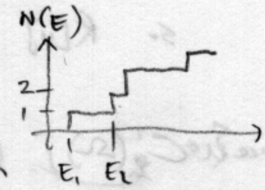
[Lec 17]

① 11/20/08

Weyl's problem: how do $\{E_j\}$ Dirichlet eigvals of domain Ω, behave as $j \to \infty$?

defn. level counting $N(E) := \#\{j : E_j \le E\}$



Thm ("Weyl's (1912) Law")

$$N(E) = \begin{cases} \underbrace{\frac{\text{area}(\Omega)}{4\pi} E}_{\text{lin. growth}} + \underbrace{O(E^{1/2})}_{\text{smaller fluctuation}} & \text{for } \Omega \subset \mathbb{R}^d,\ d=2 \\ \frac{\text{Vol}(\Omega)}{(4\pi)^{d/2}\,\Gamma(d/2+1)} E^{d/2} + O\left(E^{\frac{d-1}{2}}\right) & d \geq 2 \end{cases}$$

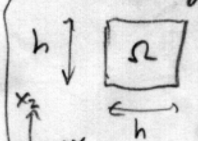
- $d=2$: asymp. const. density (mean spacing) of E_j. gamma func $\Gamma(x+1) := \int_0^\infty t^x e^{-t}\,dt$, $\Gamma(n+1) = n!$
- bound is sharp because of e.g. disk (sphere, etc) for which correction term is as large as $cE^{\frac{d-1}{2}}$
- Since $\text{Vol}(B^d)$, d-dim unit ball, is $\frac{\pi^{d/2}}{\Gamma(d/2+1)}$ (see Resources), $N(E) \sim \frac{1}{(2\pi)^d}\text{Vol}(\Omega)\cdot \underbrace{\text{Vol}(B^d)k^d}_{\text{vol. of velocity space w/ speed } |k|}$ with $k^2 = E$ wave #.

'phase space' = space of positions & velocities of point particles in Ω.

'each mode occupies fixed phase volume'

- Jeans in 19th knew this, not proven.

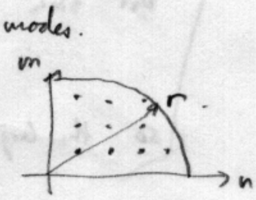
Proof for square:



$\phi_{nm} = \sin\frac{n\pi x_1}{h}\sin\frac{m\pi x_2}{h}$, $E_{nm} = \left(\frac{\pi}{h}\right)^2(n^2+m^2)$ check.

$n,m \in \mathbb{N}$ Δ separable in cartesians, so mode is product of 1d modes.

$N(E) = \#$ lattice pts of $\mathbb{N}^2$ within radius $r = \frac{h}{\pi}\sqrt{E}$ of origin.



Since each dot inside brings area 1, $N(E) \le \frac{\pi r^2}{4}$ ← $\frac14$ disc.

But $\frac{\pi r^2}{4} - N(E) \le$ area of rectangle $\frac{\pi}{2}r\cdot\sqrt{2}$ so $N(E) = \frac{\pi r^2}{4} + O(r)$

$$= \underbrace{h^2}_{\text{area}(\Omega)}\frac{E}{4\pi} + O(E^{1/2})$$

Gauss' circle problem... $N(E)$ has interesting fluct. QED.

Thm (Courant – Fischer) (Minimax characterization of eigvals) E_n of lin. op. A with complete o.n.b. of eigfuncs ϕ_n.

$$E_n = \sup_{\substack{v_1, v_2, \dots v_{n-1} \\ \in \mathcal{H}}}\left[\inf_{\substack{u \perp \text{Span}\{v_1,\dots v_{n-1}\} \\ u \in D(A)}} \underbrace{\frac{(u, Au)}{(u,u)}}_{\text{Rayleigh quotient. } R[u]}\right]$$

pf. $u = \sum c_i\phi_i$ so $R[u] = \frac{\sum E_i c_i^2}{\sum c_i^2} \geq E_1$ which proves for $n=1$. (there's no sup then).

$n>1$, $v_j = \phi_j$ $j = 1\cdots n-1$ gives optimal choice, ie largest inf.

Why? i) with this choice, $c_j = 0$ for $j = 1\cdots n-1$ so $\inf_{u \perp \text{Span}\{v_1,\cdots v_{n-1}\}} R[u] = \inf_{a_j,\, j\ge n} \frac{\sum_{j\ge n} E_j a_j^2}{\sum_{j \ge n} a_j^2}$

ii) if $V := \mathrm{Span}\{v_1, \dots v_{n-1}\} \neq \mathrm{Span}\{\phi_1 \dots \phi_{n-1}\}$ then

$\exists\, u \perp V$, $u \in \mathrm{Span}\{\phi_1, \dots \phi_n\}$ s.t. $a_j \neq 0$, $j = 1 \dots n-1$.

