher-order algebraic convergence.

If $f \in C^\infty$, then error $= O(n^{-m})$ for each $m \ge 0$, called "super-algebraic" convergence.

But if f analytic, do even better: exponential conv.

→ [2011o.pdf slides] write Davis thm. then ⟶ * First review complex: $f(z)$ holomorphic in $D \subset \mathbb{C}$: means analytic at each pt. in D.

Eg. $\frac{1}{1+25x^2}$ holomorphic in $\mathbb{C} \setminus \{i/5, -i/5\}$. ← simple poles.

simple pole @ $z=a$: $f(z) = \frac{b}{z-a}$ ← residue. $\quad$ generally at simple pole, $f(z) = \frac{b}{z-a} + \underbrace{c_0 + c_1 z + \cdots}_{\text{Taylor.}}$

Residue thm: if f holomorphic in D apart from finite # poles,

$$\underset{\text{line integral}}{\int_{\partial D} f(z)\,dz} = 2\pi i \sum_{\text{poles}} (\text{residue of each pole}).$$

Pf of thm (slides).

· May also derive from trigonometric interpolation, ie Fourier series truncated at terms $\pm n/2$, is also exp. accurate.

[Lec 7 middle of]

& choose $\{w_j\}$ as usual, ③ 1/24/12

Converse of this holds: Lemma 9.14: if $\{x_j\}$ nodes sat. $q_{n+1} \perp \mathbb{P}_n$ ", it's a Gauss. quad.

Pf: recall interpolatory quad. has $\sum w_k f(x_k) = \int_a^b (L_n f)(x)\,dx \quad \forall f \in C[a,b]$

claim each $p \in \mathbb{P}_{2n+1}$ can be written $p = L_n p + q_{n+1} q$ for some $q \in \mathbb{P}_n$

why? $p - L_n p = 0$ at $\{x_j\}$, so q can have at most $(2n+1) - (n+1) = n$ zeros.

So $\int p(x)dx = \int (L_n p)(x)\,dx + \cancel{\int q_{n+1}(x) q(x)\,dx} = \sum w_k p(x_k)$ QED.

chosen orthog. since interp. (degree n).

So, if can find q_{n+1}, a degree-$(n+1)$ poly, orthog to $\mathbb{P}_n$, with all roots in $[a,b]$,

need: the roots give the nodes!

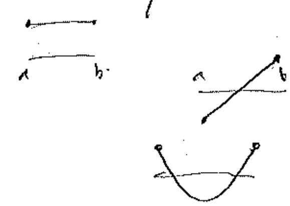
ORTHOGONAL POLYNOMIALS (useful anyway):

Lemma 9.15: $\exists$ unique seq. $(q_n)_0^\infty$ w/ $q_0 = 1$ & $q_n(x) = x^n + p(x)$, $p \in \mathbb{P}_n$

which are mutually orthog. ie $(q_n, q_m) = 0 \quad \forall m < n$, and $\text{span}\{q_0, \ldots, q_n\} = \mathbb{P}_n$.

Pf: $1, x, x^2, \ldots$ are lin. indep. on $[a,b]$, so Gram-Schmidt unique:

$$q_0 = 1$$
$$q_1 = x - \frac{(x, q_0)}{(q_0, q_0)} q_0$$
$$q_2 = x^2 - \frac{(x^2, q_1)}{(q_1, q_1)} q_1 - \frac{(x^2, q_0)}{(q_0, q_0)} q_0$$
$$\vdots$$
$$q_n = x^n - \sum_{j=0}^{n-1} \frac{(x^n, q_j)}{(q_j, q_j)} q_j$$



& these $n+1$ L.I. elements of $\mathbb{P}_n$ (an $n+1$-dim vector space) must span it.

in HW3 you'll prove this can be done via 3-term recurrence, ie q_{n+1} involves q_n & q_{n-1} only.

• 'Legendre' poly's (but above not std normalization): unique seq. of orthog poly's on $[-1,1]$ w/ unweighted inner product (f,g).

Lemma 9.16 q_n has n simple zeros all in $[a,b]$ (... good, so they give a Gauss quad.!)

pf. $\forall n \geq 1$, $q_n \perp q_0$ ie $\int q_n = 0$ so q_n has ≥ 1 zeros $x_1 \cdots x_m$ in $[a,b]$

Supp. $m < n$, then $r_m := \prod_{j=1}^m (x - x_j) \in \mathbb{P}_{n-1}$ so is $\perp q_n$

but $\int r_m q_n \neq 0$ since $r_m q_n$ has fixed sign, not $\equiv 0$.

contradiction $\Rightarrow m = n$.

In practice, how compute $\{x_j\}_{j=0}^n$? They are eigvals of

$$\begin{bmatrix} 0 & \beta_1 & & & \\ \beta_1 & 0 & \beta_2 & & \\ & \beta_2 & 0 & \beta_3 & \\ & & \beta_3 & \ddots & \ddots \\ & & & \ddots & \end{bmatrix}$$

tridiagonal matrix $\beta_n := \frac{1}{2\sqrt{1-(2n)^{-2}}}$

& $\{w_j\}$ come from eigenvectors. "Golub-Welsh"

See code gauss.m

This is $O(n^3)$ slow! ($n < 10^2$ ok, otherwise slow)

Glaser-Liu-Rokhlin 2007 has better idea which is $O(n)$: find x_{j+1} from x_j by Taylor expansion, coeffs given by Legendre poly recurrence.

Periodic numerical quadrature

The simplest rule to approximate $\int_0^{2\pi} f(t)dt$ is sometimes the best: sum N equally spaced samples of f !

Theorem (Davis '59): Let f be 2π-periodic, and *real analytic*, meaning $f(z)$ is bounded and analytic in some strip $|\operatorname{Im} z| \leq a$ of half-width $a > 0$. Then there is a const $C > 0$ (indep. of N) such that the error is

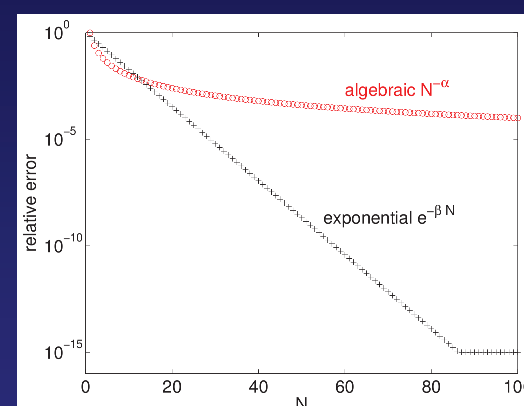
$$\left| \frac{2\pi}{N} \sum_{j=1}^{N} f\left(\frac{2\pi}{N} j\right) - \int_0^{2\pi} f(t)dt \right| \leq Ce^{-aN}$$

- exponential convergence in N:

doubling N squares your accuracy

very desirable: can get accuracies of 10^{-14}

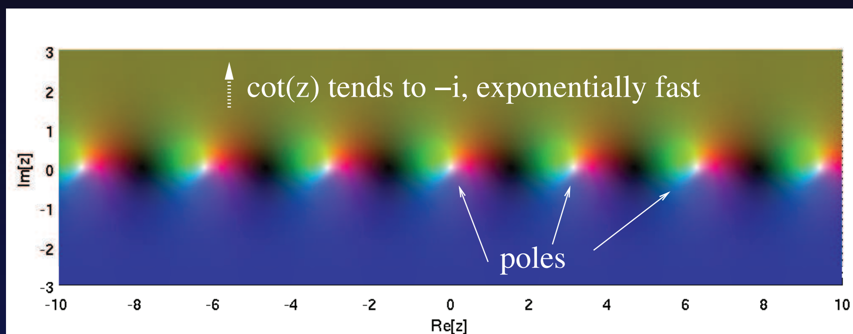
w/ little effort. Carries over to solving the PDE!

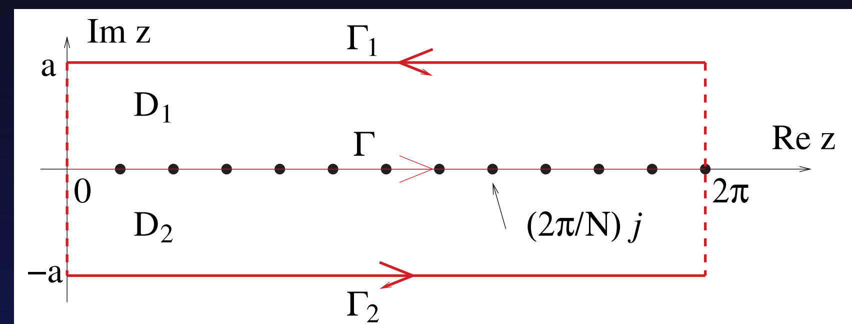


Proof

Residue Thm: $2\pi i \sum$ residues $=$ closed contour integral in $\mathbb{C}$

Beautiful cotangent function $\cot(z)$: poles at πj, $j \in \mathbb{Z}$, residues 1





f analytic $\frac{1}{2i} f(z) \cot(\frac{N}{2} z)$: poles at $\frac{2\pi}{N} j$, residues $\frac{1}{iN} f(\frac{2\pi}{N} j)$

Res. Thm in strip: $$\frac{2\pi}{N} \sum_{j=1}^{N} f\left(\frac{2\pi}{N} j\right) = \int_{\Gamma_1+\Gamma_2} \frac{1}{2i} f(z) \cot\left(\frac{N}{2} z\right) dz$$

integrand pure Im on $\mathbb{R}$, so

Re parts antisymmetric $\updownarrow$ add

Im parts symmetric $\updownarrow$ cancel

$$= \mathrm{Re} \int_{\Gamma_1} (-i) f(z) \cot\left(\frac{N}{2} z\right) dz$$

$$\frac{2\pi}{N}\sum_{j=1}^{N} f\left(\frac{2\pi}{N}j\right) \;=\; \mathrm{Re}\int_{\Gamma_1} (-i) f(z) \cot\left(\frac{N}{2}z\right) dz$$

Cauchy integral formula in D_1 (since f analytic):

$$-\int_{\Gamma} f(z)dz \;=\; \int_{\Gamma_1} f(z)dz$$

add Re part of this to previous eqn:

$$\underbrace{\frac{2\pi}{N}\sum_{j=1}^{N} f\left(\frac{2\pi}{N}j\right) - \int_{\Gamma} f(z)dz}_{\text{error of our quadrature}} \;=\; \mathrm{Re}\int_{\Gamma_1} \Big[\underbrace{1 - i\cot(\tfrac{N}{2}z)}_{\text{exp. small} \le 2/(e^{aN}-1)}\Big] \underbrace{f(z)}_{\text{bnded in } D_1} dz$$

QED

- Research: good quadrature schemes for f's with *singularities* ?

· copy 12 or page of Ch 12 NA. ① 1/31/12.

Lec. 8 · [M126]

HW3 debrief:

Integral Eqns: §12 (NA)

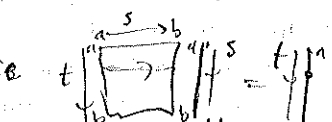
given interval $[a,b]$, func f on $[a,b]$, kernel λ func k on $[a,b]^2$

solve $\underbrace{\int_a^b k(t,s)\,u(s)\,ds}_{(Ku)(t)} = f(t) \quad \forall t \in [a,b]$ ← right hand side.

Fredholm 1st kind.

or 2nd kind $\quad u(t) + (Ku)(t) = f(t) \quad \forall t\in[a,b]$.

functional eqn: $Ku = f$, visualize like $A\vec{x} = \vec{b}$, ie



← ie $f(t)$ = inner prod of $k(t,\cdot)$ & u

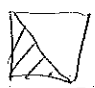
- What is $(K^2u)(t)$? $= \int k(t,s)\underbrace{(Ku)(s)}_{\text{write out}}\,ds = \int k(t,s)\int k(s,r)u(r)\,dr\,ds$

$= \int k'(t,r)\,u(r)\,dr$

where k' is kernel of K^2 so $k'(t,r) = \int k(t,s)\,k(s,r)\,ds$

[like matrix prod. $(AB)_{ik} = \sum_j a_{ij} b_{jk}$]

- if $k(t,s) = 0$ for $s > t$



diagonal. $t=s$

'lower-triangular,' they're called Volterra, not Fredholm, can be written $\int_a^{t} k(t,s)\,u(s)\,ds = f(t)$ (note) has unique soln, / won't concern us.

eg $k\equiv 1$: $\int_0^t u(s)ds = f(t)$, $t>0$ $\iff$ $u(t) = f'(t)$ soln.

Fredholm has stuff on both sides of diag

Eg $\int_0^1 t^2 s\, u(s)\,ds = \frac{t^2}{3} \quad 0<t<1.$

bring out: $t^2\int_0^1 s\,u(s)ds = \frac{t^2}{3}$ so any func u sat. $\int_0^1 s\,u(s)ds = 1/3$ is a soln.

eg $u(t) = \underset{\text{particular soln}}{t} + \underset{\text{homog. soln}}{(\text{any func} \perp t)}$

soln. highly nonunique, typ. of 1st kind.

K is rank-1 since for any u, $(Ku)(t)$ = a multiple of t^2.

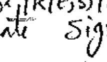
Bounded operators: $\|K\| = \sup_{\|u\|=1}\|Ku\|$ for your choice of norm, eg sup (L^∞), L^2, etc.

