

Handling quadrature for singular kernels.

Recall Helmholtz BVP (eg. for scattering): need Nyström for  $D - \epsilon \Delta S$

cont. but not analytic  $\rightarrow$  log singular on diag; PTR fails.  
periodic trap. rule lurches.

Are 'cheap' ways to correct PTR: Kapor-Rokhlin '97 changes weights near diag, sets diag  $\epsilon_{ij}$  to zero. not so good. ( $\sim 50$  nodes per wavelength needed for high acc.)

Best is 'product quadrature' (as in Kress 1991): ( $\sim 6$  nodes per wavelength gets you 14 digits!) ① 3/1/2

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

desired func. (real, smooth)  $\leftarrow$  fixed weight func (real, may be not so smooth).  $\leftarrow$  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  $f(s) = \sum_{n \in \mathbb{Z}} f_n e^{ins}$   $\leftrightarrow$   $f_n = \frac{1}{2\pi} \int_0^{2\pi} f(s) e^{-ins} ds$

$\leftarrow (\sum_n f_n e^{ins}, \sum_m g_m e^{ims}) = \sum_n \sum_m \bar{f}_n g_m \int_0^{2\pi} e^{-ins + ims} ds$

$= 2\pi \sum_m \bar{f}_m g_m$  Parseval.  $\leftarrow$  coeffs.  $\leftarrow$   $\begin{cases} 2\pi & n=m \\ 0 & \text{otherwise} \end{cases}$   $\leftarrow \{e^{ins}\}$  orthog. basis.

If  $f$  smooth &  $|f_n| \rightarrow 0$  fast as  $|n| \rightarrow \infty$ .  $\leftarrow L_2(\mathbb{Z})$  inner prod.

In particular, if  $f$  analytic in strip  $|\text{Im}(s)| < \alpha$ , then  $f_n = O(e^{-\alpha|n|})$  ex: prove this.

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

Why good? sub. F. series for  $f$ :  $\hat{f}_n = \frac{1}{N} \sum_{j=1}^N e^{-ins_j} \sum_{m \in \mathbb{Z}} f_m e^{ims_j} = \sum_{m \in \mathbb{Z}} f_m \frac{1}{N} \sum_{j=1}^N e^{i(m-n)\frac{2\pi j}{N}}$

so  $\hat{f}_n = f_n + f_{n+N} + f_{n-2N} + \dots$  So (\*) exact for  $\{e^{ins}\}_{|n| < N/2}$

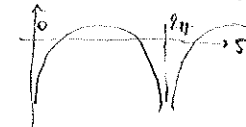
aliasing error: small if F. coeffs decay rapidly.  $\leftarrow$   $\begin{cases} 1 & m=n \pmod{N} \\ 0 & \text{otherwise} \end{cases}$

then  $\int_0^{2\pi} f(s) g(s) ds = 2\pi \sum_{n \in \mathbb{Z}} \bar{f}_n g_n \approx 2\pi \sum_{n=-N/2}^{N/2} \bar{f}_n g_n \approx \frac{2\pi}{N} \sum_{j=1}^N f(s_j) \sum_n e^{ins_j} g_n$

since  $f_n$  exp small for  $|n| > N/2$ .  $\leftarrow$  meaning  $n \in [N/2, N/2]$  but weights end by  $1/2$ .  $\leftarrow$  why truncate?  $\leftarrow$  since  $\hat{f}_n$  repeats @  $N$ :  $\frac{f_n}{N}$   $\rightarrow$   $\frac{f_{n+N}}{N}$   $\rightarrow$   $\frac{f_{n+2N}}{N}$   $\rightarrow$   $\dots$   $\leftarrow$   $\therefore w_j$

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

E.g. periodized log sing:  $g(s) = \ln(4 \sin^2 \frac{s}{2})$  has  $g_n = \begin{cases} 0 & n=0 \\ -\frac{1}{|n|} & \text{otherwise} \end{cases}$  [LIE, Thm 8.2] algebra.

note:  $g'(s) = \cot s/2$  helps proof. 

$\leftarrow$  note since  $\sum_{n \in \mathbb{Z}} |g_n|^2 < \infty$ ,  $g \in L^2(0, 2\pi)$ .

then  $w_j = \frac{2\pi}{N} \left[ \sum_{n=0}^{N/2-1} g_n e^{i s_j n} + g_{-n} e^{-i s_j n} + \frac{1}{2} (g_{N/2} e^{i s_j} + g_{-N/2} e^{-i s_j}) \right]$  ②  $2^{1/2}$

True for any real  $g$ .  
For our  $g_n$ ,  $2 \operatorname{Re}(g_n e^{i s_j n}) = g_n$  since  $g$  real.  $(-1)^j \operatorname{Re} g_{N/2}$

$$w_j = \frac{2\pi}{N} \left[ -\sum_{n=1}^{N/2-1} \frac{2}{n} \cos n s_j - (-1)^j \frac{1}{N} \right] \quad \text{done.}$$

Note: the  $x$  in above are exact for  $f \in \operatorname{span} \{ e^{i n s} \}_{n=-N/2}^{N/2}$ , can check.   
  $T_N$  'trigonometric polynomials'.