(Combine i) & ii) QED.) so $R[u] = \sum_{j=1}^{n} E_j a_j^2 \le E_n$. $\sum_{j=1}^{n} a_j^2 = 1$.

for $A = -\Delta$ in space $\{u \in C_0^2(\Omega),\ u|_{\partial\Omega} = 0\}$.

$$R[u] = \frac{1}{\|u\|^2}\int u(-\Delta)u = \frac{\int_\Omega |\nabla u|^2 dx}{\int_\Omega u^2 dx} \leftarrow \text{Dirichlet integral, or `energy'}.$$

Lec 17: [Finish Weyl's Law] give Courant-Fischer thm. in particular, choose $A = -\Delta$, $\mathcal{H} = L^2(\Omega)$, $D(A) = C_0^2(\Omega)$ with piecewise-C^1 also.

Thm: if $\Omega \subset \Omega^*$ then $E_n \geq E_n^*$ for each $n = 1, 2, \dots$ ie making domain larger can only decrease its eigvals.

pf: extend funcs $v_1 \dots v_{n-1}$, u as zero in $\Omega^* \setminus \Omega$. $\longrightarrow$ still in space of piecewise C^1.

Then $u \perp \mathrm{Span}\{v_1 \dots v_{n-1}\}$ still holds with inner prod $\int_{\Omega^*} \overline{u(x)}\, v(x)\, dx$.

also $R^*[u] = R[u]$

$\uparrow$ means $\dfrac{\int_{\Omega^*} \bar{u}(-\Delta u)\, dx}{\int_{\Omega^*} |u|^2 dx}$

but since, fixing v's, ~~subspace~~ $C_0^2(\Omega^*) \supset C_0^2(\Omega)$ ie space of trial funcs enlarged, (is a subspace)

$$\inf_{\substack{u \perp v_1 \dots v_{n-1} \\ u = 0 \text{ on } \partial\Omega^*}} R^*[u] \leq \inf_{\substack{u \perp v_1 \dots \\ u = 0 \text{ on } \partial\Omega}} R[u]$$

so the largest inf cannot exceed that of E_n.

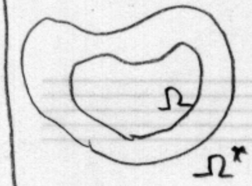
See 2006 notes. : Subtlety is the Neumann BC case.

(2006 notes)

Bounding eigenvalues by contained and containing domains:

Thm if $\Omega \subset \Omega^*$ then $E_n \geq E_n^*$ for all $n = 1, 2, \cdots$

Pf. extend funcs $\begin{cases} v_1, \cdots v_{n-1} \\ u \end{cases}$ as zero in $\Omega^* \setminus \Omega$



Then if $u \perp \mathrm{Span}\{v_1 \cdots v_{n-1}\}$ holds over Ω, also does over Ω^*

Also $R^*[u] = R[u]$, where $*$ indicates integrals in Ω^*.

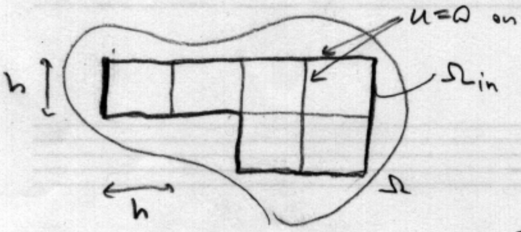
But since subspace of trial func u enlarged, $\displaystyle\min_{\substack{u \perp V \\ u=0 \text{ on } \partial\Omega^*}} R^*[u] \leq \min_{\substack{u \perp V \\ u=0 \text{ on } \partial\Omega}} R[u]$

Using minimax, E_n^* then cannot exceed E_n.

General rule: $\begin{cases} \text{enlarging} \\ \text{restricting} \end{cases}$ the linear space of trial funcs means E_n cannot $\begin{cases} \text{increase} \\ \text{decrease} \end{cases}$

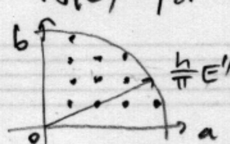
- As our restricted space choose:

$u=0$ on all boundaries of squares in lattice contained in Ω.