Eg. space $= C[a,b]$ w/ ∞-norm:

for each $t\in[a,b]$, $|(Ku)(t)| = \left|\int_a^b k(t,s)u(s)\,ds\right| \le \int_a^b |k(t,s)|\,ds$ if $\|u\|_\infty = 1$ note: $|(v,u)| \le \|v\|_1\|u\|_\infty$ again

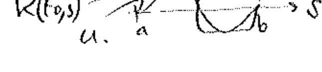
so $\|K\|_\infty \le \sup_{t\in[a,b]} |(Ku)(t)| = \sup_{t\in[a,b]}\int_a^b |k(t,s)|\,ds$ "biggest row-integral of abs.val of kernel"

eg $k\in C^2[a,b]$ has $\|K\|_\infty < \infty$.



Can say more: above $\le$ is $=$! Why? { Pick t_0 = the t which maximizes $\int_a^b|k(t,s)|ds$ (exists). Continuous funcs u can approximate sign $k(t_0,s)$ arb. well.

This is NA Thm 12.5. (explicitly gives example of this).



so $\|K\|_\infty \ge \int_a^b |k(t_0,s)|ds - \varepsilon \quad \forall\varepsilon>0.$

② 1/31/12

Kernel may blow up on diagonal, eg $k(t,s) = \frac{1}{|t-s|^\gamma}$

But if $|k(t,s)| \le \frac{C}{|t-s|^\gamma}$ $\forall s,t$, $0<\gamma<1$ then L_1 norm of each row bounded, $\Rightarrow \|K\|_\infty < \infty$ norm bnded

called 'weakly singular'. $\gamma \ge 1$ strongly singular, may be unbounded operator.

↳ rears ugly head: PDE apps.

Numerical solution method: Nyström (1930), 2^{nd} kind.

$$u(t) - \underbrace{\int_a^b k(t,s)u(s)\,ds}_{\text{quadr } Q_n \text{ w/ nodes } s_1,\cdots s_n \text{ \& weights } w_1,\cdots w_n} = f(t) \qquad t\in[a,b] \qquad \text{ie } (I-K)u=f$$

approx u by u_n which obeys

$$u_n(t) - \underbrace{\sum_{j=1}^n w_j\, k(t,s_j)\, u_n(s_j)}_{=: (K_n u_n)(t)} = f(t) \qquad (*)$$

where K_n is a rank-n operator approx to K (its range $= \text{Span}\{k(\cdot, s_j)\}_{j=1}^n$)

ie $(I-K_n)u_n = f$.

Then values at nodes $u_i^{(n)} := u_n(s_i)$ sat. the lin. sys,

$$\forall i=1,\cdots n, \quad u_i^{(n)} - \sum_{j=1}^n w_j\, k(s_i,s_j)\, u_j^{(n)} = f(s_i) \qquad (LS)$$

$$\text{ie} \quad (I - A)\,\vec{u}^{(n)} = \vec{f}$$

A: $n\times n$ matrix, $A_{ij} = k(s_i,s_j)w_j$; $\vec{u}^{(n)}$: vector; $\vec{f}$: RHS at nodes vector.

- So you've solved for u at nodes — how get back full func $u_n(s)$? Lagrange interp. poss; better since exact is:

Thm (12.11) If any vector $\{u_i^{(n)}\}_{i=1}^n$ is soln. to (LS), then $u_n(t) = f(t) + \sum_{j=1}^n w_j k(t,s_j) u_j^{(n)}$ solves $(*)$, $\boxed{\text{exactly}}$ — surprising that we have exact interpolation. ← call formula (N). for Nyström interpolant.

Pf: (Don't try & insert (N) into $(*)$!)
$u_n(s_i) = u_i^{(n)}$ $\forall i$, since set $t=s_i$ in (N), gives (LS)
Use this to sub for $u_j^{(n)}$ in (N) turns it into $(*)$, $\forall t$. Subtle!

- $(*)$ expresses u_n as f + span{column slices of kernel at nodes} ↳ $k(\cdot, s_j)$, form interpolation basis.

k:

- (LS) is equiv. of Vandermonde sys. requiring interpolant agrees at nodes; (N) is interpolation formula.
- if drop I, can apply to 1^{st} kind, but there is no interpolation formula (N) now, just get $\{u_j^{(n)}\}_{j=1}^n$.

Note: $\|K_n - K\| \not\to 0$ as $n\to\infty$ not convergent in norm topology (shame since would be easy to prove stuff).

But do have ptwise convergence ie for each $\phi\in C([a,b])$, $\|(K_n-K)\phi\| \to 0$ as $n\to\infty$. (← can still prove stuff!)

Compact operators — just the essentials: (see [IE], [NA] Ch.12) (1) 2/2/12

↳ may have ∞-dim range but behave 'like' finite-dim ops (ie, square matrices).

$X = C[a,b]$ topological space, $f \in X$ (func.) is a 'point' in X. Choose metric norm eg. $\|f\|_\infty$.

- seq $(f_n)_{n=1,2,\ldots}$ bdded if $\|f_n\| \le C$ $\forall n = 1,2,\ldots$ note: seq. goes forever, a 'long time'!
- seq (f_n) converges to $f \in X$ if $\forall \varepsilon > 0$ no matter how small, $\exists N$ st $\|f_n - f\| < \varepsilon$ $\forall n \ge N$.

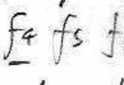
Thm (Bolzano-Weierstrass.) if $\dim(X) < \infty$, every bdded seq. contains a convergent subseq.

$f_0\ \underline{f_1}\ f_2\ \underline{f_3}\ \underline{f_4}\ f_5\ f_6\ \underline{f_7}\ \ldots$

subseq also goes on forever!

eg $X = \mathbb{R}$: the only way to avoid some limit pt is to escape to $\pm\infty$.

But ∞ dim spaces such as $C[a,b]$, $L^2(a,b)$ ← all funcs f st $\int_a^b |f|^2 dx < \infty$.

eg Fourier seq $\{\sin nx\}_{n=1}^\infty$ bdded in $L^2(0,\pi)$ but has no convergent subseq:  } mutually orthog.

Defn: linear op. $K: X \to Y$ between normed lin. spaces X, Y is compact if given any bounded seq. (f_n) in X, the seq. (Kf_n) contains a convergent subseq.
↳ "feels" finite dim.

- Eg. if K has finite-dim range $\mathbb{R}^N$: $BW \Rightarrow (Kx_n)$ has conv. subseq $\Rightarrow K$ cpt.
- But $K = Id$ in ∞-dim space $Y = X$: can feed it Fourier seq. $\Rightarrow K$ not cpt.

Useful facts: (prove later?)

Cpt op. maps unit ball to hyperellipsoid w/ successive semiaxes shrinking to zero: 
intuition.

1) Cpt ops have discrete eigenvalues w/ zero the only limit: $K\phi = \lambda\phi$ then $\lim_{j\to\infty} \lambda_j = 0$
2) Cpt $\Rightarrow$ bdded (easy to prove)
3) integral operator on $[a,b]$ w/ {continuous or weakly singular kernel, $|k(t,s)| \le \frac{C}{|t-s|^\gamma}$, $\gamma < 1$, $\forall s,t$, is cpt (in ∞- or 2-no
4) K cpt if: it is the operator norm limit of seq $K_1, K_2, \ldots$ of cpt op, ie $\lim_{n\to\infty} \|K - K_n\| = 0$ (cut?)

eg acting on sequences, $K\{a_1, a_2, \ldots\} := \{\mu_1 a_1, \mu_2 a_2, \ldots\}$ (μ_j consts) ↳ $\|K\|_\infty$. Say $\mu_n \to 0$. Then can truncate to finite-dim ops K_n & $(K - K_n)\{a_1, a_2, \ldots\} = \{0, \ldots, 0, \mu_{n+1} a_{n+1}, \ldots$ so $\|K - K_n\| \to 0$. & K is cpt.

5) Thm (Fredholm Alternative). Let $K: X \to X$ be cpt

Then either i) for each $f \in X$, $(I - K)u = f$ has unique soln. $u \in X$

or ii) homog. eqn $(I - K)u = 0$ has nontrivial soln (ie, $\lambda = 1$ is eigval of K

This asserts existence of soln to 2nd kind IE from uniqueness... amazing!

Behave like finite linear systems: $A\vec{x} = \vec{b}$ has soln. $\forall \vec{b}$ iff $A\vec{x} = \vec{0}$ has only the triv. soln (nonsingular)

6) K cpt $\Rightarrow$ convergence rate of Nyström method for 2nd kind IE is $\|u_n - u\|_\infty \le C\|Ku - K_n u\|_\infty$

see [NA Ch.12]. Ie same rate as quadrature scheme applied to $k(t,\cdot)u(\cdot)$.

Lec 9 (M126) part 2: PDEs. ② 2/2/12

Laplacian $\Delta := \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}$ in $\mathbb{R}^2$. $x = (x_1, x_2)$

$= \text{div grad}$

$\vec{n}$, length $|\vec{n}| = 1$. $\Omega \subset \mathbb{R}^2$ open bndd domain

$\Delta u = 0$ in Ω $\Leftrightarrow$ u harmonic in Ω ($\Leftrightarrow$ $u = \mathrm{Re}\, v$ for some v analytic in $\Omega \subset \mathbb{C} \simeq \mathbb{R}^2$)

Check $\ln \frac{1}{|x|} = -\ln |x|$ obeys $\Delta \ln \frac{1}{|x|} = 0$ $\forall x \neq 0$.

eg $\frac{\partial}{\partial x_1} \ln|x| = \frac{1}{2} \frac{\partial}{\partial x_1} \ln(x_1^2 + x_2^2) = \frac{1}{2(x_1^2+x_2^2)} 2x_1 = \frac{x_1}{|x|^2}$

etc.

$\Rightarrow$ Fundamental Soln. $\Phi(x, y) := \frac{1}{2\pi} \ln \frac{1}{|x-y|}$ ($x \in \mathbb{R}^2$, $y \in \mathbb{R}^2$) obeys $\Delta_x \Phi(x, y) = 0$ $\forall x \neq y$

shifts the 'spike' to sit at loc. y.

(Note: already seen in quadrature stuff in $\mathbb{C} \simeq \mathbb{R}^2$)

Divergence Thm: $\vec{a} = \begin{pmatrix} a_1(x) \\ a_2(x) \end{pmatrix}$ vector field (eg $a_1, a_2 \in C^1(\Omega)$, Ω may have corners).

then $\int_\Omega \underbrace{\vec{\nabla} \cdot \vec{a}}_{\text{div}\,\vec{a} = \frac{\partial a_1}{\partial x_1} + \frac{\partial a_2}{\partial x_2}} \, dx = \int_{\partial \Omega} \vec{n} \cdot \vec{a} \, ds$

vol.; surface (arclength measure on $\partial\Omega$)

'flux' $= \int_{\partial\Omega} \vec{n}_y \cdot \vec{a}(y) \, ds_y$

flux > 0.

$\rightarrow$ W/S.

(choose $\vec{a} = u \vec{\nabla} v$ where u, v scalar funcs).

& prod rule $\vec{\nabla} \cdot (u \vec{\nabla} v) = u \Delta v + \vec{\nabla} u \cdot \vec{\nabla} v$ check.

G1I, G2I, "zero flux" (ZF) $\int_{\partial\Omega} u_n \, ds = 0$ note $\vec{n} \cdot \vec{\nabla} u =: u_n$ normal deriv.

directional deriv. of Fund. Sol: say $\vec{n}$ is a unit vector $\nearrow$

deriv. of $\Phi(x,y)$ wrt. moving source pt. y in $\vec{n}$ direction: $\frac{\partial \Phi(x,y)}{\partial n_y} = \frac{1}{2\pi} \vec{n} \cdot \nabla_y \ln \frac{1}{|x-y|}$

$\frac{\partial}{\partial y_1} \ln \frac{1}{|x-y|} = -\frac{1}{2} \frac{\partial}{\partial y_1} \ln|x-y|^2 = -\frac{1}{2} \frac{1}{|x-y|^2} \underbrace{\frac{\partial}{\partial y_1}\left[(x_1-y_1)^2 + (x_2-y_2)^2\right]}_{-2(x_1-y_1)} = \frac{x_1 - y_1}{|x-y|^2}$

so ∇ ...

so $\frac{\partial \Phi}{\partial n_y} = \frac{1}{2\pi} \frac{\vec{n} \cdot (\vec{x} - \vec{y})}{|x-y|^2}$

is harmonic for $x \neq y$.

Lec 10 MATH 126 ① 2/7/12.

elliptic PDE & Potential theory. (LIE Ch 6)

HW5: several potential of a bunch of dipoles, check "Gauss' Law". Ido Nyström w/ kernel from this lec.

Last time

$\Omega \subset \mathbb{R}^d$ ($d\ge 2$; we did $d=2$)

G 2nd Id: $(u,v\in C^2(\bar\Omega))$ $\displaystyle\underbrace{\int_\Omega u\Delta v - v\Delta u \, dx}_{\text{vol.}} = \underbrace{\int_{\partial\Omega} u v_n - v u_n \, ds}_{\text{bdry}}$ remind $u_n = ?\ \vec n\cdot\vec\nabla u$ normal direc. deriv.