Now can split kernel of  $D - y S$  into analytic(s,t) +  $\log(4 \sin^2 \frac{s-t}{2}) \cdot \text{analytic}(s,t)$   
 $\uparrow$  usual PTR  $\uparrow$  new weights, shifted cyclically.

eg:  $S$  has kernel (rot. parameter  $0 \leq s < 2\pi$ ):

$$\frac{1}{\pi} H_0(k |y(t) - y(s)|) |y'(s)| = \frac{-1}{4\pi} J_0(k |y(t) - y(s)|) |y'(s)| \cdot \ln \left( 4 \sin^2 \frac{t-s}{2} \right) + M_2(t,s)$$

$\underbrace{\hspace{10em}}_{\text{speed.}} \quad \underbrace{\hspace{10em}}_{M_1(t,s) \text{ anal.}} \quad \underbrace{\hspace{10em}}_{\text{analytic, since the log part precisely removed!}}$

$M_2(t,s)$  defined by this, apart from  $M(s,s)$ , for which exists formula.

Similar for  $D$ ... see Kress '91, or Coltan-Kress '98.

Schwarz: Nyström matrix  $A_{ij} = \frac{2\pi}{N} M_2(s_i, s_j) + w_{|i-j|} M_1(s_i, s_j)$   
 $\uparrow$  PTR weights (fixed)

Note: incompatible w/ FMM since weights dep. on  $j$  and  $i$  so can't be treated as fixed charges.

Why? this shifts singularity to be at  $j=i$  for row  $i$ .  
Circulant matrix: each row is previous cyclically shifted 1 to right.

Other objects you should see:

A) Sobolev spaces (type of Hilbert spaces)

recall  $L^2[0, 2\pi] := \{ \text{functions } f : \int_0^{2\pi} |f(x)|^2 dx < \infty \}$ , loosely -  $\|f\|_{L^2}$

Defn: (Sobolev space order  $s$ ):

$$H^s[0, 2\pi] := \{ \text{funes } f : \sum_{n \in \mathbb{Z}} (1+n^2)^s |f_n|^2 < \infty \} \quad \text{v. common in PDE analysis.}$$

$H^0 = L^2$ ,  $s > 0$  enforces faster decay of Fourier coeffs.  $\Rightarrow$  smoother than  $L^2$ .

eg  $g(x) = \ln(4 \sin^2 \frac{x}{2}) \in H^s[0, 2\pi] \quad \forall s < 1/2$  since  $\sum (1+n^2)^s \frac{1}{n^2} < \infty$ .

Thm: Let  $s > 1/2$ ,  $f \in H^s$ , then  $f \in C[0, 2\pi]$ .  $\leftarrow$  periodic

Pf: for each  $x$ ,  $(\sum_{n \in \mathbb{Z}} |f_n e^{i n x}|)^2 \leq \underbrace{(\sum_{n \in \mathbb{Z}} \frac{1}{(1+n^2)^s})}_{\text{converges for } s > 1/2} \sum_{n \in \mathbb{Z}} (1+n^2)^s |f_n|^2$   
 So Fourier series abs. conv,  $f$  uniform lim. of cont. funes.

Thm: Let  $f \in H^s$ , then  $\frac{df}{dx} \in H^{s-1}$  ← derivative is /less smooth: one order.

pf: Fourier coeffs of  $f$  are  $\text{inf}_n$ .  $\square$

So,  $H^s(a,b) = \left\{ f : \int_a^b |f(x)|^2 dx + \int_a^b |f'(x)|^2 dx < \infty \right\}$   
 since  $2\pi \sum (1+n^2) |f_n|^2$

$H^2(\mathbb{R}^d)$  is higher-dim analog, common for PDE.

Thm: single-layer op  $S$  is bnded from  $H^s$  to  $H^{s+1}$

pf sketch: i) singularity of  $S$  is  $g(s-t) = \ln(4\pi n^2 \frac{s-t}{2})$  which has  $|g_n| \sim \frac{1}{|n|}$  → convolution kernel.

ie  $S$  behaves like "1 order of integration" (smoothing, makes coeffs decay more)

ii) Applying convolution 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:  $D : H^s \rightarrow H^s$  bnded (order 0)  
 $T : H^s \rightarrow H^{s-1}$  bnded, ie like derivative of 1 order.

see [LIE Ch-8], [CK] books

Suggests that  $TS$  is order 0.  
 order +1      order -1

Trace:  $TS = -I/4 + (D^*)^2$  called 'Calderón identity', numerically amuse to precondition nasty  $T$  into Id + c.p.t.

