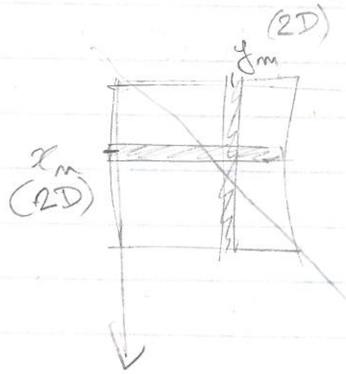
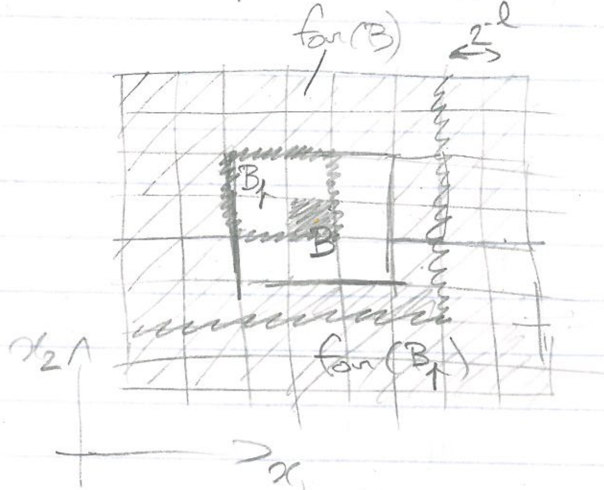
03/05/2013 FMM: fast multipole method



$> G(x_m, :)$ row
$G(:, y_m)$ column

i, x: row index / var.
j, y: column index / var.

Dyadic partitioning. $\ell = 0, 1, 2, \ldots$



Source B
Target A

Def: A and B (at the same scale) are well separated
$\Leftrightarrow$ $B \in$ far(A) (far field)
$\Leftrightarrow$ $A \in$ far(B)

when dist(A, B) $\geq$ sidelength(A) $= sl(B)$

$\rightarrow$ A, B for which canonical charges/potentials are adequate.

A, B for which interaction computed as such:

<u>Def</u>. A is in the <u>interaction list</u> of B (at the same scale as A)
($A \in IL(B)$) when
- $A \in far(B)$
- A is not the child of a box in $far(B_p)$ — parent of B.

2D : 27 boxes
3D : 189 boxes

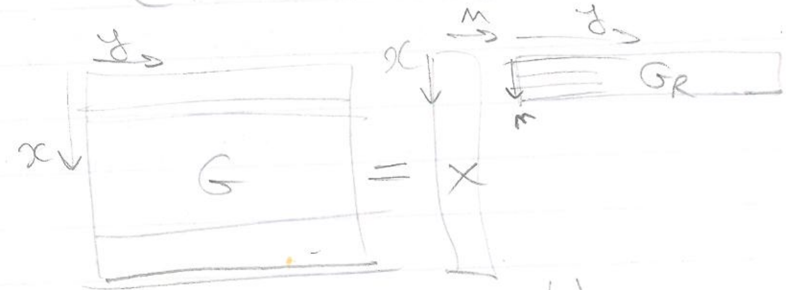
Rationale for separation property: accurate <u>interpolation</u> with few terms.

(1) $G(x,y) \simeq \sum_m P_m^A(x)\, G(x_m^A, y)$ $\quad x \in A,\ y \in far(A)$

(2) $G(x,y) \simeq \sum_m G(x, y_m^B)\, P_m^B(y)$ $\quad y \in B,\ x \in far(B)$

1) Pol. interp.
2) Harm. pol
3) Linear algebra : $G \simeq X G_R$
$G \simeq G_C Y$

R: subset of rows indexed by x_m^A
C: — cols — y_m^B

(1) 

→ low-rank, one-sided interpolative dec. of G.
Det by pivoted QR

+

Compare with $G(x,y) \simeq \sum u_j(x)\, \sigma_j\, v_j(y)$ $x \in A$, $y \in far(A)$

(SVD)

2-sided interpolative / skeleton

(3) $G(x,y) \simeq \sum_{mm} G(x, y_m^B)\, Z_{mm}\, G(x_m^A, y)$

$$G \simeq G_C\, Z\, G_R$$

<u>ex</u>. $Z = G_C^+\, G\, G_R^+$ (best LS)

or G_{CR}^+ (convenient)

compare to (1) : $P_m^A(x) = \sum G(x, y_m^B)\, Z_{m,m}$

In all cases : induced separation of G:

$m = 1, \ldots, M_\varepsilon^* \geq r_\varepsilon$, rank of G

<u>Next</u>: Why kernel is low-rank

Why adjoint harm. pol. is multipole.

BIE.

03/07/2013 FMM (interpolative view)

$B \in \mathrm{far}(A)$: block $G(x,y)$ for $\begin{cases} x \in A \\ y \in B \end{cases}$ has low rank

Interpolation:

(1) $G(x,y) \simeq \sum_m P_m^A(x)\, G(x_m^A, y)$, $x \in A$, $y \in \mathrm{far}(A)$

(2) $G(x,y) \simeq \sum_m G(x, y_m^B)\, P_m^B(y)$, $y \in B$, $x \in \mathrm{far}(B)$

Partial potentials resulting from separated interactions

From B: $u^B(x) = \int_B G(x,y)\, q(y)\, dy$, $x \in \mathrm{far}(B)$

To A: $u^{\mathrm{far}(A)}(x) = \int_{\mathrm{far}(A)} G(x,y)\, q(y)\, dy$: $x \in A$.

L2T.

Target: let $u_m^A = u^{\mathrm{far}(A)}(x_m^A)$ (can. pot)

$\boxed{\text{To A (1)}} \Rightarrow u^{\mathrm{far}(A)}(x) \simeq \sum_m P_m^A(x)\, u_m^A$ (interp (L2T))

called local expansion

Go from $u_{m'}^{A_p}$ at $x_{m'}^{A_p}$ to u_m^A at x_m^A.

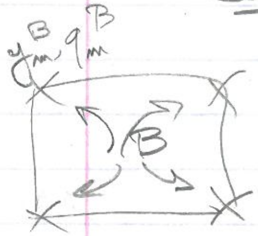
$$\boxed{u_m^A \simeq \sum_{m'} P_{m'}^{A_p}(x_m^A)\, u_{m'}^{A_p}} + (\dots)$$

(L2L)

→ downward pass

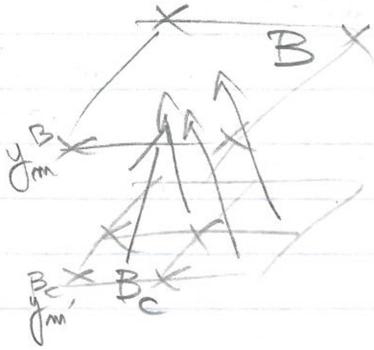
called → multipole expansion

<u>Source</u>: let q_m^B s.t. $u^B(x) \simeq \sum_m G(x, y_m^B)\, q_m^B$ (can. charges)



From B (2) ⇒ $\boxed{q_m^B = \int_B P_m^B(y)\, q(y)\, dy.}$ projection (S2M)

adjoint of L2T



Go from $q_{m'}^{B_c}$ at $y_{m'}^{B_c}$ to q_m^B at y_m^B:

$$\boxed{q_m^B \simeq \sum_{c} \sum_{m'} P_m^B(y_{m'}^{B_c})\, q_{m'}^{B_c}}$$

(M2M)

→ upward pass

<u>Conversion</u>: At each scale, $q_m^B \to u_m^A$

For each A, gather $B \in IL(A)$

$$\boxed{u_m^A \simeq \sum_{B \in IL(A)} \sum_m G(x_m^A, y_m^B)\, q_m^B} + (L2L)$$

(M2L)