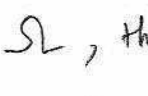
$v\equiv 1$, u harmonic? (v const, harm) $0 =$ (const)

So $\displaystyle\int_{\partial\Omega} u_n = 0$ "zero flux" (ZF)

Greens Representation Formula: Let $u\in C^2(\bar\Omega)$ be harm. in Ω, then

(GRF) LIE Thm 6.5
$$\int_{\partial\Omega} \Phi(x,y)\,u_n(y) - \frac{\partial\Phi}{\partial n_y}(x,y)\,u(y)\,ds_y = \begin{cases} u(x) & x\in\Omega \quad \text{inside} \\ \tfrac12 u(x) & x\in\partial\Omega, \ (\partial\Omega \text{ smooth}) \\ 0 & x\in \mathbb{R}^d\setminus\bar\Omega \quad \text{outside}\end{cases}$$

parse it: $\Phi(x,y)$ Fund sol $= \begin{cases}\frac{1}{2\pi}\ln\frac{1}{|x-y|} & \text{in } d=2 \\ \frac{c_d}{|x-y|^{d-2}} \end{cases}$

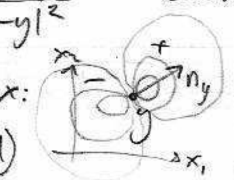


$\Phi(\cdot,y)$ harmonic in $\mathbb{R}^d\setminus\{y\}$

normal directional deriv. w.r.t. y param: $\displaystyle\frac{\partial\Phi}{\partial n_y} = \underbrace{\vec n(y)}_{\text{normal @ } y}\cdot\vec\nabla_y\Phi(x,y) \overset{(d=2)}{=} \frac{1}{2\pi}\frac{\vec n\cdot(\vec x-\vec y)}{|x-y|^2}$ check

$\partial\Phi(\cdot,y)/\partial n_y$ harm. in $\mathbb{R}^d\setminus\{y\}$.

plot vs x: (show Brad)



dipole potential

So its bdry data $u|_{\partial\Omega}$, u_n, enough to reconstruct u everywhere in Ω via a boundary integral!

Pf: $\boxed{\text{case } x\in\Omega}$ ($d=2$, $d>2$ similar) $\partial B(x;r)$:= circle radius r about x

in $R := \Omega\setminus\overline{B(x;r)}$ (closed ball), $\Phi(x,y)$ harm. as func of y. (ie now x = param, y = coord.)

$\Rightarrow$ G2nd I in R for u, $v=\Phi(x,\cdot)$,

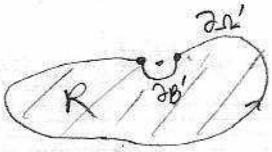
$$0 = \int_R u\,\underbrace{\Delta_y\Phi(x,y)}_{\text{harm.}} - \Phi(x,y)\underbrace{\Delta u}_{0} = \int_{\partial R = \partial\Omega + \partial B} u(y)\frac{\partial\Phi(x,y)}{\partial n_y} - \Phi(x,y)\,u_n(y)$$

$\leftarrow$ move $\partial\Omega$ bits; ∂B inwards pointing $\vec n$.

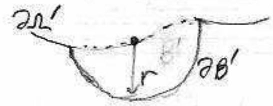
So $$\int_{\partial\Omega}\Phi(x,y)u_n(y) - \frac{\partial\Phi}{\partial n_y}(x,y)u(y) = \int_{\partial B(x;r)} \underbrace{\frac{\partial\Phi(x,y)}{\partial n_y}}_{\frac{1}{2\pi r}} u(y) - \underbrace{\Phi(x,y)}_{-\frac{1}{2\pi}\ln r} u_n(y)\,ds_y.$$

$$= \frac{1}{2\pi r}\underbrace{\int_{\partial B} u(y)\,ds_y}_{\text{by MVT } = 2\pi r\cdot u(y) \text{ for some } y\in\partial B} + \frac{1}{2\pi}\ln r\underbrace{\int u_n(y)\,ds_y}_{\text{why? ZF}} \xrightarrow{\text{take } \lim_{r\to 0}} \lim_{r\to 0} u(y)\Big|_{y\in\partial B} = u(x). \quad \square$$

$\boxed{\text{Case } x \in \partial\Omega}$: (sketch)



now $\partial R = \partial\Omega' + \partial B'$ where $\partial B' = \partial B(x;r) \cap \Omega$



so in $\lim_{r\to 0}$, $\partial\Omega$ locally flat so $\partial B' \to$ half-circle

$$\& \quad \frac{1}{2\pi r}\int_{\partial B'} u(y)\,ds_y \;\to\; \tfrac{1}{2}u(x)$$

$$\frac{1}{2\pi}\ln r \underbrace{\int_{\partial B'} u_n(y)\,ds_y}_{=\pi r\, u_n(y) \text{ for some } y\in\partial B'} \;\to\; 0 \quad \text{since } u_n \text{ bnd}, \ \& \ r\ln r \to 0.$$

& $\partial\Omega' \to \partial\Omega$.

$\boxed{\text{Case } x \in \mathbb{R}^d \setminus \overline{\Omega}}$ There is no ball, $R = \Omega$. $\square$

Useful corollaries

i) since Φ & $\frac{\partial\Phi}{\partial n_y}$ analytic funcs. of 1st var, ie $(x_1, x_2, \ldots)$, u is analytic in Ω wrt. each coord
(LIE Thm 6.6) regardless how nonsmooth bdry data is

ii) mean val. thm. for harm funcs. (LIE Thm 6.7) if u harm, $u(x) = \frac{1}{2\pi r}\int_{\partial B(x;r)} u(y)\,ds_y$ $(d=2)$
ie val. at center is mean of surface. pf: GRF, bring out $\Phi(x,y)$ const, use ZF. — for $d>2$, it's surf. area

$\Rightarrow$ Maximum principle: harm. funcs attain their max & min. on bdry

pf: let x be isolated interior max, then $\exists\, B(x;r)$, $r>0$ & mean val. $\Rightarrow$ contradiction.

$\Rightarrow$ BVP $\begin{cases}\Delta u = 0 & \text{in } \Omega\\ u = f & \text{on } \partial\Omega\end{cases}$ has <u>at most</u> one soln. Suppose u_1, u_2 solns, then $w = u_1 - u_2$ harm.
with $w|_{\partial\Omega} = 0$, so $w \equiv 0$ in Ω by Max. Princ.

iii) $$\int_{\partial\Omega} \frac{\partial\Phi}{\partial n_y}(x,y)\,ds_y = \begin{cases} -1 & x\in\Omega\\ -1/2 & x\in\partial\Omega\\ 0 & x\in\mathbb{R}^d\setminus\overline{\Omega}\end{cases}$$ pf: GRF w/ $u \equiv -1$ (is harm, $u_n \equiv 0$)

"Gauss' Law" (GL) Can also prove via ZF & small balls directly (try it).

postponed

Layer potentials (new notation)

$\partial\Omega$ closed curve, "density" $\varphi \in C(\partial\Omega)$, $(S\varphi)(x) := \int_{\partial\Omega} \Phi(x,y)\,\varphi(y)\,ds_y$ ← 'single-layer potential'

$(D\varphi)(x) := \int_{\partial\Omega} \frac{\partial\Phi(x,y)}{\partial n_y}\,\varphi(y)\,ds_y$. ← ('double-layer pot.')

are the bdry integrals from GRF.

Often use $\begin{cases}\sigma & \text{for SLP density}\\ \tau & \text{DLP}\end{cases}$

eg GRF says, in Ω, $u = S\sigma + D\tau$ where $\sigma = u_n$, $\tau = -u|_{\partial\Omega}$

eg GL says $D1$ generates potential -1 in Ω, 0 outside. ← test in HW5.

• How eval such integrals in practice? ($d=2$ case!) Change variable:

say $z(s)$ parametrizes $\partial\Omega$, $z(2\pi) = z(0)$ ie $z : [0, 2\pi) \to \mathbb{R}^2$
$(z_1(s), z_2(s))$

eg $\partial\Omega$ given by $f(\theta)$ in polars: $z_1(s) = f(s) \cos s$
$z_2(s) = f(s) \sin s$

Then (if $g: \mathbb{R}^2 \to \mathbb{R}$) $\displaystyle\int_{\partial\Omega} g(y)\, ds_y \overset{\text{change of var.}}{=} \int_0^{2\pi} g(z(s))\, \underbrace{|z'(s)|}_{\text{'speed function'}}\, ds \xrightarrow{\text{quadrature via periodic trap rule}} \frac{2\pi}{N} \sum_{j=1}^{N} g(z(s_j))\, |z'(s_j)|$

At each surface node $z(s_j)$ also need normal

$n =$ "z' rotated CW 90° & normalized"

ie $n(s) = \begin{pmatrix} n_1(s) \\ n_2(s) \end{pmatrix} = \frac{1}{|z'(s)|} \begin{pmatrix} z_2'(s) \\ -z_1'(s) \end{pmatrix}$

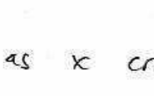
Coding: recommend you set up (inline?) funcs $\begin{cases} z(s) \\ z'(s) \\ n(s) \end{cases}$ gives

then pass the func. handles (& N) to routine that:
2) fill a_{ij} matrix els for Nyström
1) plots a potential due to given density func handle $\mu(s)$

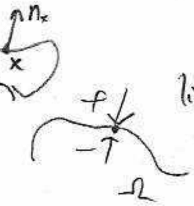
<u>Jump relations</u>: note GL: $\mathcal{D}1$ has jump of $+1$ in value as x crosses $\partial\Omega$ from inside to outside.

Define (let $x \in \partial\Omega$)

$u^\pm(x) := \lim_{h \to 0^+} u(\vec{x} \pm h\vec{n}_x)$ normal at x:



$u_n^\pm(x) := \lim_{h \to 0^+} \vec{n}_x \cdot \vec{\nabla} u(\vec{x} \pm h\vec{n}_x)$



limiting values on $\partial\Omega$ from each side

The expect DLP has $u^+(x) - u^-(x) = \tau(x)$, true:

Thm (JR's) Let $\partial\Omega$ be C^2 (ie $z_1, z_2 \in C^2$), $\sigma, \tau \in C(\partial\Omega)$, and $u = \mathcal{S}\sigma$, $v = \mathcal{D}\tau$, then for $x \in \partial\Omega$,

$$u^\pm(x) = \int_{\partial\Omega} \Phi(x,y)\, \sigma(y)\, ds_y \qquad \text{(no jump in SLP val.)}$$

$$u_n^\pm(x) = \int_{\partial\Omega} \frac{\partial \Phi(x,y)}{\partial n_x}\, \sigma(y)\, ds_y \mp \frac{\sigma(x)}{2} \qquad \text{(jump in deriv. of SLP)}$$

$\leftarrow$ note!

$$v^\pm(x) = \int_{\partial\Omega} \frac{\partial \Phi(x,y)}{\partial n_y}\, \tau(y)\, ds_y \pm \frac{\tau(x)}{2} \qquad \text{(jump in DLP val.)}$$

$$v_n^\pm(x) = \int_{\partial\Omega} \frac{\partial^2 \Phi(x,y)}{\partial n_x \partial n_y}\, \tau(y)\, ds_y \qquad \text{(no jump in DLP deriv.)}$$

Lec 11 (M126) • stop at 11:35a! • show singlelayer.m ① 2/9/12

{ finish Layer pot defns, JRs last time.
  •

Bdry integral ops: $S: C(\partial\Omega) \to C(\partial\Omega)$ has kernel $\Phi(x,y)$ ← note: weakly singular (diag $y=x \to \infty$).
(not S)

$D: C(\partial\Omega) \to C(\partial\Omega)$ kernel $\frac{\partial \Phi(x,y)}{\partial n_y}$

So JR3 says, (if $v = \mathcal{D}\tau$) $v^{\pm} = D\tau \pm \frac{1}{2}\tau$

Say want v to solve BVP $\begin{cases} \Delta v = 0 & \text{in } \Omega \\ v = f & \text{on } \partial\Omega \end{cases}$ ← already sat. by rep. $v = \mathcal{D}\tau$! ← set $v^- = f$ & we've done.

$\Rightarrow (D - \frac{1}{2})\tau = f$ Fred. IE, (which kind? 2nd due to ½), a Bdry IE (BIE)

or $\boxed{(I - 2D)\tau = -2f}$ BIE in std. 2nd kind form.

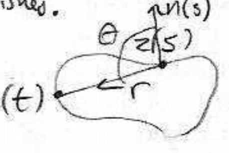
Recipe to solve BVP: i) solve BIE for τ, ii) reconstruct $v = \mathcal{D}\tau$ in interior of Ω.

Thm: let $\partial\Omega$ be C^2 smooth, in $\mathbb{R}^2$. Then kernel of D is continuous.

intuitively, y, contours of $\frac{\partial\Phi(\cdot,y)}{\partial n_y}$ are circles, local curvature of $\partial\Omega$ dictates which contour you're on. $\Rightarrow$ curvature needs to be cont. $\Rightarrow C^2$.

Pf  parametrize by $z: \mathbb{R} \to \mathbb{R}^2$, 2π-periodic. $\partial\Omega \in C^2$ means $z'(s) = \dot z(s) = \frac{dz}{ds}$, $\ddot z(s) = \frac{d^2 z}{ds^2}$ } both cont. vec. funcs of s

Demand $|\dot z| > 0$, speed never vanishes.

wrt $t, s \in [0, 2\pi)$, kernel $k(t,s) = \frac{1}{2\pi} \frac{n(s)\cdot(z(t) - z(s))}{|z(t) - z(s)|^2}$ 

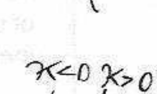
also $k(s,t) = \frac{1}{2\pi}\frac{\cos\theta}{r}$

top & bot. cont. wrt s & t, $\Rightarrow$ cont. $\forall s \neq t$.

$\lim_{t\to s} k(t,s)$ top & bot vanish $\Rightarrow$ l'Hôpital: $\frac{d}{dt}\text{top} = n(s)\cdot \dot z(t) \to 0$ also! Why?