B) Calderón projection (Helmholtz case)

Recall a "projection op."  $P$  obeys  $P^2 = P$  as operators.

Recall interior GRF  $-\mathcal{D}u^- + S u_n^- = \begin{cases} f u & \text{on } \Omega \\ 0 & \text{on } \mathbb{R}^d \setminus \Omega \end{cases}$

taking  $x \rightarrow \partial\Omega^-$ , values:  $-(\mathcal{D}-1/2)u^- + S u_n^- = u^-$   
 $x \rightarrow \partial\Omega^+$ ,  $u^-$ -derivs:  $-T u^- + (\mathcal{D}^* + 1/2)u_n^- = u_n^-$  ie  $\begin{pmatrix} -[\mathcal{D}-S] & [I/2] \\ [T-\mathcal{D}^*] & [I/2] \end{pmatrix} \begin{pmatrix} u^- \\ u_n^- \end{pmatrix} = \begin{pmatrix} u^- \\ u_n^- \end{pmatrix}$

Instead taking  $x \rightarrow \partial\Omega^+$  gives opposite jumps,  $\Rightarrow (\frac{1}{2} + H) \begin{pmatrix} u^- \\ u_n^- \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ .  $\leftarrow$  so  $P_- := (\frac{1}{2} + H)$  is identity in lin. subspace  $N_{-1}$  of interior bdm data pairs.

But haven't yet shown  $P_-$  is a projection!

Showing  $P_-$  is actually a projection:

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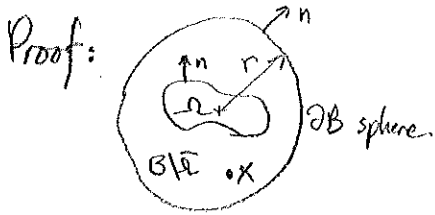
$\forall \tau, \sigma$ , know  $\begin{bmatrix} \tau \\ \sigma \end{bmatrix}$  is an interior Helmholtz solution, say  $u$ ,  
in which case  $\begin{bmatrix} u \\ u_n \end{bmatrix} \in V_-$

$\Rightarrow$  Using JKs as before,  $P_- \begin{bmatrix} \tau \\ \sigma \end{bmatrix} = \begin{bmatrix} u^- \\ u_n^- \end{bmatrix}$  since  $P_-$  acts as Id in  $V_-$

so  $P_-^2 \begin{bmatrix} \tau \\ \sigma \end{bmatrix} = P_-(P_- \begin{bmatrix} \tau \\ \sigma \end{bmatrix}) = P_- \begin{bmatrix} u^- \\ u_n^- \end{bmatrix} = \begin{bmatrix} u^- \\ u_n^- \end{bmatrix} = P_- \begin{bmatrix} \tau \\ \sigma \end{bmatrix}$  True  $\forall \tau, \sigma$ , so  $P_-^2 = P_-$  as ops.  $\square$

Since  $P_- = \frac{1}{2} - H$ ,  $(\frac{1}{2} - H)^2 = \frac{1}{4} - H + H^2 = \frac{1}{2} - H$  so  $H^2 = \frac{1}{4}$ , ie  $\begin{bmatrix} D^2 - ST & -DS + SD^* \\ TD - D^*T & -TS + DX^2 \end{bmatrix} = \begin{bmatrix} 1/4 & 0 \\ 0 & 1/4 \end{bmatrix}$  Calderón identities!

Then (exterior GRF): let  $(D+k^2)u=0$  in  $\mathbb{R}^d \setminus \bar{\Omega}$  &  $u$  sat. radiation condition @  $\infty$ ,  
then  $-\epsilon Du' + \mathcal{D}u_n' = \begin{cases} 0 & \text{in } \Omega \\ -u & \text{in } \mathbb{R}^d \setminus \bar{\Omega} \end{cases}$  (CK book Thm. 2.4)



Proof: Let  $B$  be ball centered at  $0$  enclosing  $\Omega$ , radius  $r$

i) We first show  $\int_{\partial B} |u|^2 ds = O(1)$  as  $r \rightarrow \infty$  - flux leaving sphere

we have the identity, by expanding,  $\int_{\partial B} |\frac{\partial u}{\partial r} - ik u|^2 ds = \int_{\partial B} |\frac{\partial u}{\partial r}|^2 + k^2 |u|^2 + 2k \text{Im} u \frac{\partial u}{\partial r} ds$  (+)

Also, in any region  $R$  in which  $u$  a Helmholtz soln, we have "flux balance" (FB):

$$\text{Im} \int_{\partial R} u \bar{u}_n ds = \text{Im} \int_R \frac{u \Delta \bar{u}}{1 - k^2 \bar{u}} + Du \cdot \nabla \bar{u} dx \quad \text{by GII.}$$

interpret as net flux entering  $R$ . = 0 since RHS purely real.