Don't forget the closeby interactions:
Finest scale, $B \notin far(A)$: $u^{diag}(x) = \int_{B \notin far(A)} G(x,y)\, q(y)\, dy$ for $x \in A$

<u>Ref</u>. 1) White-Phillips, Brandt
2) Greengard-Rokhlin
3) H-matrices (H^2): Hackbusch, Bebendorf, Börm

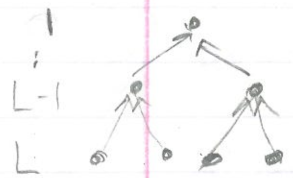
Algo: 0) Init: - choose finest scale L:

$\quad$ sidelength$(A) = 2^{-L}$ (leaves)

- bin sources into B (finest scale)

$\quad$ targets into A (—)

- For each A, build $IL(A)$



1) Upward pass to get q_m^B

Init leaves: $q_m^B = S2M$

For $l = L \ldots 1$:

$\quad$ For B at scale l

$$q_m^B = \sum_c M2M\left(q_{m'}^{B_c}\right)$$

2) Downward pass to get u_n^A

Init root: $u_n^A = 0$ $(l=0)$

For $l = 1 \ldots L$

$\quad$ For A at scale l

$$u_n^A = \sum_{B \in IL(A)} M2L\left(q_m^B\right) + L2L\left(u_{n'}^{A_p}\right)$$

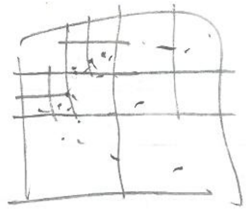
3) Termination: $u(x) = L2T(u_n^A) + u^{diag}(x)$ $\quad (x \in A)$

2D Complexity: say $n = 1, \ldots, p$ and $m = 1 \ldots p$

- single M2M: p^2 / box B_c
- single L2L: p^2 / box A
- single M2L: $p^2 \times 27$ / box A
- number of boxes: $2^{2L} + 2^{2(L-1)} + \ldots \leq 2 \cdot 2^{2L}$

$\Rightarrow O(p^2 2^{2L})$

Point of FMM: nonuniform geometries !



points: N

$$u(x_i) = \sum_{j=1}^{N} G(x_i, y_j)\, q_j \qquad i=1,\dots N$$

Adaptive quadtree: $\leq s$ sources per leaf box.
$\rightarrow O(N/s)$ leaf boxes
$\rightarrow O(N/s)$ boxes

0) Binning: $O(N)$ ops = # points

1) S2M to get $q_m^B = \int_B P_m^B(y)\, q(y)\, dy = \sum_{j=1} P_m^B(y_j)\, q_j$

Each q_j is in some box B
p coeffs per box $\rightarrow O(pN)$ ops

M2M : $O(p^2 \frac{N}{s})$ ops

2) M2L : $O(27 p^2 \frac{N}{s})$ ops

L2L : $O(p^2 \frac{N}{s})$ ops

3) L2T to get $u^{far(A)}(x_i) = \sum_{m=1}^{p} P_m^A(x_i)\, u_m^A$

Each x_i is in some box A
p coeffs per box $\rightarrow O(pN)$

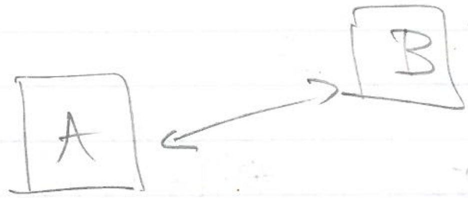
Diag: # leaf boxes $\times$ # pts per box A
$\times$ # pts per box B

$$O\left(\frac{N}{s} s^2\right) = O(Ns)$$

Complexity $= O\left(N + pN + p^2 \frac{N}{s} + Ns\right)$

Choose $s = p$, get $O(pN)$

Why is $G(x,y)$ low-rank,
$x \in A,\ y \in B$
$B \in \text{far}(A)$



ex. $G(x,y) = \log|x-y|$
obeys $\Delta_x G = 0 \quad x \neq y$

Show there exist $f_k\ g_k$, $k = 1, \ldots p$

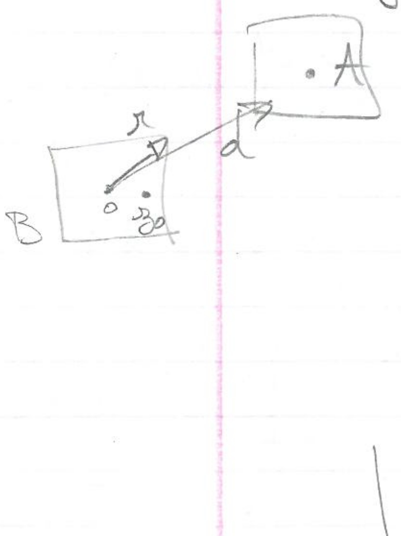
$$\max_{\substack{x\in A\\ y \in B}} \left| G(x,y) - \sum_{k=1}^{p} f_k(x)\, g_k(y) \right| \le C \left(\frac{\sqrt{2}}{3}\right)^p$$

$z = x_1 + i x_2$
$z_0 = y_1 + i y_2$

$$\log|x-y| = \operatorname{Re}\left(\log(z - z_0)\right)$$

each term is separated

$$\log(z - z_0) = \log(z) - \sum_{k=1}^{\infty} \frac{1}{k}\left(\frac{z_0}{z}\right)^k \quad \circledast$$



→ Taylor (harm pol) in z_0 (L)
Multipole in z (M)

Here $|z_0| \le r$
$|z| \ge d$

$$\left| \log(z - z_0) - \log(z) + \sum_{k=1}^{p} \frac{1}{k}\left(\frac{z_0}{z}\right)^k \right|$$

$$\le \left| \sum_{k=p+1}^{\infty} \frac{1}{k}\left(\frac{z_0}{z}\right)^k \right| \le \frac{1}{p+1} \frac{(r/d)^p}{1 - r/d}$$

with $\frac{r}{d} = \frac{\sqrt{2}/2}{3/2} = \frac{\sqrt{2}}{3}$

$$\dots \le C \left(\frac{\sqrt{2}}{3}\right)^p$$

geometric

ex Show that ⊛ can be used as an interpolation/projection scheme for FMM.

ex. Collocation by matching a multipole at ∞ is dual/adjoint to interp. by harmonic polynomials

Next lecture on BIE: - def. normal derivative

- GRF: interior only!
- 4 fundam. problems & solvability
- SLP for Dirichlet prob. + ex in 2D/3D
  (Compact op. → accumul° eig., 1st kind IE)
- DLP for Dirichlet + ex in 2D/3D
  (boundedness → compact)
  jump conditions
  ($I/2 + T_K$ → OK, 2nd kind IE)
- SLP for Neumann prob.
  jump cond.
  ($-I/2 + T_K^*$ → OK, 1 eigenvalue though)
- Exterior pb.
- Symmetric BIE
- Helmholtz & CFIE
- 3 discretization methods.

+ Ref Folland Intro PDE

03/12 BIE
Boundary Integral Equations

Ω bounded, connected
$x \in \mathbb{R}^d$ $d=2,3$
n pointing outwards

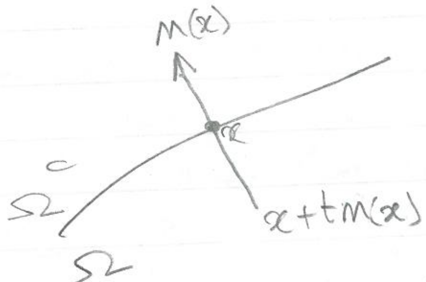
(harmonic)

treat this one first → ID $\begin{cases} \Delta u = 0 & \Omega \\ u = f & \Sigma = \partial\Omega \end{cases}$

ED $\begin{cases} \Delta u = 0 & \Omega^c \\ u = f & \Sigma \\ |u(x)| = O(|x|^{2-d}) & \text{as } |x| \to \infty. \end{cases}$

IN (mod const) $\begin{cases} \Delta u = 0 & \Omega \\ \partial_{n,-} u = g & \Sigma \end{cases}$, $\int_\Sigma g\, dS = 0$

EN (mod const) $\begin{cases} \Delta u = 0 & \Omega^c \\ \partial_{n,+} u = g & \Sigma \\ |u(x)| = O(|x|^{2-d}) & \text{as } |x| \to \infty \end{cases}$, $\int_\Sigma g\, dS = 0$ when $d=2$



$\partial_{n,\pm} u(x) = \lim_{t \to 0^\pm} n(x) \cdot \nabla u(x + t n(x))$

(ext, int normal der.)