$\Rightarrow \frac{d^2}{dt^2}\text{top} = n(s)\cdot \ddot z(t) \xrightarrow{t\to s} n(s)\cdot \ddot z(s)$

$\frac{d}{dt}\text{bot.} = 2\dot z(t)\cdot(z(t) - z(s))$, $\frac{d^2}{dt^2}\text{bot} = 2|\dot z(t)|^2 \to 2|\dot z(s)|^2$

Combine: $\lim_{t\to s} k(t,s) = \frac{1}{4\pi}\frac{n(s)\cdot \ddot z(s)}{|\dot z(s)|^2} = \frac{-\kappa(s)}{4\pi}$ κ = local curvature $= (\text{curv. radius})^{-1}$ 

• In practice BIE all done wrt $s, t \in [0, 2\pi)$, by changing arc length ds_y to $|z'(s)|ds$

$\Rightarrow f, \tau$ are funcs on $[0, 2\pi)$ (2π-periodic), and D has kernel $k(t,s) = \frac{1}{2\pi}\frac{n(s)\cdot(z(t) - z(s))}{|z(t) - z(s)|^2}\cdot|z'(s)|$ $t \neq s$, or on the diagonal, $k(s,s) = \frac{-1}{4\pi} \underbrace{\kappa(s)}_{} \cdot |z'(s)|$ ② 2/9/12

$\hookrightarrow$ in code use $-\frac{n(s)\cdot z''(s)}{|z'(s)|^2}$

Solving via Nyström $(I-A)\vec{\tau} = -2\vec{f}$ lin. sys,

where $N{\times}N$ mat. A has entries $a_{ij} = \delta_{ij} + 2k(s_i, s_j)\, w_j$ $\qquad s_j = \frac{2\pi j}{N}$

col. vec $\vec{f}$ has $f_j = f(z(s_j))$, the bdry data at the nodes. $\qquad w_j = \frac{2\pi}{N} \ \forall j$

Solution vector $\vec{\tau} = \{\tau_j\}_{j=1}^N$ is density at nodes, can be used.

Commonly, $v = \underset{\text{interior soln in } \Omega}{\mathcal{D}\tau}$ is then approximated using these same quadrature nodes.

... this isn't always accurate!
(active research by me!)

Thm: above BVP has a soln. Pf: $\mathcal{D}$ kernel cont. $\Rightarrow \mathcal{D}$ cpt
Can show $2\mathcal{D}$ doesn't have 1 as an eigvalue.
$\Rightarrow$ by Fredholm Alternative, soln. τ exists $\Rightarrow$ soln v exists

got here.

Proof of JR3 (hard): need to show $v = \mathcal{D}\tau$ can be continuously extended from

Ω to $\overline{\Omega}$ w/ lim. value $v_- = (D - 1/2)\tau$

$\mathbb{R}^2\backslash\overline{\Omega}$ to $\mathbb{R}^2\backslash\Omega$ " $\quad v_+ = (D + 1/2)\tau$

$v+$, $v-$, Ω

[1] split into GL & correction: let $x = z + hn_z$

$$v(x) = \underbrace{\tau(z)\int_{\partial\Omega} \frac{\partial\Phi}{\partial n_y}(x,y)\,ds_y}_{\text{by GL} = \begin{cases} -1 & h<0 \\ -1/2 & h=0 \\ 0 & h>0 \end{cases}} + \underbrace{\int_{\partial\Omega} \frac{\partial\Phi}{\partial n_y}(x,y)\big(\tau(y) - \tau(z)\big)\,ds_y}_{=: V(z,h)}$$

note: vanish as $y \to z$.

If show $\lim_{h\to 0} V(z,h) = V(z,0)$, uniformly in $z \in \partial\Omega$, we are done, since GL accounts for the jump.

i.e. continuous wrt h.

[2] Pick radius $r > 0$ & split y integral into 'far' & 'local' parts:

$$V(z,h) - V(z,0) = \underbrace{\int_{\substack{y\in\partial\Omega \\ |y-z|\geq r}} \left(\frac{\partial\Phi}{\partial n_y}(x,y) - \frac{\partial\Phi}{\partial n_y}(z,y)\right)\big(\tau(y)-\tau(z)\big)\,ds_y}_{a \quad \text{far}} + \underbrace{\int_{|y-z|<r} \left(\frac{\partial\Phi}{\partial n_y}(x,y) - \frac{\partial\Phi}{\partial n_y}(z,y)\right)\big(\tau(y)-\tau(z)\big)\,ds_y}_{b \quad \text{local}}$$

Assume $2|h| \leq r$, then $|a| \leq 2\|\tau\|_\infty \underbrace{\int_{|y-z|\geq r} \left|\frac{\partial\Phi}{\partial n_y}(x,y) - \frac{\partial\Phi}{\partial n_y}(z,y)\right| ds_y}_{\text{HW: } \leq\, C h/r^2}$, so $|a| \leq C\frac{|h|}{r^2}$

dep. on τ, not z.

Lemma (local part) (L-PL): $\exists h_0 > 0$ & C (indep of h) s.t. $\int_{|y-z|<r} \left|\frac{\partial\Phi}{\partial n_y}(z + hn_z, y)\right| ds_y \leq C \quad \forall |h| \leq h_0$

(pf of LPL to follow.)

③ 2/9/12

Then $|v(z,h) - v(z,0)| \le C\frac{|h|}{r^2} + 2C \cdot \underbrace{\max_{\substack{z\in\partial\Omega \\ |y-z|<r}} |\tau(y) - \tau(z)|}$

given $\varepsilon > 0$ can choose $r > 0$ s.t. $\le \frac{\varepsilon}{4C}$

since τ cont. on $\partial\Omega$ ($\Rightarrow$ unif. cont.)

then choose $h_0 = \frac{\varepsilon r^2}{2C}$

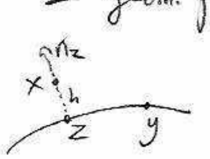
$\Rightarrow |v(z,h) - v(z,0)| \le \varepsilon \quad \forall z \in \partial\Omega$ & $|h| \le h_0$. such an $h_0 > 0$ exists for each $\varepsilon > 0$

$\Rightarrow v(\cdot,h) \longrightarrow v(\cdot,0)$ uniformly $\square$

$\boxed{3}$

Finally, pf of LPL:

2 geom. facts i) "Normal lemma" (NL): $\exists L$ st. $n_y\cdot(z-y) \le L|z-y|^2 \quad \forall z,y \in \partial\Omega$
($\partial\Omega \in C^2$)



in $d=2$ pf is simply that doublelayer kernel is continuous.
$d\ge 2$: Taylor Thm wrt. s, param.

ii) "Lower bnd on distance" (LBD): $|x-y|^2 = |z-y+hn_z|^2 = |z-y|^2 + 2h\underbrace{n_z\cdot(z-y)}_{\le L|z-y|^2 \text{ (NL)}} + h^2$

$x-y = z-y + x-z$

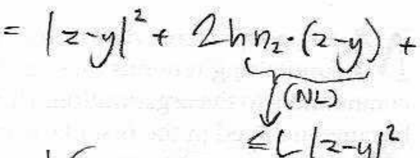
$\ge \frac{1}{2}(|z-y|^2 + h^2) \quad \forall |h| < h_0$, for some $h_0 > 0$

Then $\left|\frac{\partial\Phi}{\partial n_y}(x,y)\right| \le \frac{|n_y\cdot(z-y)|}{2\pi|x-y|^2} + \frac{|n_y\cdot(\cancel{x}-z)|}{2\pi|x-y|^2}$

NL, LBD; $\le h$; LBD.

$\le C + C\frac{h}{|z-y|^2+h^2}$

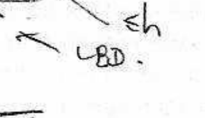
h^2 in denom makes integrable!



Cauchy distn

Pick patch Γ_r around z where $n(z)\cdot n(y) \ge 1/2, \ \forall y \in \Gamma_r$.

patch means $\Gamma_r := \{y : |z-y| < r, \ y \in \partial\Omega\}$. Can project onto line w/ at most factor 2 in variable change $ds_y \to ds$



So $\int_{\Gamma_r} \left|\frac{\partial\Phi}{\partial n_y}(x,y)\right| ds_y \le 2C\underbrace{\int_{-r}^{r} 1 + \frac{h}{s^2+h^2}\, ds}_{2r+\pi} \le Cr + C\underbrace{\int_{-\infty}^{\infty}\frac{h}{s^2+h^2}ds}_{\pi} \le C$, indep of h

$\square$

M126 Lec12 — ① 2/14/12.

OH Tu 2-3.

- Prove JR3 from Lec 11 — Discuss project.txt. — HW5: Neu int?

HW5: convergence rate worse nr. $\partial\Omega$ — error research prob har determinants!

Other BVPs.

We did interior Dirichlet : "what temperature dist does uniformly conducting body settle to when bdry values set to func. f ?"

- Interior Neumann: $\begin{cases} \Delta u = 0 & \text{in } \Omega \\ u_n = f & \text{on } \partial\Omega \end{cases}$ equilibrium temp. distn, f = specified heat input flux at each pt on $\partial\Omega$.

What if pumping in more heat than extracting? blow up!

Already know u harm. $\Rightarrow$ ZF: $\int_{\partial\Omega} u_n = 0$ ie $\int_{\partial\Omega} f = 0$ for existence.

Then if u_1, u_2 are solns, $w = u_1 - u_2$ sat $\begin{cases} \Delta w = 0 & \text{in } \Omega \\ w_n = 0 & \text{on } \partial\Omega \end{cases}$ w = const. a soln. [the only soln: GI: $\int w \underbrace{\Delta w}_{0} - \nabla w \cdot \nabla w = \int \underbrace{w w_n}_{0}$ so $\nabla w \equiv 0$.

$\Rightarrow$ when exists, soln. is unique only up to a const. (Δ op has $\lambda = 0$ a Neumann eigenvalue).

BIE solution? if use $u = \mathcal{D}\tau$ as before, BC is $\underbrace{\int_{\partial\Omega} \frac{\partial^2 \Phi}{\partial n_x \partial n_y}(x,y)\, \tau(y)\, ds_y}_{\text{deriv of DLP: } T\tau} = f$ hypersingular: kernel $\sim \frac{1}{|x-y|^2}$ nr diag, not integrable! unbounded op.

instead try? $u = \mathcal{S}\sigma$ so $\underbrace{\int_{\partial\Omega} \frac{\partial \Phi}{\partial n_x}(x,y)\, \sigma(y)\, ds_y}_{D^T\sigma} + \frac{\sigma(x)}{2} \overset{\text{JR2}}{=} u_n^- = f$

IE is $(I + 2D^T)\sigma = 2f$. 2^{nd} kind again. D cpt $\Leftrightarrow D^T$ cpt.

But we know nonunique since BVP is, but in practice, backwards-stable lin. solver should give a $\vec{\sigma}$ which satisfies.
can prove via ext. GRF. → cond # of matrix → ∞.

Got here.

Danger: the const will be large ⇒ loss of digits in $\vec{\sigma}$.

Atkinson book: (p. 336-7) solve $(I + 2D^T)\sigma + \sigma(x_0) = 2f$

where $x_0 \in \partial\Omega$ fixed.

Proves uniquely solvable $\forall f \in C(\partial\Omega)$.

- Exterior BVPs : eg Dirichlet (ED) $\begin{cases} \Delta u = 0 & \text{in } \mathbb{R}^2 \setminus \overline{\Omega} \\ u = f & \text{on } \partial\Omega \\ u(x) = O(1) & \text{as } |x| \to \infty \end{cases}$ ie bounded. (harmonic at ∞)

has unique soln $\forall f \in C(\partial\Omega)$

for $d > 2$ this is $o(1)$. → physically this needed since potential at ∞ needs to be specified.

Follows from $\tilde{u}(x) := u\left(\frac{x}{|x|^2}\right)$ "Kelvin xform of u" maps $\mathbb{R}^2 \setminus \overline{\Omega}$ to $\tilde{\Omega}$ ← works in $\mathbb{R}^d$. (Folland PDE book)

$\tilde{u}$ is harmonic in $\tilde{\Omega} = \{x : \frac{x}{|x|^2} \in \mathbb{R}^2 \setminus \overline{\Omega}\}$ (d=2 only!)

Condition at ∞ mapped to 'analytic at 0'

Lec 13 M126 · Colloq today ① 2/16/12

OH 2:30 Th.

Laplace variants 2 Fr

Helmholtz, scattering

last time: · int. Dir BVP $\xLeftarrow[u=\mathcal{D}\tau]{u \text{ solves (w/ data } f)}$ $(I - 2D)\tau = -2f$

(proven unique)

· int Neu BVP $\xLeftarrow[u=\mathcal{S}\sigma]{}$ $(I + 2D^T)\sigma = 2f$

(proven unique up to const, needs $\int_{\partial\Omega} f = 0$)

inherits nonuniqueness of BVP, ie $\dim \mathrm{Nul}(I+2D^T) = 1$

But can solve lin. sys. fine (try it).

These are both "indirect" BIE: pick a representation for soln. u as LP, so that BIE for unknown density comes out 2nd kind.

Why not 1st kind? eg try $u = \mathcal{S}\sigma$ for int. Dir, want BC $S\sigma \underset{JR1}{=} u^- = f$

but S cpt $\Rightarrow$ ∞ # eigvals accumulating at zero, $\Rightarrow$ ill-conditioned in a bad way (for N large, use iterative rather than $O(N^3)$ direct lin. solvers; they hate such a matrix).

