The Fast Multipole Method

Lexing Ying
University of Texas at Austin

July, 2008

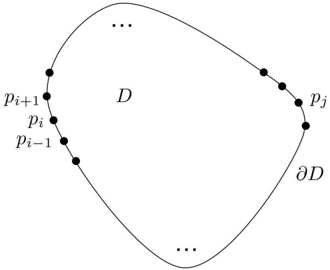
Problem statement

Given

- $\{f_i\}$ a set of charges at $\{p_i\}$,
- $G(x, y)$ a smooth kernel,

we want to compute

$$u_i = \sum_{j=0}^{N-1} G(p_i, p_j) f_j.$$



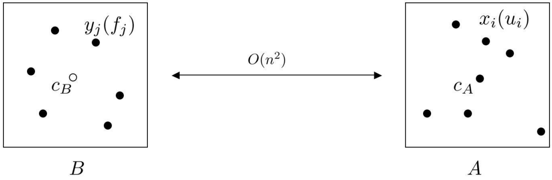
Naive algorithm takes $O(N^2)$. Our goal is to make it $O(N)$.

Solution: The fast multipole method by Greengard and Rokhlin.

Geometric part

Two sets A and B are well-separated if the distance between A and B are greater than their diameters.

Consider interaction from B to A. ($\{x_i\}$ and $\{y_j\}$ are subsets of $\{p_i\}$.)

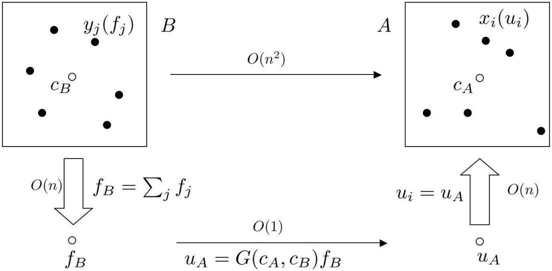


We use the following approximation. For each x_i, its potential u_i

$$u_i \approx u(c_A) = \sum_j G(c_A, y_j) f_j \approx G(c_A, c_B) \sum_j f_j.$$

Do not worry about the accuracy of this approximation for the time being. This is good when A and B are really well-separated.

Three step procedure:



Two representations:

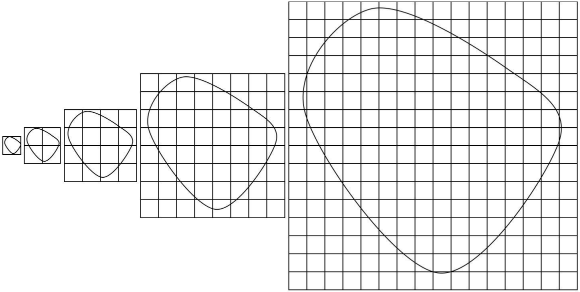
- Far field representation $f_B = \sum_j f_j$.
- local field representation $u_A = G(c_A, c_B) f_B$.

Interaction is approximately low rank. Here it is a rank-1 approximation.

However, each p_i is both a source and a target. $\{p_i\}$ are mixed up.

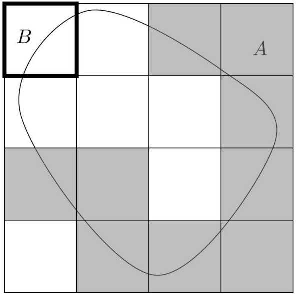
Solution: octree.

- Each leaf box contains a small number ($O(1)$) of points,
- The number of levels of the tree is $O(\log N)$.
- For each B, near field = adjacent boxes.
- Far field F^B = all well-separted boxes.
- Interaction list = boxes in B's far field but not B's parent's far field (i.e., boxes that can be addressed by B but not by B's parent).



Top level, fix a box B, we have $O(1)$ well-separated boxes (e.g. A).

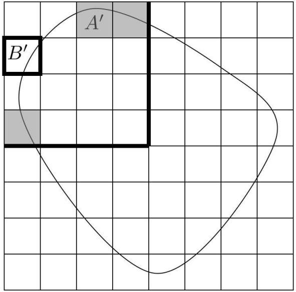
The interaction between B and A is computed using the previous 3-step procedure.



What about the nearby boxes? Go to the next level.

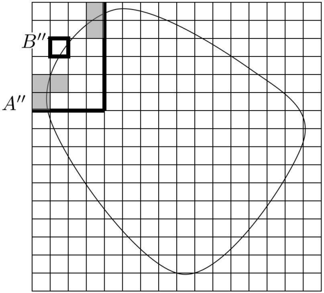
B' (a child of B) has $O(1)$ boxes in its interaction list (e.g. A') that have not been taken care of.