BIE: reduce to $\partial\Omega$ with G.

Green's function: $\Delta_{x,y} G(x,y) = \delta(x-y)$

$$G = \begin{cases} \frac{1}{2\pi} \log|x-y| & d=2 \\ \frac{1}{4\pi}\frac{1}{|x|} & d=3 \end{cases}$$

Green's identities Div thm to $v\nabla u$:

$$\int_\Omega \nabla\cdot(v\nabla u)\,dV = \int_\Sigma v\,\partial_n u\,dS$$

$$\overset{\parallel}{\int(\nabla v\cdot\nabla u + v\Delta u)\,dV}$$

$$\int_\Sigma (v\,\partial_{n_y} u - u\,\partial_{n_y} v)\,dS_y = \int_\Omega (v\Delta u - u\,\Delta v)\,dV_y$$

(Green's 2^{nd} id.)

Put $v(y) = G(x,y)$ for some $y \in \Omega$.

$\Rightarrow \Delta_y v(x) = \delta(x-y)$

and $\Delta u = 0$

$$u(x) = \int_\Sigma \left(\partial_{n_y} G(x,y)\,u(y) - G(x,y)\,\partial_n u(y)\right) dS_y$$

$\rightarrow$ express sol. from bdy values $u\,\partial_n u$.

Idea 1 let $u(x) = \int_\Sigma G(x,y)\,\phi(y)\,dS_y = T_G\,\phi$

$\hookrightarrow$ unknown charge density

$\rightarrow$ single layer potential

(seek surface charges that reproduce potential inside)

Check integrable $(d=3)$: $\int_{|x-y|\le\varepsilon} |G(x,y)|\,dy \qquad y\in B_\varepsilon(x)$

$$\int_0^{2\pi}\int_0^{\varepsilon} \frac{1}{r}\, r\,dr\,d\theta = \varepsilon\, 2\pi$$

e.g. $G(x,y) = \dfrac{1}{|x-y|^\alpha}$ integrable for $\alpha < 2$ (weakly singular)

<u>Conseq 1</u> u is continuous for $x\in\mathbb{R}^d$, when ϕ is bounded.

Solution of ID : take $x\in\Sigma$:

$$f(x) = \int_\Sigma G(x,y)\,\phi(y)\,dS_y \quad , x\in\Sigma$$

→ solve for ϕ.

→ get u everywhere from SLP !

Called first kind (Fredholm) IE.

<u>Conseq 2</u> of integrability :

$$T_G\phi(x) = \int_\Sigma G(x,y)\,\phi(y)\,dS_y \quad \text{is } \underline{\text{compact}} :$$

(i) norm lim. of finite rank op.

(ii) turns bdd seq. into conv. subseq.

(iii) "eigenvalues decay" possibly infinite # of eqval w/ zero as only accumulation point

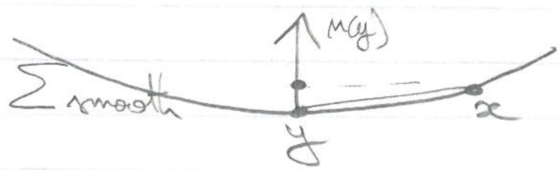
→ ill-posed inversion (large cond)

<u>Idea 2</u>. Let $u(x) = \int \underbrace{\partial_{n_y} G(x,y)}_{\text{dipoles}} \underset{\downarrow}{\varphi(y)}\, dS_y$

dipole density

→ double-layer potential

$$G(x,y) \begin{cases} \frac{1}{2\pi}\log|x-y| \to & \partial_{n_y} G(x,y) = -\frac{(x-y)\cdot n(y)}{2\pi|x-y|^2} \\ \frac{1}{4\pi}\frac{1}{|x-y|} \to & -\frac{(x-y)\cdot n(y)}{4\pi|x-y|^3} \end{cases}$$



$|(x-y)\cdot n(y)| \leq c|x-y|^2$

→ $\partial_{n_y} G$ bounded, $d=2$
weakly sing, $d=3$
when $x \in \Sigma$.

<u>But</u>, as $x \to \Sigma$ from Ω or Ω^c, stronger singularity.
$u(x)$ <u>not</u> continuous as x crosses Σ!

Jump conditions: Let $K(x,y) = \partial_{n_y} G(x,y)$ when $\underline{x \in \Sigma}$

$$u(x) = T_K \psi(x) = \int_\Sigma K(x,y)\, \psi(y)\, dS_y \quad , x \in \Sigma.$$

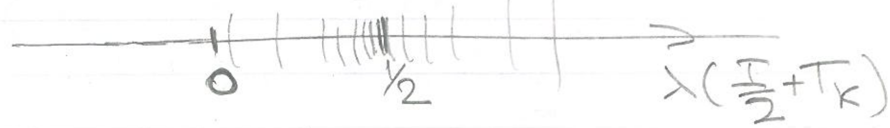
Then $u_-(x) = \left(\frac{I}{2} + T_K\right)\psi$ (from Ω)

$u_+(x) = \left(-\frac{I}{2} + T_K\right)\psi$ (from Ω^c)

Impose Dirichlet data: solve

$$f(x) = \left(\frac{I}{2} + \underbrace{T_K}_{\text{compact}}\right)\psi \quad , \text{get } u \text{ from DLP}$$

→ second-kind integral equation



0 is not an eigenvalue.

→ much better posed.

<u>Next</u>: interior Neumann: $\begin{cases} \Delta u = 0 & \Omega \\ \partial_{n_-} u = g & \Sigma \end{cases}$

let $u(x) = \int G(x,y)\, \phi(y)\, dS_y$ (SLP)

$$\forall x \notin \Sigma : \partial_n u(x) = \int \underbrace{\partial_{n_x} G(x,y)}_{\text{adjoint of } \partial_{n_y} G(x,y)} \phi(y)\, dS_y$$

Jump conditions : $K^*(x,y) = \partial_{n_x} G(x,y) = K(y,x)$

$$x \in K \quad : \quad T_K^* \phi \,(x) = \int_\Sigma K(y,x)\,\phi(y)\,dS_y .$$

Then $\partial_{n_-} u = \left(-\frac{I}{2} + T_K^*\right)\phi$

$$\partial_{n_+} u = \left(\frac{I}{2} + T_K^*\right)\phi$$

$\rightarrow$ impose $g = \left(-\frac{I}{2} + T_K^*\right)\phi$, solve for ϕ, get u from SLP

$\triangle$ T_K^* has one eigenvalue $\frac{1}{2}$
corresp. to solvability issue of IN.

<u>Next</u> : Exterior pb : use + limits

<u>Discretization</u> of $u(x) = \int K(x,y)\,\psi(y)\,dS_y$

(a) Nyström : $u(x_i) \simeq \sum_{j \neq i} K(x_i, y_j)\, w_j\, \psi(y_j)$

(b) Collocation : $\psi(y) = \sum \alpha_j v_j(y)$ ← basis set.

$$u(x_i) \simeq \sum_j \alpha_j \underbrace{\int K(x_i,y)\, v_j(y)\, dS_y}_{\text{do explicitly}}$$

(c) Galerkin : $\psi(y) = \sum \alpha_j v_j(y)$

$$u(x) = \sum \beta_i v_i(x)$$

$$\sum \beta_i \langle v_k, v_i \rangle \simeq \sum \alpha_j \langle v_k, T_K v_j \rangle$$

$\rightarrow$ solve for α.