"Direct" BIE also possible: GRF in interior, $x \in \Omega$ then $(\mathcal{S}u_n - \mathcal{D}u|_{\partial\Omega})(x) = u(x)$ (*)

take $x \to \partial\Omega^-$ & use JR1 & 3, get $Su_n^- - (D - 1/2)u^- = u^-$

$\Rightarrow$ $(I + 2D)u^- = \underbrace{Su_n^-}$ say you want to solve int Neu BVP then $u_n^- = f$, so RHS Sf known

as here, direct give adjoint of indirect. the unknown isn't a density, rather, the value.

When BIE solved, use (*) to reconstruct u in Ω.

Note: since we know homog. int. Neu BVP has only const. solns, ie $u^- =$ const, then $\mathrm{Nul}(I+2D) = \{\text{the const. funcs}\}$

Exterior probs: eg Dirichlet BVP $\begin{cases} \Delta u = 0 & \text{in } \mathbb{R}^2\setminus\overline{\Omega} \\ u = f & \text{on } \partial\Omega \\ u(x) \text{ bnded as } |x| \to \infty \end{cases}$ ← extra condition needed for uniqueness.

(physically: zero total charge on body)

Proof unique soln exists $\forall f \in C(\partial\Omega)$:

let $\tilde{u}(x) := u\left(\frac{x}{|x|^2}\right)$ "Kelvin xform of u", turns outside in, yet $\tilde{u}$ harmonic too, now on bnded domain $\Rightarrow$ existence & unique.

condition "bnded at ∞" becomes "analytic at 0".

Indirect BIE: $u = \mathcal{D}\tau$ (sat bnded at ∞ cond), JR3 gives $(D + 1/2)\tau = u^+ \overset{BC}{=} f$ ie $(I + 2D)\tau = 2f$

signs differ from int Dir BVP, that's all!

expect BIE unique? No! Just showed op $I+2D$ singular.

② 2/16/12

Worse, BIE has <u>no</u> soln. for certain f, even though BVP <u>does</u> have (unique) soln! (Helmholtz will have similar story)

For, suppose $(I+2D)\tau = 2f$

"complementary BVP haunts the solvability!" ↳ ie int Neu for ext Dir.

then inner prod $(\phi, (I+2D)\tau) = 2(\phi, f)$

"Ghost of int Neu haunts BIE for ext. Dir.!" the single-layer σ's which generate const funcs

← move over

$$= (\underbrace{(I+2D^T)\phi}_{\text{zero } \forall \phi \in \mathrm{Nul}(I+2D^T)}, \tau)$$

$\Rightarrow$ contradiction unless $f \perp \mathrm{Nul}(I+2D^T)$

(easy part of full version of Fredholm Alternative) Thm 39, Ch.5, Colton.

Literature: various fixes, eg Colton, replace D kernel by $\frac{\partial \Phi(x,y)}{\partial n_y} + 1$ ← not Id, rather the "1 kernel"

can prove: exists, unique $\forall f$. (Colton §5.3)

<u>Helmholtz eqn.</u> $\underbrace{(\Delta + k^2)}_{\text{plays role of Laplace op}} u = 0$

k = wavenumber $= \frac{2\pi}{\text{wavelength}}$

homog. int. Dir BVP $\begin{cases} (\Delta + k^2)u = 0 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$

there exist discrete $k_1 < k_2 \le k_3 \le \cdots \nearrow \infty$ s.t. has nontriv. soln

Pf: Δ acting on $\{u \in L^2(\Omega), u|_{\partial\Omega} = 0\}$ has <u>cpt</u> inverse — prove since Greens function integral kernel of Δ^{-1}, weakly singular.

$\Rightarrow -\Delta u = k^2 u$ has a set discrete 'Dirichlet eigvals' k_j^2, accum only at ∞.

To solve int. Dir BVP $\begin{cases} (\Delta + k^2)u = 0 & \text{in } \Omega \\ u = f & \text{on } \Omega \end{cases}$ proceed as Laplace, but new kernel; that's it!

kernel: $\Phi(x,y) = \frac{i}{4} H_0^{(1)}(k|x-y|)$ $d=2$ $\quad H_0^{(1)\prime} = -H_1^{(1)}$

↳ 'outgoing' Hankel function, a special func, — see DLMF.

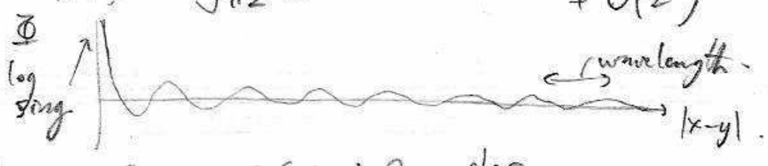
Matlab: besselh$(\nu, z) = H_\nu^{(1)}(z)$

$$\frac{\partial \Phi(x,y)}{\partial n_y} = -\frac{ik}{4} \underbrace{\frac{n_y \cdot (x-y)}{|x-y|}}_{\cos\theta} H_1^{(1)}(k|x-y|)$$

show

Asymptotics: $\Phi(x,y) \underset{x \to y}{=} \frac{1}{2\pi} \log \frac{1}{|x-y|} + O(1)$ ie same singularity as Laplace ⇒ same JRs!

large-dist: $H_\nu^{(1)}(z) = \sqrt{\frac{2}{\pi z}} e^{i(z - \frac{\nu\pi}{2} - \pi/4)} + O(z^{-1})$ as $z \to +\infty$.



Where from? say $u(r,\theta) = f(kr)e^{i\nu\theta}$ polar sep. of var, fix $\nu \in \mathbb{Z}$ & find $f(z)$ st. u sat Helm. Eqn.

$$0 = (\Delta + k^2)u = \frac{1}{r}\partial_r(r\partial_r u) + \frac{1}{r^2}\partial_{\theta\theta} u - k^2 u = \left(k^2 f'' + k\frac{f'}{r}\right)e^{i\nu\theta} + (i\nu)^2 \frac{f}{r^2} e^{i\nu\theta} - k^2 f e^{i\nu\theta}$$

gather $kr = z$: $z^2 f'' + z f' + (z^2 - \nu^2) f = 0$ Bessel's eqn (ν^{th} order), $H_\nu^{(1)}(z)$ is soln. to ODE w/ certain asymptotics

③ 2/16/12

Ext Dir BVP:
for u^s

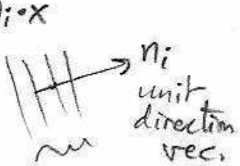
$$(ED)\begin{cases} (\Delta + k^2) u^s = 0 & \text{in } \mathbb{R}^2 \setminus \Omega \qquad d = 2, 3, \cdots \\ u^s = f & \text{on } \partial\Omega \\ \lim_{r\to\infty} r^{\frac{d-1}{2}} \underbrace{\left(\frac{\partial u^s}{\partial r} - iku^s\right)}_{\text{ie in } d=2,\ \text{this} = o\left(\frac{1}{\sqrt{r}}\right)} = 0 & \end{cases}$$

radiation condition: outgoing (e^{+ikr}) rather than incoming (e^{-ikr}) as $r \to \infty$.

has unique soln. $\forall f \in C(\partial\Omega)$, Colton-Kress Thm 3.7.

Scattering: say 'incident wave' $u^i : \mathbb{R}^d \to \mathbb{C}$, eg. $u^i(x) = e^{ik n_i \cdot x}$

sat $(\Delta + k^2) u^i = 0$ in $\mathbb{R}^d$. plane wave



then if u^s solves (ED) w/ $f = -u^i|_{\partial\Omega}$, $u := u^i + u^s$ solves Helm. eqn in $\mathbb{R}^d \setminus \overline{\Omega}$ & $\underbrace{\text{vanishes on } \partial\Omega}_{\text{the physical BC}}$.

why? $u^s|_{\partial\Omega} = f = -u^i|_{\partial\Omega}$ cancelling the inc. wave.

Note: u^i doesn't sat. radiation cond, but new waves due to obstacle (u^s) do.

M126 lec 14   finish Helmholtz · start fast algorithms.   · Mike O'Neil talk 1-2pm. · show { dlp-eigvalsweep.m, Neumann-eigfuncs., lowrank-curve.m }   ① Tu. 2/21/12.

• Where do Hankel funcs come from? want $\underbrace{(\Delta_x + k^2)}_{\text{Helm op.}}\Phi(x,y) = 0$ for $\forall x \neq y$.

$d=2$: wlog $y=0$. call $u = \Phi(\cdot,0)$, want sat. Helm. eqn.

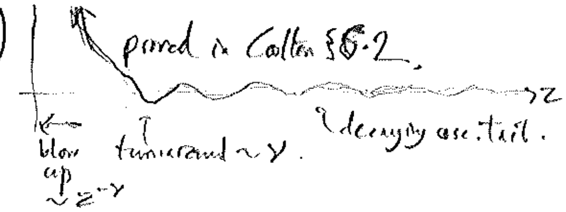
$u(r,\theta) = f(kr)e^{i\nu\theta}$ polar sep. of var., $\nu \in \mathbb{Z}$ so single-valued, solve for f:

$0 = (\Delta + k^2)u = \underbrace{\frac{1}{r}\partial_r(r\partial_r u) + \frac{1}{r^2}\partial_{\theta\theta}u}_{\text{laplacian}} + k^2 u = (\underbrace{k^2 f''}_{\text{chain rule}} + \frac{k}{r}f')e^{i\nu\theta} + \frac{(i\nu)^2}{r^2}fe^{i\nu\theta} + k^2 f e^{i\nu\theta}$

cancel $e^{i\nu\theta}$, gather $kr = z$: (& mult. by r^2) $z^2 f'' + zf' + (z^2 - \nu^2)f = 0$ Bessel's eqn., order ν (ODE)

$H_\nu^{(1)}(z)$ is soln. w/ log singular @ $z \to 0^+$

large-argument: ($z \to \infty$) $H_\nu^{(1)}(z) = \sqrt{\frac{2}{\pi z}}\, e^{i(z - \frac{\nu\pi}{2} - \pi/4)} + O\left(\frac{1}{z}\right)$ proved in Colton §5.2



Are also solutions regular at $z=0$: $J_\nu(z)$ Bessel funcs.

Fixing nonuniqueness in BIE for scattering

In HW6 you saw ext Dir BIE haunted by ghost of complementary BVP: let $u^s = \mathcal{D}\tau$, sat. Helm in $\mathbb{R}^2\setminus\bar\Omega$, radiative, solves ext BVP if (BIE): $\underbrace{(I + 2D)\tau}_{2u^s \text{ by JR3.}} = 2f = -2u^i|_{\partial\Omega}$ from inc. field.

Haunting is: $I + 2D$ singular for certain set of k → cond'n-ise, no soln. for some RHS's.

• We'll need GRF (interior), same as Laplace: (same log. sing.)   { Let $(\Delta + k^2)u = 0$ in Ω, then $\mathcal{S}u_n - \mathcal{D}u|_{\partial\Omega} = \begin{cases} u & \text{in } \Omega \\ 0 & \text{in } \mathbb{R}^d\setminus\bar\Omega \end{cases}$

Suppose $\phi \not\equiv 0$ sat. $\begin{cases}(\Delta + k^2)\phi = 0 & \text{in } \Omega \\ \phi_n = 0 & \text{on } \partial\Omega\end{cases}$ then ϕ is interior Neumann eigenfunc. & k^2 its eigenvalue. ("acoustic resonance of cavity" Ω).

then by GRF, $\mathcal{S}\underset{0}{\phi_n} - \mathcal{D}\phi|_{\partial\Omega} = \phi$ in Ω.

take $x \to \partial\Omega^-$ & use JR3: $-(D - \tfrac{1}{2})\phi|_{\partial\Omega} = \phi|_{\partial\Omega}$ ie $(I + 2D)\phi|_{\partial\Omega} = 0$.

since $\phi|_{\partial\Omega}$ nontriv. (otherwise $\phi \equiv 0$ by GRF), $\dim \mathrm{Nul}\,(I + 2D) > 0$, singular, not soluble $\forall f$! (Fred. Alt. (just like sq. matrix))

Show evolving eigval of $2D$ vs k: when hit $\begin{cases}-1 \\ +1\end{cases}$ $k^2 = \begin{cases}\text{Neu} \\ \text{Dir}\end{cases}$ eigval of Ω

↳ project: use smooth evolution to find such k^2's.

Fix it: rep. $u^s = (\mathcal{D} - i\eta\mathcal{S})\tau$, $\eta > 0$ Brakhage–Werner, Leis, Panich, '60s,

solves ext Dir BVP if $(\underset{\text{JR3 as before}}{I + 2D} - \underset{\text{JR1 (no jump for S val.)}}{2i\eta S})\tau = 2f$

Thm: $I + 2D - 2i\eta S$ injective $\forall k > 0$

Pf: let τ solve $(\tfrac{1}{2} + D - i\eta S)\tau = 0$, wish to show $\tau \equiv 0$.

from τ create potential $v := (\mathcal{D} - i\eta\mathcal{S})\tau$, then $v^+ = 0$ by construction of BIE $\left(\overset{\text{RHS}}{2f = 0}\right)$.

$\Rightarrow$ $v = 0$ in $\mathbb{R}^2 \setminus \bar{\Omega}$ by uniqueness of ext. Dir. BVP for radiative solns.
← a PDE result (Colton §6.5)

$\Rightarrow$ $v_n^+ = 0$ on $\partial\Omega$

$\Rightarrow$ JR 1, 3 $\Rightarrow$ $v^- = -\tau$
JR 2, 4 $\Rightarrow$ $v_n^- = -i\eta\tau$ } (a)

GII in Ω:
$$\underbrace{\int_{\partial\Omega} \bar{v}^- v_n^- \, ds}_{\text{by (a)} \; +i\eta\int_{\partial\Omega}|\tau|^2 ds} = \underbrace{\int_\Omega \bar{v}\Delta v + \vec{\nabla}\bar{v}\cdot\vec{\nabla}v \, dx}_{-k^2|v|^2 + |\vec{\nabla}v|^2 \text{ pure real.}}$$

Take Im part: $\tau \equiv 0$. (& $\eta \neq 0$). QED.