Each Dirichlet square has spectrum $E_n = \left(\frac{\pi}{h}\right)^2 (a^2+b^2)$
(modes: $\sin a\frac{\pi x}{h} \sin b\frac{\pi x}{h}$) for $a, b \in \mathbb{N}$

Then $N(E)$ for each square $= \#$ lattice points of $\mathbb{N}^2$



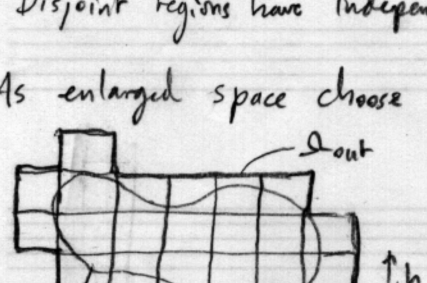
$\frac{h}{\pi}E^{1/2} = r$ lying within radius $\frac{h}{\pi}E^{1/2}$ of origin.

Thus $N(E) = \frac{\pi}{4} r^2 + O(r)$
$= \frac{h^2}{4\pi} E + O(E^{1/2})$

Ie each square already obeys Weyl's Law. (area $= h^2$)

Disjoint regions have independent spectra $\Rightarrow N_{in}(E) = \frac{\mathrm{vol}(\Omega_{in})}{4\pi} E + O(E^{1/2})$

- As enlarged space choose covering squares,



each with Neumann BCs ('free' membranes),
similar argument gives $N_{out}(E) = \frac{\mathrm{vol}(\Omega_{out})}{4\pi} E + O(E^{1/2})$

Thus asymptotically, $\lim_{E\to\infty} \frac{N_{in}(E)}{E} = \frac{\mathrm{vol}(\Omega_{in})}{4\pi}$

$$\lim_{E\to\infty} \frac{N_{out}(E)}{E} = \frac{\mathrm{vol}(\Omega_{out})}{4\pi}$$

Our bounds on eigenvalues E_n mean

$$N_{in}(E) \leq N(E) \leq N_{out}(E)$$

ie $\frac{\mathrm{vol}(\Omega_{in})}{4\pi} \leq \lim_{E\to\infty} \frac{N(E)}{E} \leq \frac{\mathrm{vol}(\Omega_{out})}{4\pi}$

Finally we may take arbitrarily small squares h, giving $\mathrm{vol}(\Omega_{in}) \to \mathrm{vol}(\Omega)$
$\mathrm{vol}(\Omega_{out}) \to \mathrm{vol}(\Omega)$

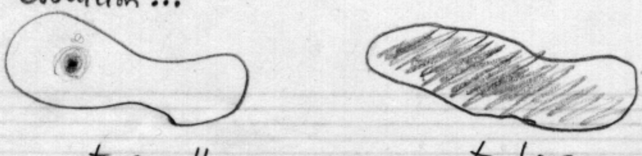
Thus. $\underline{\lim_{E\to\infty} \frac{N(E)}{E} = \frac{\mathrm{vol}(\Omega)}{4\pi}}$ QED. "Exhaustion method".

Heat trace asymptotics:

Historically, the next step (Carleman, '30's)
[see Baltes & Hilf, Spectra of Finite Systems, book (1976)]

Heat equation
$$u_t = \Delta u \quad \text{in } \Omega \times [0,\infty)$$
$$u = 0 \quad \text{on } \partial\Omega \times [0,\infty)$$

Time evolution ...



t small t large

initial condition $u(x,0) = u_0(x)$
$u_0 \in L^2(\Omega)$

Solution by mode decomposition : (1) $u(x,t) = \sum_{j=1}^{\infty} a_j e^{-E_j t} \phi_j(x)$ sep. of variables.

check satisfies PDE ! $a_j = \langle \phi_j, u_0 \rangle$

Write as evolution operator, $u(x,t) = (K_t u_0)(x,t) = \int_\Omega K(x,y;t)\, u_0(y)\, dy$ (2)

where $K_t = e^{t\Delta}$ has kernel $K(x,y;t) = \sum_{j=1}^{\infty} e^{-E_j t} \phi_j(x) \phi_j(y)$ (3)
(formally solves PDE)

Why? Check (1) correctly given when stick kernel into (2).

~~M1116~~ Lec 18 ① 12/2/08.

Fast Multipole Methods (FMM): modern technology to solve large-scale numerical PDE problems.

Recall BIE, eg. scattering via DLP rep. $(I + 2D)\tau = f$

{ Nyström w/ N quadr. pts.

$(I + A)\vec{\tau} = \vec{f}$ $\qquad A_{ij} = \dfrac{\partial \Phi(y_i, y_j)}{\partial n_{y_j}} w_j$

$\llcorner_{N\times N}$ dense matrix.

effort: $O(N^2)$ to fill A

$+\,O(N^3)$ to solve dense linear system via 'direct' methods (eg Gaussian elim).