Rmk Symmetric BIE: $\quad x \in \Omega \setminus \Sigma$

$$u = \int \left((\partial_{n_y} G) u - G (\partial_{n_y} u) \right) dS_y$$

$x \in \Sigma$: $\boxed{u = \frac{u}{2} + T_K u - T_G (\partial_n u)}$ (1)

Then $\partial_n u = \int \left((\partial_{n_x} \partial_{n_y} G) u - \partial_{n_x} G \, \partial_{n_y} u \right) dS_y$

$x \in \Sigma$: $\boxed{\partial_n u = T_H u - T_K^* \partial_n u + \frac{\partial_n u}{2}}$ (2)

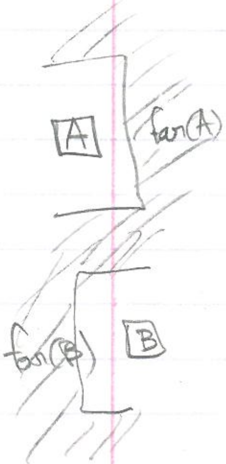
hypersingular (eval w/ Maue id.)

$\rightarrow$ use $u = f$ on Σ_D
$\partial_n u = g$ on Σ_N

Rmk: Helmholtz: DLP $- i\omega$ SLP
(CFIE)

03/21 Low-rank representations $u(x) = \int G(x,y)\, f(y)\, dy$

Kernel separation:

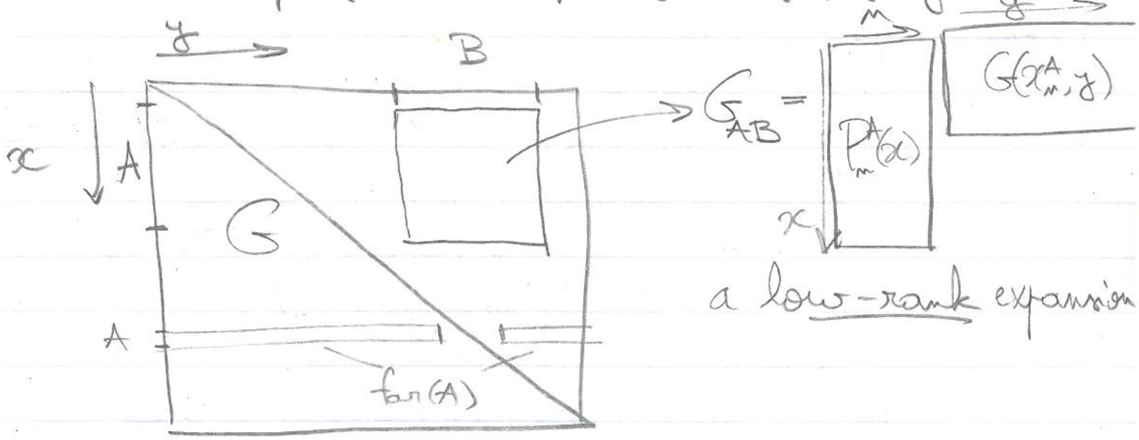


$$G(x,y) \simeq \sum_m P_m^A(x)\, G(x_m^A, y), \quad x \in A,\ y \in far(A)$$

$$G(x,y) \simeq \sum_m G(x, y_m^B)\, P_m^B(y), \quad y \in B,\ x \in far(B)$$

Consequence

- interpolation: $u(x) \simeq \sum_m P_m^A(x)\, u_m^A$ (L2L)
- projection: $q_m^B \simeq \int P_m^B(y)\, q(y)\, dy$ (M2M)



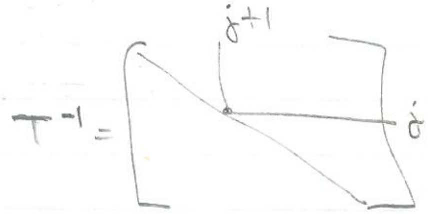
a low-rank expansion

Others: (best) $G_{AB} = U\, \Sigma\, V^T$ (sing. val. dec.)

— algebraic in 1D

<u>Ex</u>. 1D Green's matrices. $G = T^{-1}$

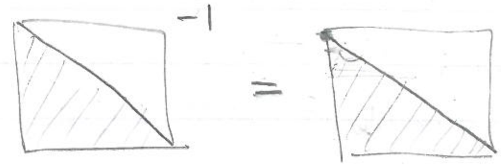
$$T = \begin{bmatrix} \alpha_1 & \beta_1 & & \\ \gamma_1 & \ddots & \ddots & \\ & \ddots & \ddots & \beta_{n-1} \\ & & \gamma_{n-1} & \alpha_n \end{bmatrix} \qquad T^{-1} =$$



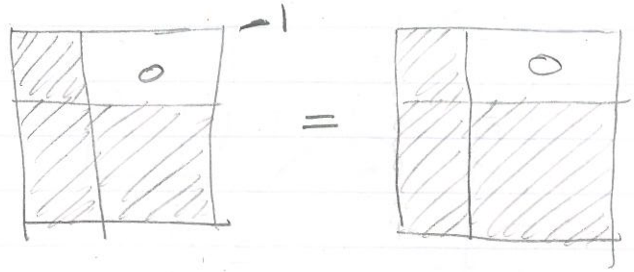
$3n-2$ d.o.f.

<u>Lemmas</u>:

a)

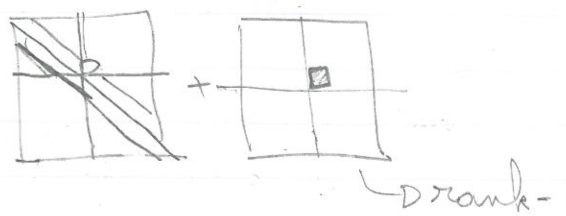


b)

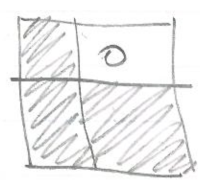


(2×2 block version of a))

View $T = U + \beta_j e_j e_{j+1}^T$ $\qquad e_j = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \leftarrow j$



$U^{-1} =$



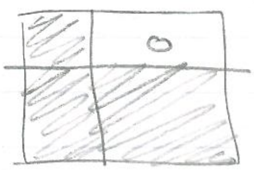
Call $\overbrace{\beta_j e_j}^{u}\,\overbrace{e_{j+1}^T}^{v^T} = u v^T$

$$T^{-1} = (U + u v^T)^{-1} = U^{-1} - U^{-1}\frac{u v^T}{1 + v^T U^{-1} u} U^{-1}$$

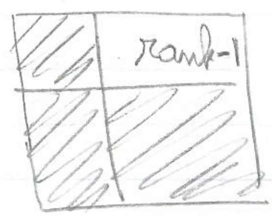
$$= U^{-1} - \frac{(U^{-1}u)(U^{-T}v)^T}{1 + v^T U^{-1} u}$$

$\rightarrow$ rank-1 update too!

