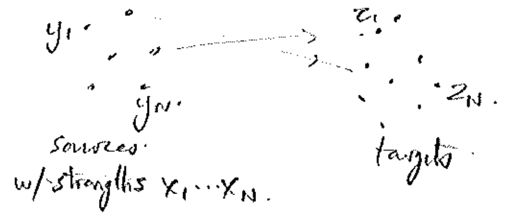
M126 lec. 5 *fast algs.* (for Laplace kernel in $\mathbb{R}^2$). ① 2/23/12

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 $z = z_i$, $i = 1 \ldots N$.

$z \in \mathbb{R}^2$; x_j = charge strengths of sources

$\mathbb{R}^2$:



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

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

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

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

z in polars; $c_0 \ln\frac{1}{r}$: monopole; 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 $\mathbb{R}^2 \cong \mathbb{C}$, $u(z) = \mathrm{Re}\left[c_0 \ln\frac{1}{z} + \underbrace{\sum_{n=1}^{\infty} c_n z^{-n}}_{\text{Laurent expansion ("Taylor exp." about } \infty)} \right]$

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

$= \ln\frac{1}{z} + yz^{-1} + \frac{y^2}{2} z^{-2} + \frac{y^3}{3} z^{-3} + \ldots$ 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!

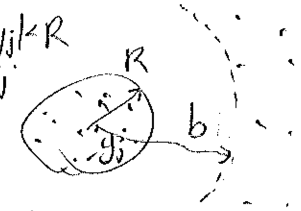
Use this bnd for each charge in disc B, get:

<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: $\left(\frac{R}{b}\right)^p (\text{tot. charge}) \approx \varepsilon$. ← typ. $p \sim 20$ to 40.
ii) compute multipole coeffs due to sources:
$$c_0 = \sum_{j=1}^N x_j \;, \quad c_n = \sum_{j=1}^N \frac{y_j^n}{n} x_j \,, \; n = 1, \ldots p-1 \qquad \Big\} \text{ does } \vec{c} = Q\vec{x}$$
iii) evaluate multipole expansion at targets:
$$u(z_i) \approx u^{(p)}(z_i) = c_0 \ln \frac{1}{z_i} + \sum_{n=1}^{p-1} c_n z_i^{-n} \qquad i = 1, \ldots N. \qquad \Big\} \text{ does } \vec{u} = P\vec{c}, \; \tilde{A} \approx PQ.$$

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

$N\overset{N}{\boxed{\tilde{A}}} \approx N\boxed{P}\,p\overset{N}{\boxed{Q}}$ ⇒ $O(N)$. for fixed error.

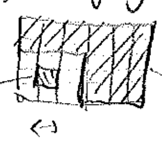
compare original $O(N^2)$! eg $N = 10^6$, $p = 10^{1.5}$ $(\varepsilon = 10^{-9})$, then speedup is $10^{4.5} \approx 30000$! That's a good algorithm ;)

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:

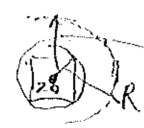
Cover by M square boxes:

box. B_i



L

all these boxes are well-separated from B_i



$b = \frac{3}{2}L$, $R = \frac{b}{\sqrt{2}}$ $\Big\}$ $\frac{b}{R} = \frac{3\sqrt{2}}{2} \approx 2.1$ 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
↖ terms each charge affects.
$z - z_0$ replaces z in expansion, where $z_0 =$ box center.

Then $u_i = \sum_{j=1}^N A_{ij} x_j = \sum_{j \text{ in } B \text{ or touching box}} A_{ij} x_j + \sum_{j \text{ in box for which } B \text{ is well-sep}} A_{ij} x_j$

y_i in same box B

do direct sum, effort $\approx 9\frac{N}{M}$

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

Total effort $(i = 1, \ldots N)$
$$= \underbrace{pN}_{\text{get coeffs (cheap)}} + \underbrace{9\frac{N^2}{M}}_{\text{local, direct}} + \underbrace{pMN}_{\text{distant}}$$
← 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.