N^3 limits you to $N <$ few$\cdot 10^3$ (& takes ~1 hr) on usual workstation.

Linear sys. can be solved by 'iterative' methods, eg. GMRES (Tref. & Bau)

where each iter involves $\vec{x} \to A\vec{x}$ ie the matrix-vec mult, which is $2N^2$ flops.

GMRES converges fast iff cond(A) small. $\Rightarrow$ why 2nd kind preferred over 1st kind or MPS for large probs.

Then, can get good accuracy ($\varepsilon \sim 10^{-9}$) in 10-20 iters. $\approx \underbrace{20}_{\text{small const.}} N^2$ flops.

The whole method is now $O(N^2)$ ... you could go to $N \sim 10^4$, where A occupies ~1Gb RAM.

This is useless for $N \sim 10^6$ or 10^7, which can be done ... how?

- Never fill the matrix A, instead find a 'fast' way to do $\vec{x} \to A\vec{x}$ given any vector $\vec{x}$. ... eg if A were sparse would be easy but it's not
- Starting with Greengard & Rokhlin, late 80s, this can be done in $O(N \ln N)$, so whole solution $O(N \ln N)$ with similar storage $O(N \ln N)$.

True for Laplace, Helmholtz, other kernels, 2D or 3D.

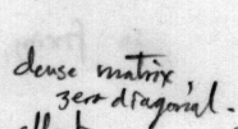
Toy problem: $A_{ij} = \begin{cases} \Phi(z_i, z_j) := \ln \dfrac{1}{|z_i - z_j|} & i \neq j \\ 0 & i = j. \end{cases}$ $\quad i,j = 1 \cdots N.$ dense matrix, zero diagonal.

Given $z_i \in \mathbb{R}^2$, $i = 1 \cdots N$, vector $\vec{\sigma} \in \mathbb{C}^N$, compute $A\vec{\sigma}$ in less than $O(N^2)$ effort

Apps:
- 2D laplace eqn solve via SLP. (ignoring quadrature).
- electrostatic potential energy of N pt. charges in 2d, or line charges in 3d.
- the 3D equivalent v. important for gravitational simulation of galaxies ($N > 10^6$), fluids.

Clue: if $y_i \in \mathbb{R}^2$, $z_i \in \mathbb{R}^2$, $i = 1 \cdots N$, $\tilde{A}_{ij} = \ln \dfrac{1}{|y_j - z_i|}$ $\quad i,j = 1 \cdots N$

sources $\neq$ targets



N	numerical rank($\tilde{A}$)
0	10
21	21
00	21
000	21

} means $\tilde{A}$ can be approx to $\varepsilon_{\text{mach}}$ by $\tilde{A} \approx PQ = {}_N\big[\,\big]_{21}\,{}_{21}\overset{N}{\big[\quad\big]}$, via SVD.

however, if z_i are mingled in with y_i, full rank. $\Rightarrow$ Low-rank approx. requires src-target separation

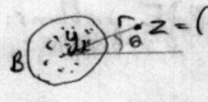
Field due to sources,

$u(z) = \sum \sigma_j \ln \frac{1}{|z-y_j|}$ is harmonic ($\Delta u = 0$) for $z \neq y_j$, $j = 1 \dots N$

since this is the fund soln.

Goal is to eval. $u(z_i)$ at targets z_i, $i = 1 \dots N$.

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



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

monopole — complete set, regular at ∞.

or considering $z \in \mathbb{C}$, $\quad u(z) = c_0 \ln \frac{1}{|z|} + \mathrm{Re} \underbrace{\sum_{n=1}^{\infty} c_n z^{-n}}_{\text{Laurent expansion}}$

Sums absolutely convergent in $\mathbb{R}^2 \setminus \overline{B}$

Say, truncate sum to p terms, how bad is error?

Consider single unit charge at y: $\quad u(z) = \ln \frac{1}{|z-y|}$

$$= \ln \frac{1}{|z|} - \ln \left| 1 - \frac{y}{z} \right|$$

when $\left|\frac{y}{z}\right| < 1$ may use Taylor expansion $-\ln(1-x) = x + \frac{x^2}{2} + \frac{x^3}{3} + \dots$

(use $\ln(ae^{ib}) = \ln a + ib$)

$$= \ln \frac{1}{|z|} - \mathrm{Re} \ln \left(1 - \frac{y}{z}\right)$$

$$= \ln \frac{1}{|z|} + \mathrm{Re}\left[y z^{-1} + \frac{y^2}{2} z^{-2} + \frac{y^3}{3} z^{-3} + \dots \right] \quad \text{for } |z| > |y|.$$

is multipole exp, proves above thm.