Apply FB to  $R = B \setminus \bar{\Omega}$  gives  $2k \text{Im} \int_{\partial B} u \frac{\partial \bar{u}}{\partial r} ds = 2k \text{Im} \int_{\partial \Omega} u \bar{u}_n ds$

Combine w/ (+) gives  $\lim_{r \rightarrow \infty} \int_{\partial B} |\frac{\partial u}{\partial r}|^2 + k^2 |u|^2 ds = -F + \lim_{r \rightarrow \infty} \int_{\partial B} |\frac{\partial u}{\partial r} - ik u|^2 ds$   
 LHS is sum of nonneg. terms, so each bounded,  $O(1)$  a bounded number  $F$ , dep on  $u$ .  
 = 0 by rad. cond.

ii) Now use this to show surface term in GRF on  $\partial B$  vanishes as  $r \rightarrow \infty$ : Let  $x \in B \setminus \bar{\Omega}$ ,

$$\int_{\partial B} [u(y) \frac{\partial \Phi(k, y)}{\partial n_y} - u_n(y) \Phi(k, y)] ds_y = \underbrace{\int_{\partial B} u \left[ \frac{\partial \Phi}{\partial n_y} - ik \Phi \right] ds_y}_{=: I_1} - \underbrace{\int_{\partial B} \Phi (u_n - ik u) ds_y}_{=: I_2}$$

claim  $I_1, I_2 \rightarrow 0$  as  $r \rightarrow \infty$ :

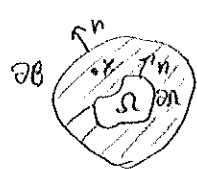
$$\frac{\partial \Phi(x,y)}{\partial n_y} - ik \Phi(x,y) = o\left(\frac{1}{r^{\frac{d-1}{2}}}\right) \text{ since } \Phi(x,\cdot) \text{ radiating soln.}$$

by G.S.  $I_1^2 \in \underbrace{\int_{\partial B} |u|^2 ds}_{o(1)} \cdot \int_{\partial B} \underbrace{\left| \frac{\partial \Phi(x,y)}{\partial n_y} - ik \Phi(x,y) \right|^2 ds_y}_{o\left(\frac{1}{r^{d-1}}\right)} = o(1) \text{ as } r \rightarrow \infty.$

↑ 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  $I_2 \rightarrow 0$  as  $r \rightarrow \infty$ .

iii) We apply interior GRF to  $B \setminus \Omega$  gives,



$$-\int_{\partial \Omega + \partial B} u_n(y) \Phi(x,y) - u(y) \frac{\partial \Phi(x,y)}{\partial n_y} ds_y = \begin{cases} \int u(x) & x \in \partial \Omega \\ 0 & x \in \Omega \end{cases}$$

↑ since  $\partial \Omega$  normal points into  $B \setminus \Omega$       ↑ in ii) we showed this term vanishes as  $r \rightarrow \infty$

True for each  $r$ . Finally take  $\lim r \rightarrow \infty$ . QED.

May now finish Calderón Projectors:

apply exterior GRF, take  $x \rightarrow \partial \Omega^+$  & use JK'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  $\mathbb{R}^d \setminus \Omega$ )

by identical proof as  $P_-$ , we then get  $P_+$  is a projection.  $\mathbb{Z}$  holds for all  $\begin{bmatrix} u^{++} \\ u_n^{++} \end{bmatrix} \in V_+$

Lemma:  $V_+ \oplus V_- = \begin{bmatrix} L^2(\partial \Omega) \\ L^2(\partial \Omega) \end{bmatrix}$  Pf:  $I = \frac{1}{2} + H + \frac{1}{2} - H = P_+ + P_-$

so,  $\forall \delta, \tau$ ,  $\begin{bmatrix} -\tau \\ \delta \end{bmatrix} = P_+ \begin{bmatrix} -\tau \\ \delta \end{bmatrix} + P_- \begin{bmatrix} -\tau \\ \delta \end{bmatrix}$ , is a decomposition into  $V_+$  &  $V_-$ .  $\square$

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 paper, eg. 2003, have clear explanation of this.
  - contrary to statement of Kress in his acoustic notes,  $2H$  is not a projection. (it is a reflection, since  $(2H)^2 = I$ )
  - We haven't shown  $V_+ \perp V_-$ , ie that projections are orthogonal. This would require  $P_+ = P_+^*$ , etc; I don't believe holds.

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