(Woodbury, Sherman - Morrison)

$T^{-1} =$ 

$+$ (rank-1)

$=$ 

<u>Thm</u> Let T tridiagonal, invertible

Then T^{-1} has rank-1 off-diagonal blocks

(make sure $1 + v^T U^{-1} u \neq 0$ in the proof

$\Leftrightarrow$ T invertible)

<u>Thm</u> Let T be banded with band width $2p+1$

then T^{-1} has rank-p off-diag blocks

<u>Def.</u> T is called rank-1 semiseparable when

$$T_{ij} = \begin{cases} a_i b_j & i \geq j \\ c_i d_j & i \leq j \end{cases}$$

$$\rightarrow \underbrace{4n}_{\#a,b,c,d} - \underbrace{n}_{a_i b_i = c_i d_i} - \underbrace{2}_{a_1 = 1,\ c_1 = 1} = 3n - 2 \text{ d.o.f.}$$

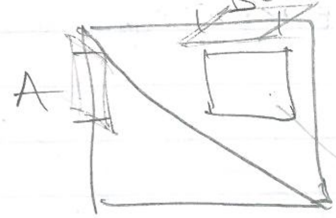
<u>Thm</u>. T invertible

T rank-1 semiseparable $\Leftrightarrow$ T^{-1} rank-1 semiseparable

<u>Ref</u>. Strang, Nguyen, 2004.

analytical in 2D

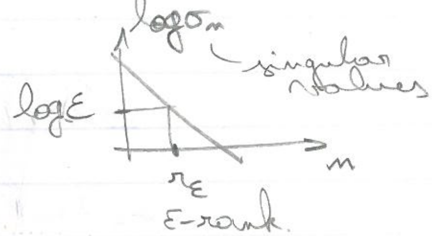
<u>Ex</u>. 2D, $G(x,y) = \log \|x-y\|$, $x,y \in R^2$



blocks do not touch the diagonal

$+ O(\varepsilon)$

$\Delta G(x,y) = 0$, $x \neq y$



<u>Thm</u>. Let $B \in \text{far}(A)$

$x \in A : \ |x| \geq d$

$y \in B : \ |y| \leq r$

There exist $f_k(x)$, $g_k(y)$ $k = 1, \ldots, 2p+1$ such that

$$\max_{\substack{x \in A \\ y \in B}} \left| \log \|x-y\| - \sum_{k=1}^{2p+1} f_k(x) g_k(x) \right| \leq C_{AB} \left(\frac{\sqrt{2}}{3}\right)^p.$$

Pf $\quad z = x_1 + i x_2 \qquad i = \sqrt{-1}$

$z_0 = y_1 + i y_2$

$$\log \|x-y\| = \operatorname{Re} \log(z - z_0)$$

because $z - z_0 = \rho e^{i\theta}$ with $\rho = \sqrt{(x_1-y_1)^2 + (y_1-y_2)^2}$

$\|x-y\| = |z-z_0| = \rho \qquad = |z - z_0|$

$$\begin{aligned} \operatorname{Re} \log(z-z_0) &= \operatorname{Re} \log \rho e^{i\theta} \\ &= \operatorname{Re} (\log \rho + i(\theta + 2m\pi)) \\ &= \log \rho \\ &= \log \|x-y\| \end{aligned}$$

(Harmonic) Taylor expansion in z_0:

$$\log(z - z_0) = \log(z) - \sum_{k=1}^{\infty} \frac{1}{k} \left(\frac{z_0}{z}\right)^k \quad (*)$$

(Multipole expansion in z)

$$\begin{aligned} \operatorname{Re}(z_0^k z^{-k}) &= \left|\frac{y}{x}\right|^k \operatorname{Re}\left(e^{i(\arg y - \arg x)}\right) \\ &= \left|\frac{y}{x}\right|^k \cos(\arg y - \arg x) \\ &= \left|\frac{y}{x}\right|^k \left(\cos \arg y \cos \arg x + \sin \arg y \sin \arg x\right) \\ &= 2 \text{ terms of the form } f_k(x) g_k(y) \end{aligned}$$

Truncate at $k = p$. $|z_0| \le r$, $|z| \ge d$. with $r/d = \frac{\sqrt{2}/2}{3/2}$

$$\left| \log(z - z_0) - \log(z) + \sum_{k=1}^{p} \frac{1}{k} \left(\frac{z_0}{z}\right)^k \right| \le \left| \sum_{k=p+1}^{\infty} \frac{1}{k} \left(\frac{z_0}{z}\right)^k \right| \le \frac{1}{p+1} \frac{(r/d)^p}{1 - \frac{r}{d}}$$

$$\le C \left(\frac{\sqrt{2}}{3}\right)^p$$

+

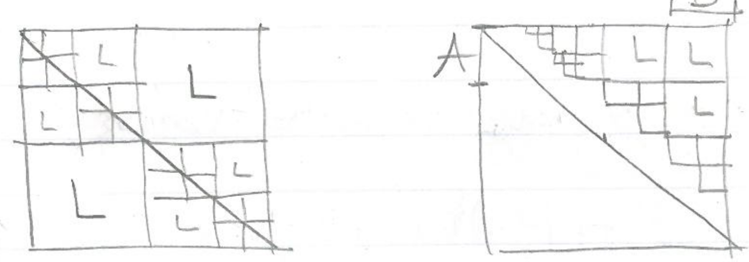
$$\frac{1}{z} = \frac{d}{dz}\log z \quad \text{e.g. } \frac{\partial}{\partial x_1}\log(x_1 + i x_2)$$

is a <u>dipole</u>

<u>04/02/2013</u> H-matrices: algebra of hierarchical low-rank matrices

H: hierarchical

<u>H structure</u>: consider square blocks



H-matrices: Compute the inverse in H form (like circulant, unlike Toeplitz)

Form 1 (strong)
Good for 1D.

Form 2 (weak)
Blocks don't touch diagonal (well separated)
→ nD

<u>Form 1 algebra (ring)</u> +, ×, inv

1) Matvec:

$$\begin{bmatrix} H & L \\ L & H \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} H x_1 + L x_2 \\ L x_1 + H x_2 \end{bmatrix}$$

Recurse for Hx_1, Hx_2
$\to O(N \log N)^2$

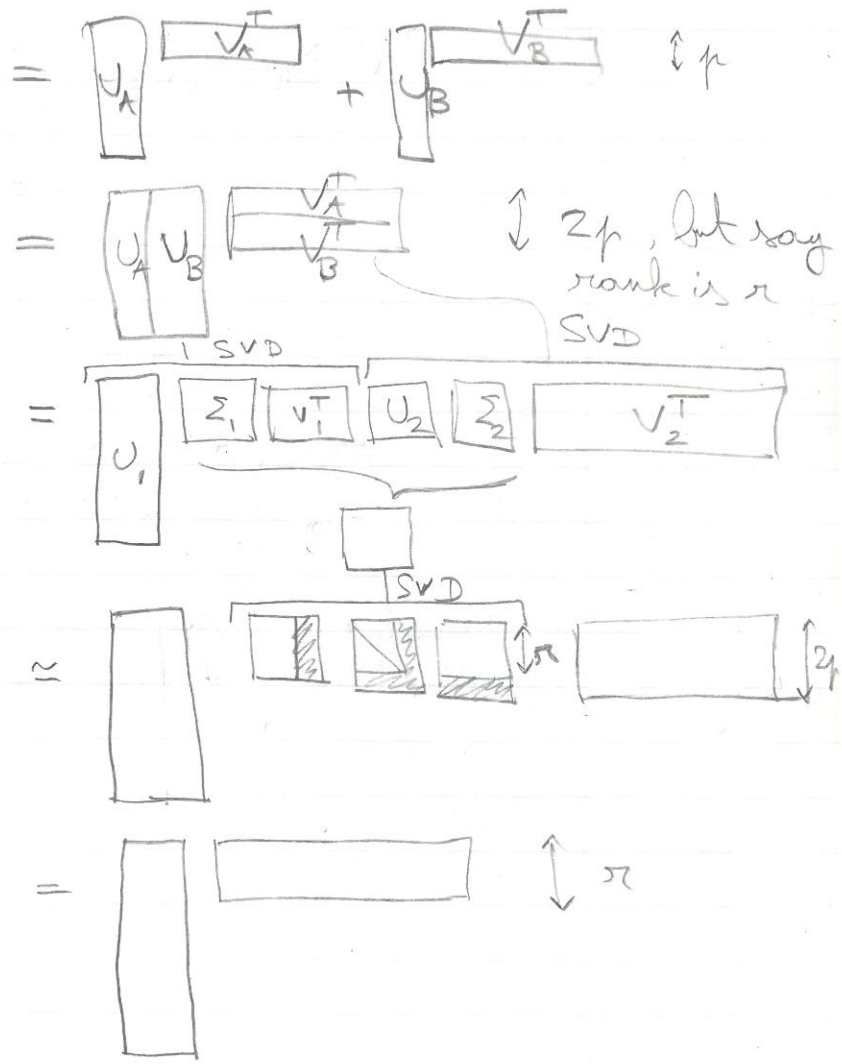
2) Addition: $H + H \to H$ (ranks may increase)