↑ but complex k messes this up.

Notes:

i) Call such a scheme robust since provably never fails; similar exist for Neu ext BVP, transmission, etc. Maxwell (ACMS!)

ii) Quadrature of BIE now harder: S has log singularity

Approaches: a) use 'correction' of periodic trap. rule weights near diagonal, so omits diagonal $i=j$ & integrates smooth + $\log|s-t|\cdot$ smooth to high order.
Kapur–Rokhlin '97.

b) find exact weights to integrate log · smooth globally: 'product quadrature'
Kress '91, better but more analytic work.

c) other ways to correct near singularity using new set of nodes; sing, replace.
Alpert '99.

projects, research.

These also make D quadr. high order (HW6: noticed only 3rd order, unlike Laplace $k=0$ case was exponential).

Fast Algorithms:

how people solve big problems.

eg $N = 10^6$: can't even fill Nyström matrix A ($10^{12} \times 16$ bytes $= 16000$ GB)
demanded by complex geom or 3d surface.
let alone do dense linear solve ($N^3 = 10^{18}$ flops)! $A\vec{x} = \vec{b}$

Instead: iterative methods. eg. 'GMRES' (NLA ch. 35), each iter. involves $\vec{x} \mapsto A\vec{x}$
converges, stop when residual error $\|A\vec{x} - \vec{b}\|$ small enough for you.

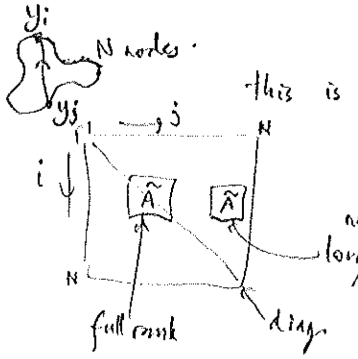
For well-conditioned 2nd kind IE, takes only $\underbrace{10\text{–}20}_{O(1), \text{ ie indep. of } N!}$ iters to get many digits (10^{-14}) accuracy.
But 1st kind terrible convergence rate, unless

So now, whole scheme to solve for $\vec{\tau}$ is $O(N^2)$ since $x \mapsto Ax$ is.

Can we apply the dense $N\times N$ Nyström matrix to a vector $\vec{x}$ faster than $O(N^2)$? Yes!

③ 2/21/12

Toy problem { Let $y_i \in \mathbb{R}^2$ be set of nodes.
A has elements $a_{ij} = \begin{cases} \ln\frac{1}{|y_i-y_j|} & i\neq j \\ 0 & i=j \end{cases}$



this is off-diag part of Nyström matrix for S operator (Laplace), without weights w_j.

↳ also apps to

run lowrank_curve.m w/ N = 1e3, 5e3

numerical lowrank: small (~10) & indep. of N!

low rank requires source — target separation.

$\tilde A$ low num. rank means $\tilde A \approx PQ = \underbrace{N \times \sim 10}_{} \; \underbrace{\sim 10 \times N}_{}$ eg via SVD, (but that's too slow in practice)

Fix an off-diag block, call it size N×N: sources $y_j \in \mathbb{R}^2$, $j=1\ldots N$, targets $z_i \in \mathbb{R}^2$, $i=1\ldots N$.

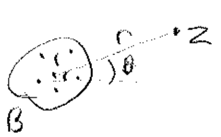
wish to compute $u_i = \sum_{j=1}^{N} x_j \ln\frac{1}{|z_i-y_j|} = (\tilde A \vec x)_i$, $i=1\ldots N$.

'charge strength' at each node.

Potential due to sources $u(z) = \sum_{j=1}^{N} x_j \ln\frac{1}{|z-y_j|}$ harmonic for $z \neq y_j$, $j=1\ldots N$.

Goal is eval u @ targets z_i, $i=1\ldots N$.

Thm (multipole expansion): outside a disc B centered at 0, containing all $\{y_j\}$, we can write



$$u(r,\theta) = \underbrace{c_0 \ln\frac{1}{r}}_{\text{monopole}} + \sum_{n=1}^{\infty} (a_n \cos n\theta + b_n \sin n\theta)\, r^{-n}$$

← Fourier series on each circle r = const

or writing $z = re^{i\theta}$,
$$u(z) = \mathrm{Re}\left\{ c_0 \ln\frac{1}{z} + \underbrace{\sum_{n=1}^{\infty} c_n z^{-n}}_{\text{Laurent expansion}} \right\}$$

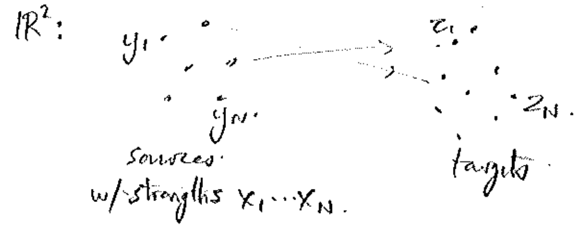
sums abs. convergent in $\mathbb{R}^2 \setminus \overline{B}$

M126 lec. 5 fast algs. (for Laplace kernel in $\mathbb{R}^2$). ① 2/23/12

last time empirically observed low-rank property of off-diag blocks, but how exploit this? (without doing an SVD, which is $O(N^3)$!)

last time: want eval potential $u(z) = \sum_{j=1}^{N} x_j \ln \frac{1}{|z-y_j|}$ at $z = z_i$, $i = 1 \cdots N$.

$\uparrow$ $\in \mathbb{R}^2$; x_j: charge strengths of sources



- since N sources, N targets, N^2 interactions (have to eval ln dist N^2 times, naively)
- if $u_i := u(z_i)$ then $\vec{u} = \hat{A}\vec{x}$, where $\hat{A}$ is some $N \times N$ off-diagonal block of eg Nyström matrix.

Note: $u(z)$ harmonic for $z \neq y_j$, $j = 1 \cdots N$.

<u>Thm (multipole expansion)</u>: Let B be a disc containing all y_j, centered at O, radius R,

then for $r > R$, $\underbrace{u(r,\theta)}_{z \text{ in polars}} = \underbrace{c_0 \ln \frac{1}{r}}_{\text{monopole}} + \underbrace{\sum_{n=1}^{\infty} (a_n \cos n\theta + b_n \sin n\theta) r^{-n}}_{\text{Fourier series at each radius } r.}$

sums abs. convergent in $r > R$.

Note: setting $c_0 = 0$, true for any func u harmonic in $r \geq R$ w/ $u = o(1)$ as $r \to \infty$.

Or considering $\mathbb{R}^2 \simeq \mathbb{C}$, $u(z) = \text{Re}\left[c_0 \ln \frac{1}{z} + \underbrace{\sum_{n=1}^{\infty} c_n z^{-n}}_{\text{Laurent expansion}} \right]$ ("Taylor exp. about ∞")

Say truncate to p terms, how bad is error?

Consider single unit charge @ y: $u(z) = \ln \frac{1}{z-y}$ let's work w/ complex-valued potential, take Re at end.

$= \ln \frac{1}{z} - \ln(1 - y/z)$

Taylor $-\ln(1-x) = x + \frac{x^2}{2} + \frac{x^3}{3} + \cdots$ when $|x| < 1$.

$= \ln \frac{1}{z} + y z^{-1} + \frac{y^2}{2} z^{-2} + \frac{y^3}{3} z^{-3} + \cdots$ abs. conv. for $|z| > |y|$

is multipole expansion, proves above thm.

P'wise truncation error $e_p(z) := \underbrace{\ln \frac{1}{z} + \sum_{n=1}^{p-1} \frac{y^n}{n} z^{-n}}_{p\text{-term approx.}} - \underbrace{\ln \frac{1}{z-y}}_{\text{true}} = \underbrace{\sum_{n=p}^{\infty} \frac{y^n}{n} z^{-n}}_{\text{tail of sum.}}$

so $|e_p(z)| \leq \sum_{n=p}^{\infty} \frac{1}{n} \left|\frac{y}{z}\right|^n \underset{\text{shift sum.}}{=} \left|\frac{y}{z}\right|^p \sum_{n=0}^{\infty} \underbrace{\frac{1}{n+p}}_{\leq \frac{1}{n} \text{ for } n>0.} \left|\frac{y}{z}\right|^n \leq \left|\frac{y}{z}\right|^p \underbrace{\left(\frac{1}{p} + \ln \frac{1}{1 - |y/z|} \right)}_{O(1) \text{ as } p \to \infty, \text{ for fixed } y, z \in \mathbb{C}.}$

so $|e_p(z)| = O\left(\left|\frac{y}{z}\right|^p\right)$ as $p \to \infty$ exponential conv. in p!

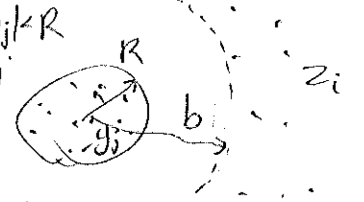
Use this bnd for each charge in disc B, get:

<u>Thm (multipole error)</u>: potential due to N charges x_j, locations y_j, in disc rad. R can be rep. by p^{th}-order multipole expansion in $|z| > b > R$ w/ pointwise error $\leq C \left(\sum_{j=1}^{N} |x_j| \right) \cdot \left(\frac{R}{b}\right)^p$

② 2/23/12

Use to apply offdiagonal blocks $\tilde{A}$: $|z_i| > b$, $|y_j| < R$ $\forall j$

Say $\{z_i\}_{i=1}^{N}$ 'well-separated' from $\{y_j\}_{j=1}^{N}$, ie
targs sources



$\frac{b}{R}$ significantly larger than 1, eg. 2.

Recipe: (HW7!)

i) decide p based on desired accuracy: $\left(\frac{R}{b}\right)^p$(tot. charge) $\approx \varepsilon$. ← typ. $p \sim 20$ to 40.

ii) compute multipole coeffs due to sources:
$$c_0 = \sum_{j=1}^{N} x_j \ , \quad c_n = \sum_{j=1}^{N} \frac{y_j^n}{n} x_j, \ n = 1, \dots p-1$$
} does $\vec{c} = Q\vec{x}$

iii) evaluate multipole expansion at targets:
$$u(z_i) \approx u^{(p)}(z_i) = c_0 \ln\frac{1}{z_i} + \sum_{n=1}^{p-1} c_n z_i^{-n} \qquad i = 1, \dots N.$$
} does $\vec{u} = P\vec{c}$, $\tilde{A} \approx PQ$.

Complexity: ii) $O(pN)$, iii) $O(pN)$ ⇒ $O(pN)$ total, but $p = O(\ln\frac{1}{\varepsilon})$
⇒ $O(N)$. for fixed error.

$$N\,\boxed{\tilde{A}}_N \approx N\,\boxed{P}_p \ p\,\boxed{Q}_N$$

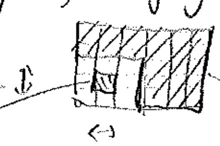
compare original $O(N^2)$! eg $N = 10^6$, $p = 10^{1.5}$ $(\varepsilon = 10^{-9})$, then speedup is $10^{4.5} \approx 30000$! That's a good algorithm ;)

Unfortunately, applying whole of A, interaction matrix between $\{y_j\}_{j=1}^{N}$ ← ie sources = targets
is trickier since not all clumps of points well-separated.

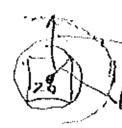
Say all y_j's lie in rectangle, roughly uniformly distributed:

Cover by M square boxes:

box. B_i



all these boxes are well-separated from B_i



$b = \frac{3}{2}L$, $R = \frac{L}{\sqrt{2}}$ } $\frac{b}{R} = \frac{3\sqrt{2}}{2} \approx 2.1$ controls convergence rate.

if uniform, $\approx \frac{N}{M}$ charges per box.

Effort to get multipole coeffs about each box due to charges in it $=$ pN ← tot charges
(about: $z - z_0$ replaces z in expansion, where z_0 = box center.) (p: terms each charge affects.)

Then $u_i = \sum_{j=1}^{N} A_{ij} x_j = \underbrace{\sum_{j \text{ in } B \text{ or touching box}} A_{ij} x_j}_{\text{do direct sum, effort} \approx 9\frac{N}{M}} + \underbrace{\sum_{j \text{ in box for which } B \text{ is well-sep.}} A_{ij} x_j}$

y_i in same box B

approx by sum of multipole expansions from each of $M-9$ other boxes,
effort $\approx p(M-9) = O(pM)$.

Total effort $(i = 1, \dots N)$
$$= \underset{\text{get coeffs (cheap)}}{pN} + \underset{\text{local, direct}}{9\frac{N^2}{M}} + \underset{\text{distant.}}{pMN}$$
← how choose M to scale with N so best?
$M = N^\gamma$, balance $\frac{N^2}{N^\gamma} \approx N^\gamma N$
ie $2 - \gamma = \gamma + 1$, $\gamma = 1/2$.

optimal here is $O(pN^{3/2})$

Fixing p, this is $O\left(\frac{N^{1/2}}{p}\right)$ times faster than naive, eg $N = 10^6$, $p = 10^{1.5}$, is $10^{1.5} \approx 30\times$ faster

Ok, but not as great as before.