Ptwise error $\quad e_p(z) := \underbrace{\ln \frac{1}{|z-y|}}_{\text{true}} - \underbrace{\ln \frac{1}{|z|} - \mathrm{Re} \sum_{n=1}^{p-1} \frac{y^n}{n} z^{-n}}_{\text{(approx by p-terms)}}$

$$= \mathrm{Re} \sum_{n=p}^{\infty} \frac{y^n}{n} z^{-n} \quad \text{just the omitted tail of sum.}$$

so $\quad |e_p(z)| \le \sum_{n=p}^{\infty} \frac{1}{n} \left|\frac{y}{z}\right|^n \underset{\text{shift sum}}{=} \left|\frac{y}{z}\right|^p \sum_{n=0}^{\infty} \underbrace{\frac{1}{n+p}}_{\le \frac{1}{n} \text{ for } n>0} \left|\frac{y}{z}\right|^n \le \left|\frac{y}{z}\right|^p \Bigg(\underbrace{\frac{1}{p} + \sum_{n=1}^{\infty} \frac{1}{n} \left|\frac{y}{z}\right|^n}_{= \frac{1}{p} + \ln \frac{1}{1 - |y/z|}} \Bigg)$

so fixing y, z, $\quad |e_p(z)| \le c \left|\frac{y}{z}\right|^p \quad$ for $p = 1, 2, \dots$ $\quad \to$ some $O(1)$ const c as $p \to \infty$, for y, z fixed

$$= O\left(\left|\frac{y}{z}\right|^p\right) \quad \text{as } p \to \infty.$$

since $\left|\frac{y}{z}\right| < 1$ this is exponential convergence.

Thm: field due to N sources y_j, strengths σ_j, inside disc radius $|y_j| < a$, is rep. by p^{th}-order multipole expansion in $|z| > b > a$ with pointwise error $\le c \underbrace{\left(\sum_j |\sigma_j|\right)}_{\text{total charge.}} \cdot \left(\frac{a}{b}\right)^p$

Eg say we have L-sized grid, sources in one box,

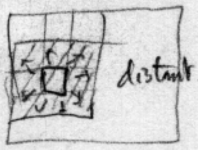
non-touching boxes are $b = \frac{3}{2} L$ away.

sources within radius $a = \frac{\sqrt{2}}{2} L$

So error $\varepsilon \le c \left(\frac{a}{b}\right)^p \simeq c \left(\frac{\sqrt{2}}{3}\right)^p \approx c\,(0.47)^p$

choose desired $\varepsilon \sim 10^{-9}$, require $p \approx |\log_{3/\sqrt{2}} \varepsilon| \approx 27$.

Recipe: say want $\vec{u} = A\vec{\sigma}$ for targets = sources = $\{z_j\}^{j=1\ldots N}$, randomly distributed in some region.

local →  ← distant.

choose $M = N^\gamma$ boxes, $0<\gamma<1$ as yet unknown.

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

we find multipole expansion coeffs of charges in each box : effort $\approx p\overset{\text{terms each charge affects}}{N}$ # charges.

then $u_i = \sum_{j=1}^{N} A_{ij}\sigma_j = \underbrace{\sum_{j \text{ in touching box or self}} A_{ij}\sigma_j}_{\text{effort} \approx 9\frac{N}{M} \text{ local, direct sum.}} + \underbrace{\sum_{j \text{ in distant box}} A_{ij}\sigma_j}_{\text{approx by sum of multipoles from each of } O(M) \text{ boxes}}$

effort $\approx pM$

Total effort $(i=1\cdots N)$ $= \overset{\text{local}}{9\frac{N^2}{M}} + \overset{\text{distant}}{pMN}$

$= \underbrace{9N^{2-\gamma} + pN^{1+\gamma}}$ these balance (same order) when $\gamma = 1/2$, minimize overall order to $O(N^{3/2})$

so if $N=10^6$ choose $M \approx 10^3$

Can improve 'distant' part to p^2M^2 by using 'local' expansions $u(z) = \mathrm{Re}\sum c_n(z-z_0)^n$ inside disc due to distant charges.

Then $\gamma = 2/3$ is best, giving $O(N^{4/3})$

Multilevel scheme gets $O(N \ln N)$ .. virtually linear in problem size! ($O(N)$ can never be beaten).