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} + \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} \to \begin{bmatrix} H & L \\ L & H \end{bmatrix}$$

$$\left.\begin{array}{l} A_{11} + B_{11} \to H \\ A_{22} + B_{22} \to H \end{array}\right\} \text{recurse}$$

$A_{12} + B_{12} \to L$ (or $A_{21} + B_{21} \to L$)

$A_{12} + B_{12} =$



keep matrices in thin form

(3 SVD trick)

$= L$

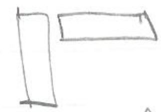
+

3) Mult. $H \cdot H \to H$ (ranks may increase)

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} \to \begin{bmatrix} H & L \\ L & H \end{bmatrix}$$

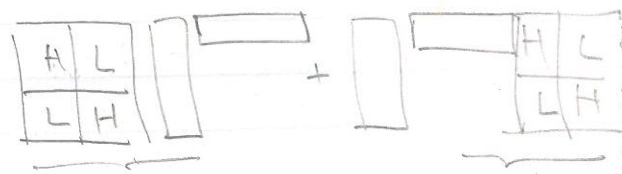
$$= \left[\begin{array}{c|c} A_{11}B_{11} + A_{12}B_{21} & A_{11}B_{12} + A_{12}B_{22} \\ \hline \text{ok} & \text{ok} \end{array}\right]$$

$A_{11}B_{11}$: recurse $\to H$

$A_{12}B_{21}$ =  =  $\to L$

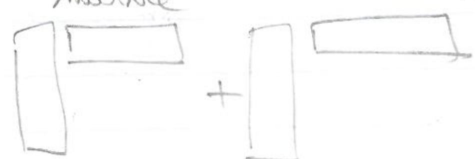
(no rank increase)

$A_{11}B_{11} + A_{12}B_{21} = H + L = H + H \xrightarrow{\text{use } +} H$

$A_{11}B_{12} + A_{12}B_{22}$ = 

use matvec

use matvec

= 

$\to L$ (use 3 SVD)

4) Inverse $A^{-1} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}^{-1} \longrightarrow \left[\begin{array}{c|c} H & L \\ \hline L & H \end{array}\right]$

GE: 2^{nd} row $- A_{21}A_{11}^{-1}$ (1^{st} row)

$$= \begin{bmatrix} A_{11} & A_{12} \\ 0 & \boxed{A_{22} - A_{21}A_{11}^{-1}A_{12}} \end{bmatrix}$$

S, Schur compl

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}^{-1} = \left[\begin{array}{c|c} A_{11}^{-1} + A_{11}^{-1}A_{12}S^{-1}A_{21}A_{11}^{-1} & -A_{11}^{-1}A_{12}S^{-1} \\ \hline S^{-1}A_{21}A_{11} & S^{-1} \end{array}\right]$$

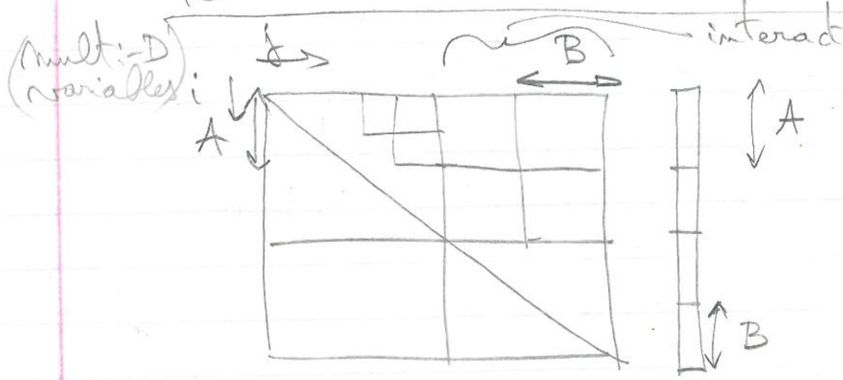
Compute S: in H form
- A_{11}^{-1} : recurse
- $A_{21}\times$, $\times A_{12}$, minus
- use ops. $\times$, $+$

invert S : recurse

compute A^{-1} : ops.

Ranks may temporarily increase, but OK in the end (Closedness of H matrices)

Form 2 H-matrices : matvec



$u = Gq$

$G_{AB}(x,y) = G(x,y),\quad x \in A,\ y \in B$

$u_A(x),\quad q_B(y)$

Have $G_{AB} \simeq U_{AB}\, N_{AB}\, V_{AB}^T$

(i) e.g. interpolative: $P_A\, G^R_{AB}$

rows from G_{AB}

(ii) double-interpolative:

$P_A\, G^{RC}_{AB}\, P_B^T$

rows, cols from G_{AB}

(iii) skeleton $G^C_{AB}\, (G^{RC}_{AB})^+\, G^R_{AB}$

+

Algo matvec: Init $u = 0$

for l, for A at l

$$u_A = \sum_{B \in IL(A)} U_{AB} N_{AB} V_{AB}^T q_B$$

for x, $u(x) = \sum_{A \ni x} u_A(x)$

diag: $u(x) := u(x) + \sum_{B \in NL(A)} G_{AB} q_B$ where $A \ni x$ (leaf)

$\longrightarrow O(N \log N)$ ops

Inefficient $\to$ Uniform $\mathcal{H}$-matrix:

$$G_{AB} \simeq \boxed{U_A} \boxed{N_{AB}} \boxed{V_B^T}$$

$\to$ reuse U_A for other B

V_B for other A

$\to$ interpolative & skeleton are like that.

(M) V_B^T projection onto canonical charges

(L) U_A: interpolation from canonical potentials

N_{AB}: M2L

matvec: for l, for B at level l,

$\tilde{q}_B = V_B^T q_B$

for l, for A at l,

$\tilde{u}_A = \sum_{B \in IL(A)} N_{AB} \tilde{q}_B$

for x, $u(x) = \sum_{A \ni x} U_A \tilde{u}_A$

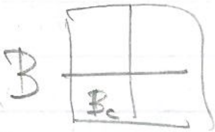
+ diagonal part

Compl $O(N \log N)$ still

⚠ Change all $f_B \to q_B$ +

② ③

H^2 matrices: $\boxed{V_B^T(:, B_c) = \overset{p\times p,\ \text{M2M}}{T_{B_c}}\, V_{B_c}^T}$



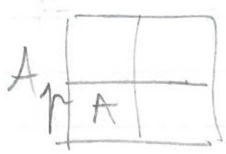
$B_c \to B$

because $\tilde{f}_{B_c} = V_{B_c}^T f_{B_c}$

$\tilde{f}_B = V_B^T f_B$
$= \sum_c V_B^T(:, B_c)\, f_{B_c}$

Want $\tilde{f}_B = \sum_c T_{B_c} \tilde{f}_{B_c}$

→ reuse generating vectors from one scale to the next.



