November 8, 2017

Lecture 6

Will use complex representation for coordinates

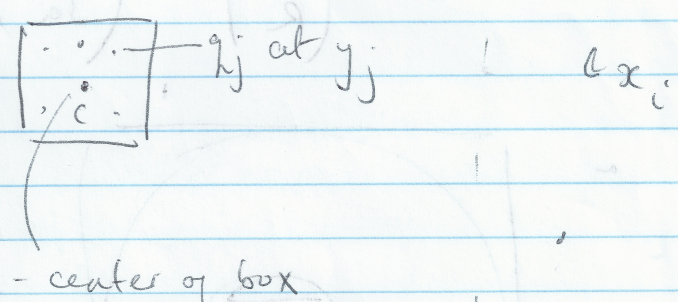
$$\underline{x} = x_1 + i x_2$$

Then must ^remember to^ use the identity

$$\log|x-y| = Re\left(\log(x-y)\right)$$

at the end of our calculations.

Consider the well-separated case



Charges q_j at $\{y_j\}_{j=1}^{n}$

Potentials ~~at~~ evaluated at $\{x_i\}_{i=1}^{m}$

$$u(x_i) = \sum_{j=1}^{n} \log(x_i - y_j)\, q_j, \qquad i = 1, \dots, m$$

Direct evaluation $- O(mn)$

$\log(x-y)$ possesses the expansion

$$\log(x-y) = \log(x-c) - \sum_{p=1}^{\infty} \frac{1}{p} \frac{(y-c)^p}{(x-c)^p}$$

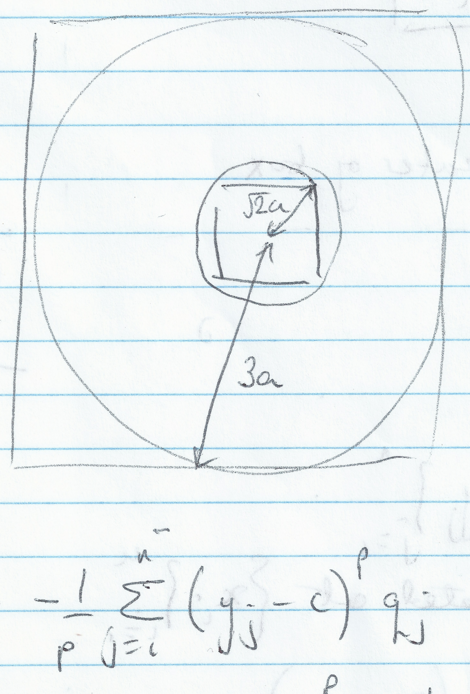
It follows that

truncated at $P+1$ terms.

$$u(x_i) = \underbrace{\log(x_i - c)\,\hat{q}_0 + \sum_{p=1}^{P} \frac{1}{(x-c)^p}\,\hat{q}_p}_{\text{"Multipole expansion"}} + E_p$$

where $\hat{q}_0 = \sum_{j=1}^{n} q_j$ and $\hat{q}_p = -\frac{1}{p}\sum_{j=1}^{n}(y_j - c)^p q_j$.

The error $E_p \sim \left(\frac{r}{R}\right)^p = \left(\frac{\sqrt{2}a}{3a}\right)^p = \left(\frac{\sqrt{2}}{3}\right)^p$.



$r = \sqrt{2}a$ is radius of small circle

$R = 3a$ radius of big circle.

__Cost__

$$\hat{q}_p = -\frac{1}{p}\sum_{j=1}^{n}(y_j - c)^p q_j \quad - O(n) \text{ for } p = 0, 1, \ldots, P$$

$\Rightarrow O(np)$

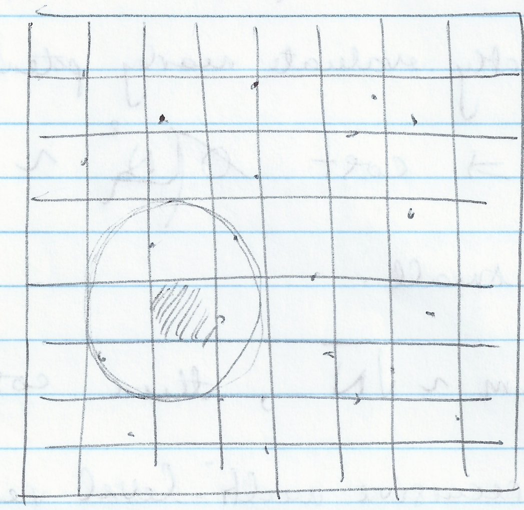
$$u(x_i) = \log(x_i - c)\,\hat{q}_0 + \sum_{p=1}^{P} \frac{1}{(x_i - c)^p}\,\hat{q}_p \quad - O(mp)$$

Hence have reduced cost from

$$O(mn) \text{ to } O(p(m+n)).$$

Can view multipole expansion as matrix factorization (✱) see page

<u>What about near interactions?</u>



N boxes

Seek to evaluate pairwise interactions between n charges at $\{x_i\}_{i=1}^{n}$.

Can be viewed as matrix-vector product

$$u = Aq$$

where $A(i,j) = \log(x_i - x_j)$.

Place square grid over comp. box.

Assume each box contains m particles $\Rightarrow \frac{N}{m}$ boxes.

Given tolerance ε, choose p s.t. $\left(\frac{\sqrt{2}}{3}\right)^p < \varepsilon$.

3 (*) Matrix Factorization view

Let $\underline{A}$ be $m \times n$ matrix

$$A(i,j) = \log(x_i - y_j)$$

Then

$$\underset{m\times n}{A} \approx \underset{m\times(P+1)}{B} \; \underset{\cancel{n(P+1)}\,(P+1)\times n}{C}$$

where

C is $(P+1)\times n$ matrix

$$C(p,j) = \begin{cases} 1 & p=0 \\ -\frac{1}{p}(y_j - c)^p, & p \neq 0 \end{cases}$$

B is $m\times(P+1)$ matrix

$$B(i,p) = \begin{cases} \log(x_i - c), & p=0, \\ \dfrac{1}{(x_i - c)^p}, & p \neq 0 . \end{cases}$$

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Consider highlighted box. m particles.

For each particle:

1: evaluate P expansion moments $O(P)$

2: evaluate potentials ~~from~~ in well-separated boxes $O\left(\left(\frac{N}{m}-9\right)P\right)$

3: directly evaluate nearby potentials: $O(9m)$

N particles $\Rightarrow$ cost $\cancel{O(N^2}$ $\sim \frac{N^2}{m} + Nm$

assuming P small.

If we set $m \sim \sqrt{N}$, then cost $\sim N^{3/2}$

By doing a recursive multi-level version of this, can reduce the complexity to $O(N \log N)$, then $O(N)$.
A matter of book keeping.