AM126 lec 16

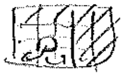
· ACMS 4pm
· X-hr: LaTeX for slides!

· projects — start putting slides together — can use LaTeX.
short write-up due Fri 9th, 5pm.

① 2/28/12

Last time: $O(N^{3/2})$ alg. for applying interaction matrix to vector x_j of charges, the $a_{ij} = \ln\frac{1}{|y_i - y_j|}$ (2d Laplace kernel) between N particles

Assuming? uniformly distributed in rectangle.

Trick: (M boxes)  nearby: sum directly.
far boxes: eval multipole expansion.

Relies on A matrix coming from elliptic PDE.

Why is $\vec{x} \mapsto A\vec{x}$ important to apply fast?

- enables iterative soln. ("Krylov" methods: apply A repeatedly) of large Nyström lin. sys. for BVP.
- Other apps: compute forces in large gravitational, fluid (point vortices), molecular (electrostatic) simulation. Timestep to evolve.

note: methods are either iterative or direct

don't know how many iters needed... (ill-cond = bad!)

eg { $O(N^3)$ algs. for dense solves, Gaussian elim.
{ fast direct solvers — Gillman colloq. this Thu } fixed effort, even for ill-cond.

Bottleneck: each target box has many $\left(\frac{N}{M}\right)$ targets at which many (M) m'pole exps have to be eval'ed.

Better: combine to 'local expansion' before eval'ing at targets in box:

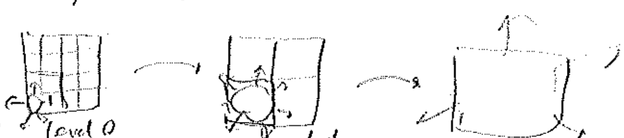
→ ③ 2/23/12. (see next page).

— break.

Hierarchical (multilevel) versions:

'Tree code':

(small boxes w/ O(1) particles per box)



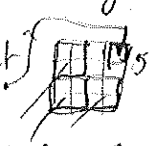
level 0 level 1 level 2

once got src box m'pole exps, gather in groups of 4 to give new m'pole exps (M2M)

(all have same order p)

requires 'quad tree' structure: each box has a level, a list of children (unless level 0, a 'leaf' box), a parent.

↑ gathering up the tree

to eval. at targ. box  near: do directly O(1)

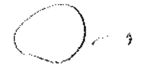
3 level 1 m'poles. (no local exps used).

get $O(N \ln N)$ effort ~ close to linear in N.
↳ (optimal, since must operate on each charge, & N of them).

Adaptivity:

what if not uniform? Subdivide to different levels until O(1) charges per box.

harder to code, but same scaling w/ N.

'Fast multipole method' (FMM): gather m'pole exps on way up the tree, translate (M2L) to local exps. on top-level boxes, " separate local exps on way down tree.  etc.

Finally eval. local exps. on leaves at all targets; excluding O(1) nearby sources which are summed directly.

Bookkeeping tricky! at each level there are boxes not well-sep. for M2L; have to do using child boxes: interaction lists.

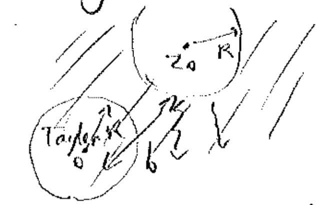
Effort: $O(N)$, Greengard-Rokhlin '87. Also adaptive version. 3d is much messier!

Where's the bottleneck? If could make smaller box size L, less interactions could be done directly. But currently would have more boxes hence more effort evaluating all their m'pole exp's at the $O(N)$ distant pts! ③ 2/28/12

$\Rightarrow$ Need a way to combine m'pole exp's so all target pts in a box can be eval'ed from single expansion... a 'local expansion' = Taylor expansion.

start

Say $z_0 \in \mathbb{C}$ is source box center, rep. by m'pole $@ z_0$, $|z_0| \geq 2R$, then can be rep. by Taylor @0 in $|z|<R$,



Consider terms in m'pole,

eg monopole $\ln \frac{1}{z-z_0} = \ln \frac{1}{z_0} - \ln\left(\frac{z}{z_0} - 1\right)$ $\quad \ln(x-1) = x - \frac{x^2}{2} + \frac{x^3}{3} - \dots$ for $|x|<1$.

$$= \ln \frac{1}{z_0} - \frac{1}{z_0} z + \frac{1}{2z_0^2} z^2 - \frac{1}{3z_0^3} z^3 + \dots$$

n^{th}-pole $(z-z_0)^{-n}$ has

0^{th} Taylor coeff $= (z-z_0)^{-n}\big|_{z=0} = (-z_0)^{-n} = (-1)^n z_0^{-n}$

1^{st} " " $\frac{d}{dz}\big|_{z=0} (z-z_0)^{-n} = -n(z-z_0)^{-n-1}\big|_{z=0} = -n(-z_0)^{-n-1} = (-1)^n z_0^{-n-1} n$

m^{th} " " $\frac{1}{m!} \frac{d^m}{dz^m}\big|_{z=0} (z-z_0)^{-n} = \frac{1}{m!}(-1)^n n(n+1)\cdots(n+m-1)\, z_0^{-n-m}$

So,

$$= (-1)^n \binom{n+m-1}{n-1} z_0^{-n-m}$$

Thm (M2L, "multipole to local"): m'pole exp. $u(z) = c_0 \ln \frac{1}{z-z_0} + \sum_{n\geq 1}^{\infty} c_n (z-z_0)^{-n}$ can be written as Taylor expansion $\sum_{n=0}^{\infty} a_n z^n$, abs. convergent in $|z| < |z_0|$, with coeffs

$$\begin{cases} a_0 = c_0 \ln \frac{1}{z_0} + \sum_{n=1}^{\infty} (-1)^n z_0^{-n} c_n \\ a_m = c_0 \frac{(-1)^m}{m} z_0^{-m} + \sum_{n=1}^{\infty} (-1)^n \binom{n+m-1}{n-1} z_0^{-n-m} c_n, \quad m = 1, 2, \dots \end{cases}$$

Thm (error of M2L): if sources $\{y_j\}_{j=1}^N$ lie in $|z-z_0|<R$, $|z_0| > b+R$ for some $b>R$, then error of truncating above sums to p terms is, in $|z|<R$, bnded by $c\left(\sum_{j=1}^N |x_j|\right)\left(\frac{R}{b}\right)^p$

Pf: Greengard–Rokhlin '87 $\quad$ dep on $\frac{R}{b}$ $\quad$ tot. charge

Same exponential convergence rate as before;

'Far' eval. can now become:
- for each target box compute a_m coeffs due to each m'pole src box c_n's
- evaluate local (Taylor) exp at all targets in the target box.

Effort is $O(p^2 M^2)$ since p^2 to map c_n's to a_m's, & M^2 translations z_0 (many are actually same)

$+ O(pN)$ eval. p^{th}-order local exp. at all N target pts.

Total effort now $\underset{\text{S2M src-to-m'pole}}{pN} + \underbrace{\underset{\text{direct}}{9\frac{N^2}{M}} + \underset{\text{M2L}}{p^2 M^2}} + \underset{\text{L2T}}{pN}$ $\rightarrow$ balance, $M = N^\gamma$

$2-\gamma = 2\gamma$, $\gamma = 2/3$

Overall scaling $O(p^2 N^{4/3})$

$= O(N^{4/3})$ if fixed p. Best yet.

Can do even better w/ heirarchical version: FMM.

Lec (7) M126. ① 3/1/12.

Handling quadrature for singular kernels.

Recall Helmholtz BVP (e.g. for scattering): need Nyström for $D - i\eta S$

cont. but not analytic ⇒ periodic trap. rule low order.

log singular on diag; PTR fails.

Are 'cheap' ways to correct PTR: Kapur-Rokhlin '97 changes weights near diag, sets diag $i=j$ to zero. Not v. good. (~ 50 nodes per wavelength needed for high acc.).

Best is 'product quadrature' (as in Kress '91): (~ 6 nodes per wavelength gets you 14 digits!). ① 3/1/12

Eg $\displaystyle\int_0^{2\pi} f(s)\, g(s)\, ds \approx \sum_{j=1}^{N} w_j f(s_j)$ where restrict $s_j = \frac{2\pi j}{N}$ ie PTR.

desired func. (real, smooth)

fixed 'weight' func (real, may be not smooth).

modified, not all just $\frac{2\pi}{N}$ for our g

Given g, how get $\{w_j\}_{j=1}^{N}$? Let's assume N even. (odd similar).

realize it's (f, g) & use Fourier series $f(s) = \sum_{n\in\mathbb{Z}} f_n e^{ins}$ (coeffs) $\longleftrightarrow f_n = \frac{1}{2\pi}\int_0^{2\pi} f(s) e^{-ins} ds$

$$\left(\sum_n f_n e^{ins}, \sum_m g_m e^{ims}\right) = \sum_n \sum_m \bar{f}_n g_m \underbrace{\int_0^{2\pi} e^{-ins+ims} ds}_{=?\ \begin{cases} 2\pi & n=m \\ 0 & \text{otherwise}\end{cases}}$$

$\{e^{ins}\}$ orthog. basis.

$$= 2\pi \sum_m \bar{f}_m g_m \quad \text{Parseval.}$$

$\ell_2(\mathbb{Z})$ inner-prod.

If f smooth, $|f_m| \to 0$ fast as $|m| \to \infty$.

In particular, if f analytic in strip $|\mathrm{Im}\, s| \le \alpha$, & bdd, then $f_m = O(e^{-\alpha|m|})$ Ex: prove this.

Use usual PTR to approx coeff formula: $f_n = \frac{1}{2\pi}\int_0^{2\pi} e^{-ins} f(s) ds \approx \tilde{f}_n := \frac{1}{N}\sum_{j=1}^{N} e^{-ins_j} f(s_j)$ (*)

Why good? sub. F. series for f: $\tilde{f}_n = \frac{1}{N}\sum_{j=1}^{N} e^{-ins_j} \sum_{m\in\mathbb{Z}} f_m e^{ims_j} = \sum_{m\in\mathbb{Z}} f_m \underbrace{\frac{1}{N}\sum_{j=1}^{N} e^{i(m-n)\frac{2\pi j}{N}}}_{\begin{cases} 1 & m = n \pmod N \\ 0 & \text{otherwise.}\end{cases}}$

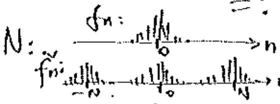
so $\tilde{f}_n = f_n + \underbrace{f_{n+N} + f_{n-N} + f_{n+2N} + f_{n-2N} + \cdots}_{\text{aliasing error: small if F. coeffs decay rapidly.}}$ So (*) exact for $\{e^{ins}\}_{|n|<N/2}$

then $\displaystyle\int_0^{2\pi} f(s) g(s)\, ds = 2\pi \sum_{n\in\mathbb{Z}} \bar{f}_n g_n \approx 2\pi \sum_n{}' \bar{f}_n g_n \underset{(*)}{\approx} \frac{2\pi}{N}\sum_{j=1}^{N} f(s_j) \underbrace{\sum_n{}' e^{ins_j} g_n}_{=: w_j}$

since f_n exp small for $|n| > N/2$.

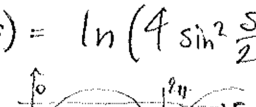
meaning $n \in [-N/2, N/2]$ but weighting ends by 1/2.

why truncate? since $\tilde{f}_n$ repeats @ N:



So $w_j = \frac{2\pi}{N}\sum_n{}' g_n e^{ins_j}$, $e^{ins_j} \to e^{\frac{2\pi i j n}{N}}$ ie $\{w_j\}$ = size N DFT of first N Fourier coeffs of g.

E.g. periodized log sing: $g(s) = \ln\left(4\sin^2\frac{s}{2}\right)$ has $g_n = \begin{cases} 0 & n = 0 \\ -\frac{1}{|n|} & \text{otherwise.}\end{cases}$ [LKE, Thm 8.21, algebra].



note: $g'(s) = \cot s/2$ helps proof.

← note since $\sum_{n\in\mathbb{Z}} |g_n|^2 < \infty$, $g \in L^2(0, 2\pi)$.

Then $w_j = \frac{2\pi}{N}\Big[\sum_{n=0}^{N/2-1} \underbrace{g_n e^{\frac{2\pi i j n}{N}} + g_{-n} e^{-\frac{2\pi i j n}{N}}}_{2\,\mathrm{Re}(g_n e^{\frac{2\pi i j n}{N}})} + \underbrace{\tfrac{1}{2}\left(g_{N/2} e^{\pi i j} + g_{-N/2} e^{-\pi i j}\right)}_{(-1)^j\,\mathrm{Re}\, g_{N/2}} \Big]$

$\frac{2\pi i j n}{N} = i s_j n$; $g_{-n} = \overline{g_n}$, since g real.

True for any real g.

For our g_n,

$$w_j = \frac{2\pi}{N}\left[-\sum_{n=1}^{N/2-1} \frac{2}{n}\cos n s_j \;-\; (-1)^j \frac{1}{N} \right]$$

done.

Note: the $\approx$ in above are exact for $f \in \underbrace{\mathrm{Span}\{e^{ins}\}_{n=-N/2}^{N/2}}_{T_N \text{ 'trigonometric polynomials'}}$, can check.