$\boxed{U_{A_p}(A, :) = U_A\, S_A^T}$ $p\times p$, L2L

$A_p \to A$

because $u_A = U_A \tilde{u}_A$
$u_{A_p} = U_{A_p} \tilde{u}_{A_p}$

$u_A = U_{A_p}(A, :)\, \tilde{u}_{A_p}$

Want $\tilde{u}_A = S_A^T \tilde{u}_{A_p}$

then matvec is exactly FMM.

do ← Algo matvec: M2M, M2L, L2L

Symmetric: $U_A = V_A$
$S_A = T_A$

+

High frequency case : separation is λ-dependent

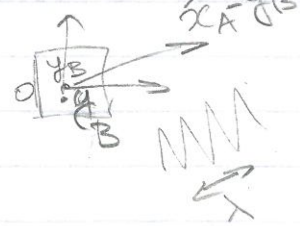
$\frac{r}{d} < 1$

Next Separation high ω

any $G(x,y)$ smooth (expand in Cheb. pol)

$x = x_A + \delta x$

Pick diam (A) = diam (B)



$y = y_B + \delta B$

$$G(x,y) = \frac{e^{ik|x-y|}}{|x-y|}$$

$\lambda = \frac{2\pi}{k}$, $\omega = kc$

Say $|y| \ll |x|$
($k|y|^2 \ll |x|$)

$$\left(\begin{array}{l} |x-y| = |x| - \hat{x}\cdot y + \frac{1}{2}\frac{|y|^2}{|x|} + \dots \\ e^{ik|x-y|} = e^{ik|x|}\, e^{-ik\hat{x}\cdot y}\, e^{ik|y|^2/|x|} (\dots) \\ \text{(ignore } \frac{1}{|x-y|}) \end{array} \right)$$

$$|x-y| = |(x_A - y_B) + (\delta x - \delta y)|$$

$$= |x_A - y_B| - \widehat{x_A - y_B}\cdot(\delta x - \delta y) + \frac{1}{2}\frac{|\delta x - \delta y|^2}{|x_A - y_B|}$$

$e^{ik|x_A - y_B|}$: const in x, y

$e^{ik(\widehat{x_A - y_B})\cdot(\delta x - \delta y)}$: separable, rank 1

$e^{ik\frac{1}{2}\frac{|\delta x - \delta y|^2}{|x_A - y_B|}}$ trouble with $\frac{2\delta x \delta y\, k}{|x_A - y_B|}$

(relate to curvature of spherical wave)

$\rightarrow$ make smooth by asking

$$\boxed{\frac{k\, d_A d_B}{\text{dist}} < 1}$$

Fresnel number $\frac{\text{diam}^2}{\lambda\ \text{dist}}$

$\Rightarrow$ dist $\sim$ diam$^2/\lambda$

Change all $f_B \to q_B$ +

<u>Algo $\mathcal{H}^2$:</u>

Init $\tilde{f}_B = V_B^T f_B$ (leaves), $u_A = 0$ (root)

for $l \uparrow$, for B at l,

$$\tilde{f}_B = \sum_c T_{B_c} \tilde{f}_{B_c} \qquad \text{(M2M)}$$

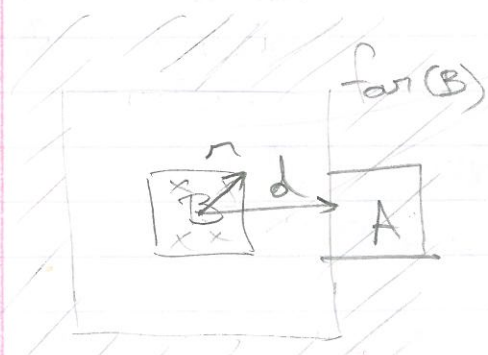
for $l \downarrow$, for A at l,

$$\tilde{u}_A := \underbrace{S_A^T \tilde{u}_{A_\uparrow}}_{\text{L2L}} + \underbrace{\sum_{B \in IL(A)} N_{AB} \tilde{f}_B}_{\text{M2L}}$$

Term: $u_A = U_A \tilde{u}_A$ (leaves)

+ diag part

04/09/2013. Butterfly ①



$y \in B$, $x \in A$

$$G(x,y) = \sum P_m^A(x)\, G(x_m^A, y)$$

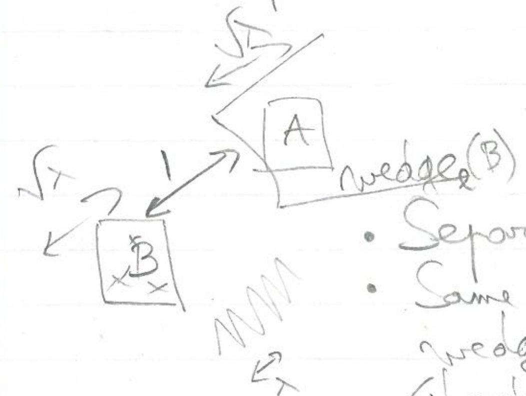
(local in x)

$$G(x,y) = \sum G(x, y_m^B)\, P_m^B(y)$$

(multipole in x)

Low frequency:

- Same expansion used in all boxes $A \in \text{far}(B)$
- Separation criterion: $\begin{cases} \text{diam}(B) < \text{dist}(A,B) \\ \text{diam}(A) < \text{dist}(A,B) \end{cases}$



High frequency: $k = \frac{2\pi}{\lambda}$

- Separation: $\text{diam}(A) \times \text{diam}(B) < \lambda \times \text{dist}(A,B)$
- Same expansion used in a wedge $x \in \text{wedge}_\ell(B)$ (shadows of A seen from B)

Ideas of the butterfly:

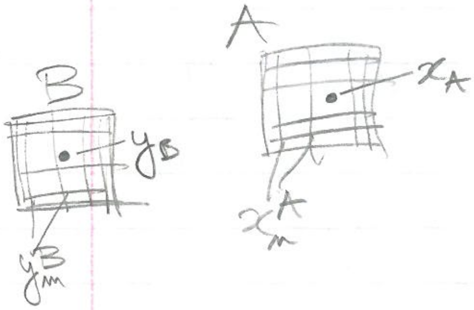
- Target-dependent multipole expansion

(1) $$G(x,y) = \sum_m G(x, y_m^B)\, P_m^{AB}(y)$$

Source-dependent local expansion

(2) $$G(x,y) = \sum_m P_m^{AB}(x)\, G(x_m^A, y)$$

ex. $G(x,y) = \dfrac{e^{ik|x-y|}}{|x-y|}$ $\quad x = x_A + \delta x$, $y = y_B + \delta y$



$$\simeq e^{ik|x_A - y_B|}\, e^{ik\widehat{x_A - y_B}\cdot(\delta x - \delta y)} \times \underbrace{\frac{e^{ik|\delta x - \delta y|^2/|x_A - y_B|}}{|x-y|}}_{\text{smooth indep. of } k \text{ because of the separation condition}} \times (\ldots)$$

negl

$\rightarrow$ use $P_m^{AB}(x) = e^{ik\widehat{x_A - y_B}\cdot\delta x}\, T_m(x - x_A)$ new

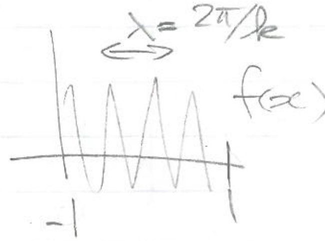
$P_m^{AB}(y) = e^{-ik\widehat{x_A - y_B}\cdot\delta y}\, T_m(y - y_B)$ new

ex. use $P_m^{AB}(x) = \sum_m G(x, y_m^B)\, Z_{mm}^{AB}$

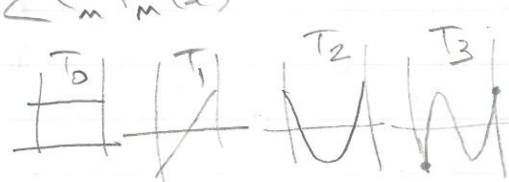
and $P_m^{AB}(y) = \sum_m Z_{mm}^{AB}\, G(x_m^A, y)$

results in skeleton decomposition : $G \simeq G_C\, Z\, G_R$

Why polynomials would fail



$$f(x) = \sum c_m T_m(x)$$



etc. m zeros

$\rightarrow$ need $M = O(k)$

+

$$u = \int G f$$

- Canonical charges split into directional contributions (looking at different A) q_m^{AB}