Now can split kernel of $D - \eta S$ into $\underset{\text{usual PTR}}{\text{analytic}(s,t)} + \underbrace{\log\left(4\sin^2\frac{s-t}{2}\right)}_{\text{new weights, shifted cyclically.}} \cdot \text{analytic}(s,t)$

eg S has kernel (wrt. parameter $0 \le s < 2\pi$):

$$\frac{i}{4} H_0(k|y(t)-y(s)|)\underbrace{|y'(s)|}_{\text{speed.}} = \underbrace{\frac{-1}{4\pi} J_0(k|y(t)-y(s)|)\,|y'(s)|}_{M_1(t,s)\text{ anal.}} \cdot \ln\left(4\sin^2\frac{t-s}{2}\right) + \underbrace{M_2(t,s)}_{\text{analytic, since the log part precisely removed!}}$$

$M_2(t,s)$ defined by this, apart from $M(s,s)$, for which exists formula.

Similar for D... see Kress '91, or Colton-Kress '98.

Scheme: Nyström matrix $A_{ij} = \underset{\text{PTR weights (fixed)}}{\frac{2\pi}{N}} M_2(s_i, s_j) + \underbrace{w_{|i-j|}}_{\text{why? this shifts singularity to be at } j=i \text{ for row } i.} M_1(s_i, s_j)$

Note: incompatible w/ FMM since weights dep. on j and i so can't be treated as fixed charges.

'Circulant' matrix: each row is previous cyclically shifted 1 to right.

Other objects you should see:

A) Sobolev spaces (type of Hilbert space)

recall $L^2[0,2\pi) := \{ \text{functions } f : \underbrace{\int_0^{2\pi} |f(x)|^2 dx}_{\|f\|_{L^2}^2 = 2\pi \sum_{n\in\mathbb{Z}} |f_n|^2} < \infty \}$, loosely.

Defn: (Sobolev space order s)

$H^s[0,2\pi) := \{ \text{funcs } f : \underbrace{\sum_{n\in\mathbb{Z}} (1+n^2)^s |f_n|^2}_{\|f\|_{H^s}^2} < \infty \}$ v. common in PDE analysis.

$H^0 = L^2$, $s > 0$ enforces faster decay of Fourier coeffs. $\Rightarrow$ smoother than L^2.

Eg $g(x) = \ln\left(4\sin^2\frac{x}{2}\right) \in H^s[0,2\pi] \quad \forall s < 1/2$ since $\sum (1+n^2)^s \frac{1}{n^2} < \infty$.

Thm: Let $s > 1/2$, $f \in H^s$, then $f \in C[0,2\pi]$. ← periodic

Pf: for each x, $\left(\sum_{n\in\mathbb{Z}} |f_n e^{inx}|\right)^2 \overset{C.S.}{\le} \underbrace{\left(\sum_{n\in\mathbb{Z}} \frac{1}{(1+n^2)^s}\right)}_{\text{converges for } s>1/2} \sum_{n\in\mathbb{Z}} (1+n^2)^s |f_n|^2$

So Fourier series abs. conv, f uniform lim. of cont. funcs.

Thm: Let $f \in H^s$, then $\frac{df}{dx} \in H^{s-1}$ ← derivative is one order less smooth.

pf: fourier coeffs of f' are $i n f_n$. □

So, $H^1(a,b) = \{ f : \underbrace{\int_a^b |f(x)|^2 dx + \int_a^b |f'(x)|^2 dx}_{\text{since } 2\pi \sum (1+n^2)|f_n|^2} < \infty \}$

$H^1(\mathbb{R}^d)$ is higher-dim analog, common for PDE.

Thm: single-layer op. S is bnded from H^s to H^{s+1}, ie S behaves like "1 order of integration." (smoothing, makes coeffs decay more)

pf sketch: i) singularity of S is $g(s-t) = \ln\left(4 \sin^2 \frac{s-t}{2}\right)$ ↳ convolution kernel.
which has $|g_n| \sim \frac{1}{|n|}$

ii) Applying confolution op. $h(t) = \int g(t-s) f(s) ds = (g * f)(t)$, is $h_n = f_n g_n$ in Fourier space. (check it!).

Thm: $D : H^s \to H^s$ bnded (order 0)
$T : H^s \to H^{s-1}$ bnded, ie like derivative of 1 order.

see [LIE Ch. 8], [CK] books

Suggests that $\underset{\text{order} +1}{T}\underset{\text{order} -1}{S}$ is order 0. True: $TS = -I/4 + (D^*)^2$

called 'Calderón identity'; numerically can use to 'precondition' nasty T into Id except.

B) Calderón projection (Helmholtz case) Recall a "projection op." P obeys $P^2 = P$ as operators.

Recall interior GRF $-Du^- + Su_n^- = \begin{cases} u & \text{in } \Omega \\ 0 & \text{in } \mathbb{R}^d \setminus \overline{\Omega} \end{cases}$

taking $x \to \partial\Omega^-$, & using JR1-4, $\begin{cases} \text{values:} & -(D - 1/2)u^- + Su_n^- = u^- \\ \text{n-derivs:} & -Tu^- + (D^* + 1/2)u_n^- = u_n^- \end{cases}$ ie $\left(- \underbrace{\begin{bmatrix} D & -S \\ T & -D^* \end{bmatrix}}_{H} + \underbrace{\begin{bmatrix} I/2 & \\ & I/2 \end{bmatrix}}_{\frac{1}{2}\mathrm{Id}} \right) \begin{bmatrix} u^- \\ u_n^- \end{bmatrix} = \begin{bmatrix} u^- \\ u_n^- \end{bmatrix}$

Instead taking $x \to \partial\Omega^+$ gives opposite jumps, ⇒ $\underbrace{(1/2 + H)}_{=: P_+} \begin{bmatrix} u^- \\ u_n^- \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$.

so $P_- = (1/2 - H)$ is identity in lin. subspace V_- of interior bdry data pairs.

But haven't yet shown P_- is a projection!

④ 3/1/12

Showing P_- is actually a projection:

$\forall \tau, \sigma$, know $\mathcal{D}\tau + \mathcal{S}\sigma$ is an interior Helmholtz solution, say u, in which case $\begin{bmatrix} u^- \\ u_n^- \end{bmatrix} \in V_-$

$\Rightarrow$ Using JRs as before, $P_- \begin{bmatrix} -\tau \\ \sigma \end{bmatrix} = \begin{bmatrix} u^- \\ u_n^- \end{bmatrix}$

so $P_-^2 \begin{bmatrix} -\tau \\ \sigma \end{bmatrix} = P_-\left(P_- \begin{bmatrix} -\tau \\ \sigma \end{bmatrix}\right) = P_- \begin{bmatrix} u^- \\ u_n^- \end{bmatrix} \overset{\text{since } P_- \text{ acts as Id in } V_-}{=} \begin{bmatrix} u^- \\ u_n^- \end{bmatrix} = P_- \begin{bmatrix} -\tau \\ \sigma \end{bmatrix}$ True $\forall \tau, \sigma$, so $P_-^2 = P_-$ as ops. □

Since $P_- = \frac{1}{2} - H$, $(\frac{1}{2} - H)^2 = \frac{1}{4} - \cancel{H} + H^2 = \frac{1}{2} - \cancel{H}$ so $H^2 = 1/4$, ie $\begin{bmatrix} D^2 - ST & -DS + SD^* \\ TD - D^*T & -TS + D^{*2} \end{bmatrix} = \begin{bmatrix} 1/4 & 0 \\ 0 & 1/4 \end{bmatrix}$ Calderón identities!

Thm (exterior GRF): let $(\Delta + k^2)u = 0$ in $\mathbb{R}^d \setminus \overline{\Omega}$ & u sat. radiation condition @ ∞, then

$$-\mathcal{D}u^+ + \mathcal{S}u_n^+ = \begin{cases} 0 & \text{in } \Omega \\ -u & \text{in } \mathbb{R}^d \setminus \overline{\Omega} \end{cases}$$

[CK book Thm. 2.4]

Proof:

Let B be ball centered at 0 enclosing Ω, radius r

i) We first show $\int_{\partial B} |u|^2 ds = O(1)$ as $r \to \infty$

we have the identity, by expanding, $\int_{\partial B} \left|\frac{\partial u}{\partial r} - iku\right|^2 ds = \int_{\partial B} \left|\frac{\partial u}{\partial r}\right|^2 + k^2|u|^2 + \overbrace{2k \,\mathrm{Im}\, u \frac{\partial \bar{u}}{\partial r}}^{\text{flux leaving sphere}} ds$ (†)

Also, in any region R in which u a Helmholtz soln, we have "flux balance" (FB):

$$\mathrm{Im} \int_{\partial R} u \bar{u}_n \, ds = \mathrm{Im} \int_R u \underbrace{\Delta \bar{u}}_{-k^2 \bar{u}} + \nabla u \cdot \nabla \bar{u} \, dx \quad \text{by G1I.}$$

interpret as net flux entering R. $= 0$ since RHS purely real.

Apply FB to $R = B \setminus \overline{\Omega}$ gives $2k \,\mathrm{Im} \int_{\partial B} u \frac{\partial \bar{u}}{\partial r} ds = \underbrace{2k \,\mathrm{Im} \int_{\partial \Omega} u \bar{u}_n \, ds}_{\text{a bounded number } F, \text{ dep on } u.}$

Combine w/ (†) gives $\lim_{r \to \infty} \int_{\partial B} \left|\frac{\partial u}{\partial r}\right|^2 + k^2 |u|^2 ds = -F + \underbrace{\lim_{r \to \infty} \int_{\partial B} \left|\frac{\partial u}{\partial r} - iku\right|^2 ds}_{=0 \text{ by rad. cond.}}$

LHS is sum of nonneg. terms, so each bounded, $O(1)$

ii) Now use this to show surface term in GRF on ∂B vanishes as $r \to \infty$. Let $x \in B \setminus \overline{\Omega}$,

$$\int_{\partial B} \left[u(y) \frac{\partial \Phi(x,y)}{\partial n_y} - u_n(y) \Phi(x,y)\right] ds_y = \underbrace{\int_{\partial B} u \left[\frac{\partial \Phi}{\partial n_y} - ik\Phi\right] ds_y}_{=: I_1} - \underbrace{\int_{\partial B} \Phi (u_n - iku) \, ds_y}_{=: I_2}$$

claim $I_1, I_2 \to 0$ as $r \to \infty$:

⑤ 3/1/12

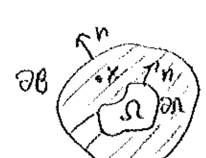
$$\frac{\partial \Phi(x,y)}{\partial n_y} - ik\Phi(x,y) = o\left(\frac{1}{r^{\frac{d-1}{2}}}\right) \quad \text{since } \Phi(x,\cdot) \text{ radiating soln.}$$

by C-S. $$I_1^2 \le \underbrace{\int_{\partial B} |u|^2 ds}_{O(1)} \cdot \underbrace{\int_{\partial B} \left| \frac{\partial\Phi(x,y)}{\partial n_y} - ik\Phi(x,y)\right|^2}_{o\left(\frac{1}{r^{d-1}}\right)} ds_y = o(1) \quad \text{as } r\to\infty.$$

surf. area is $O(r^{d-1})$

for I_2, $\Phi(x,\cdot) = O\left(\frac{1}{r^{\frac{d-1}{2}}}\right)$ & u radiating, so $I_2 \to 0$ as $r\to\infty$.

iii) We apply interior GRF to $B\setminus\overline{\Omega}$ gives,



$$-\int_{\partial\Omega + \partial B} u_n(y)\Phi(x,y) - u(y)\frac{\partial\Phi}{\partial n_y}(x,y)\, ds_y = \begin{cases} u(x) & x\in B\setminus\overline{\Omega} \\ 0 & x\in\Omega \end{cases}$$

since $\partial\Omega$ normal points into $B\setminus\overline{\Omega}$

in ii) we showed this term vanishes as $r\to\infty$

True for each r. Finally take $\lim r\to\infty$. QED.

May now finish Calderón Projectors;

apply exterior GRF, take $x\to\partial\Omega^+$ & use JR's gives, $P_+\begin{bmatrix}u^+\\u_n^+\end{bmatrix} = \begin{bmatrix}u^+\\u_n^+\end{bmatrix}$, $P_-\begin{bmatrix}u^+\\u_n^+\end{bmatrix} = \begin{bmatrix}0\\0\end{bmatrix}$
(for u any radiative Helm. soln. in $\mathbb{R}^d\setminus\overline{\Omega}$)

holds for all $\begin{bmatrix}u^+\\u_n^+\end{bmatrix}\in V_+$

by identical proof as P_-, we then get P_+ is a projection.

<u>Lemma</u>: $V_+ \oplus V_- = \begin{bmatrix}L^2(\partial\Omega)\\L^2(\partial\Omega)\end{bmatrix}$ Pf: $I = \tfrac12 + H + \tfrac12 - H = P_+ + P_-$

so, $\forall\sigma,\tau$, $\begin{bmatrix}-\tau\\\sigma\end{bmatrix} = P_+\begin{bmatrix}-\tau\\\sigma\end{bmatrix} + P_-\begin{bmatrix}-\tau\\\sigma\end{bmatrix}$, is a decomposition into V_+ & V_-. □

Summary: $P_+V_+ = V_+$, $P_+V_- = \{0\}$ and $P_+P_- = P_-P_+ = 0$
$P_-V_+ = \{0\}$, $P_-V_- = V_-$

Thus P_+, P_- are complementary projectors.

Notes:
- Shipman-Venakides papers, eg. 2003, have clear explanation of this.
- contrary to statement of Kress in his acoustic notes, $2H$ is <u>not</u> a projection. (it is a reflection, since $(2H)^2 = I$)
- We <u>haven't</u> shown $V_+ \perp V_-$, ie that projections are <u>orthogonal</u>. This would require $P_+ = P_+^*$, etc; I don't believe holds.

FIN