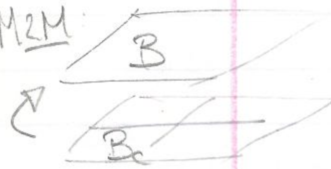
(3) $$u^B(x) = \sum_m G(x, y_m^B)\, q_m^{AB} \quad \text{for } x \in A$$

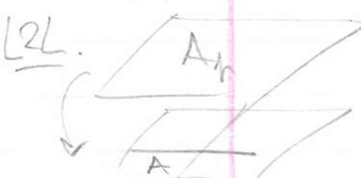
- Canonical potentials split into directional contributions (coming from different B) u_m^{AB}

(4) $$u_m^{AB} = \int_B G(x_m^A, y)\, q(y)\, dy$$

Question: which couples (A, B) to pick?

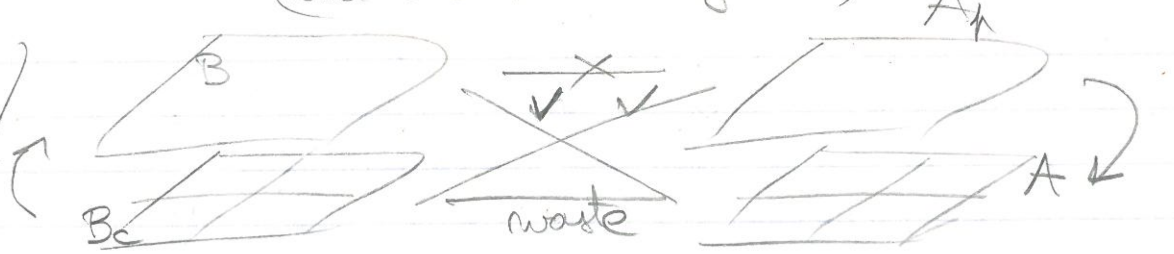
	FMM	Butterfly
Projection (1), (3) ⇒	$q_m^B = \int P_m^B(y)\, q(y)\, dy$	$q_m^{AB} = \int P_m^{AB}(y)\, q(y)\, dy$
M2M	$q_m^B = \sum_{m'} P_m^B(y_{m'}^{B_c})\, q_{m'}^{B_c}$	$\boxed{q_m^{AB} = \sum_{m'} P_m^{AB}(y_{m'}^{B_c})\, q_{m'}^{A_p B_c}}$
Interpolation (2), (4) ⇒	$u(x) = \sum_m P_m^A(x)\, u_m^A$	$u^B(x) = \sum_m P_m^{AB}(x)\, u_m^{AB}$
L2L	$u_m^A = \sum_{m'} P_{m'}^{A_p}(x_m^A)\, u_{m'}^{A_p}$	$\boxed{u_m^{AB} = \sum_{m'} P_{m'}^{A_p B_c}(x_m^A)\, u_{m'}^{A_p B_c}}$
M2L	$u_m^A \mathrel{+}= \sum G(x_m^A, y_m^B)\, q_m^B$ (same scale, $B \in IL(A)$)	$u_m^{AB^\uparrow} \mathrel{+}= \sum G(x_m^A, y_m^B)\, q_m^{A^\uparrow B}$ (same scale, $(A, B^\uparrow)$ $(A^\uparrow, B)$ admissible)



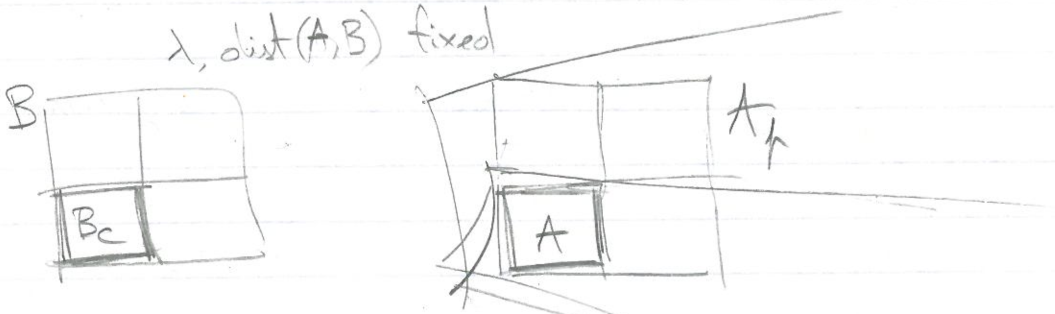


+ handle the diagonal

Admissible couples of boxes:
A, B have inversely proportional dimensions
(and are sufficiently far)



λ, dist(A,B) fixed

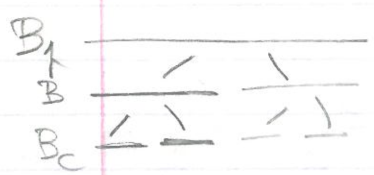


<u>Claim</u>: (A,B) admissible
$\Rightarrow (A_p, B_c)$ admissible.

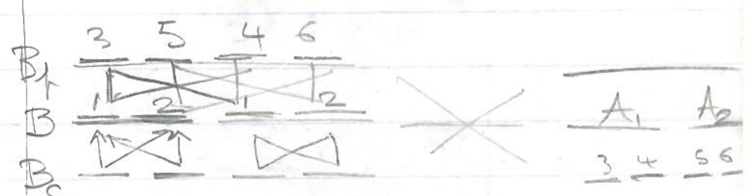
Traversal up the B (source) tree must be accompanied by a traversal down the A (target) tree to preserve admissibility.

admissible boxes per scale: $O(N)$, $N = k^2$
(discretize at wavelength level, finest scale)

FMM	Butterfly



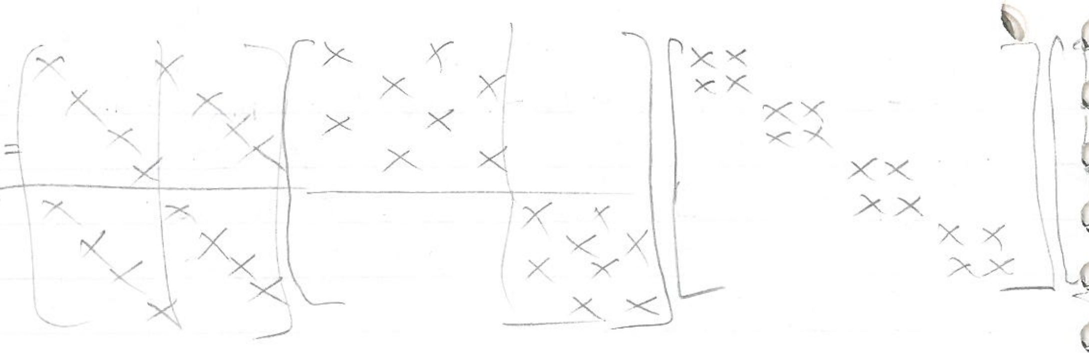
→ tree structure



→ butterfly

$G_{AB} = U_{AB} N_{AB} V_{AB}^T$

Re-use U, V from one block to the next? \ Link U, V from one scale to the next?	No	YES
No	H^1	Butterfly
YES	H^1-uniform	H^2 (FMM)

$q_m^{AB} =$ 

→ product of $O(N \log N)$ sparse matrices