The interaction between B' and A' is computed using the previous 3-step procedure.



For the nearby boxes, go to the next level.

B'' (a child of B') has $O(1)$ boxes in its interaction list (e.g. A'') that need to be taken care of.



Now B'' is also a leaf. The interaction between B'' and its neighbors is evaluated directly.

The full algorithm is:

1. At each level, for each box B, compute $f_B = \sum_{p_j \in B} f_j$.
2. At each level, for each pair A and B in each other's interaction list, add $G(c_A, c_B) f_B$ to u_A (F2L translation)
3. At each level, for each box A, add u_A to u_j for each $p_j \in A$.
4. At the leaf level, nearby computation.

Complexity analysis:

1. Each point belongs to a box in each of $O(\log N)$ levels. The complexity is $O(N \log N)$.
2. $O(N)$ boxes in total. Each box has $O(1)$ boxes in the interaction list. $O(1)$ operation per F2L translation. The complexity is $O(N)$.
3. Each point belongs to a box in each of $O(\log N)$ levels. The complexity is $O(N \log N)$.
4. $O(N)$ leaf boxes in total. Each one has $O(1)$ points in its neighbors. Direct computation is $O(N)$.

Total complexity is $O(N \log N)$.

Can we do better? Yes. Let us look at a box B and its children $B_1, \cdots, B_4$.

$$f_B = \sum_{p_j \in B} f_j = \sum_{p_j \in B_1} f_j + \sum_{p_j \in B_2} f_j + \sum_{p_j \in B_3} f_j + \sum_{p_j \in B_4} f_j = f_{B_1} + f_{B_2} + f_{B_3} + f_{B_4}.$$

So f_B can be computed from f_{B_i} of its children

- $O(1)$ complexity,
- far field rep of $B_i \Rightarrow$ far field rep of B, called F2F translation
- bottom-up traversal of the octree.

Similarly, instead of putting u_A to each of its points, simply do

$$u_{A_i} \Leftarrow u_{A_i} + u_A \quad i = 1, 2, 3, 4.$$

What is added to u_{A_i} will eventually be added to the individual points.

- $O(1)$ complexity,
- local field rep $A \Rightarrow$ local field rep of A_i, called L2L translation
- top-down traversal of the octree.

The full algorithm is:

1. Bottom up. For each level, each box B,
   - if leaf, compute f_B from its points,
   - if non-leaf, compute f_B from its children (F2F).
2. On each level, for each pair A and B in each other's interaction list, add $G(c_A, c_B) f_B$ to u_A (F2L).
3. Top down. For each level, each box A,
   - if leaf, add u_A to u_j for each point p_j in A,
   - if non-leaf, add u_A to its children (L2L).
4. At the leaf level, local computation.

Let us compute the complexity:

1. $O(N)$ boxes. $O(1)$ per F2F. Totally $O(N)$.
2. Same $O(N)$.
3. $O(N)$ boxes. $O(1)$ per L2L. Totally $O(N)$.
4. Same $O(N)$.

Total complexity is $O(N)$.

Analytic Part

Come back to the question that total mass (charge)

$$f_B = \sum_{p_j \in B} f_j$$

is not a good approximation.

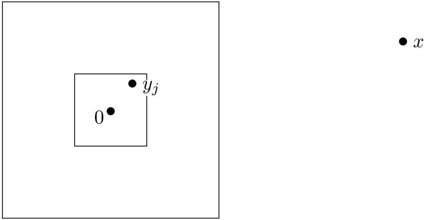
We can do better. This is the analytic part of the FMM: given a prescribed accuracy ε, all representations and translations shall have accuracy $O(\varepsilon)$.

2D case. One considers x and y to be complex numbers. Up to a constant,

$$G(x, y) = \ln|x - y| = \text{Re}(\ln(x - y)).$$

We will regard $G(x, y) = \ln(x - y)$ and throw away the complex part at the end.

Far field representation



$$G(x,y) = \ln(x-y) = \ln(x) + \ln(1-y/x) = \ln(x) + \sum_{k=1}^{\infty}(-1/k)(y/x)^k.$$

$$u(x) = \sum_j G(x,y_j)f_j = \ln(x)(\sum_j f_j) + \sum_{k=1}^{p} 1/x^k(-1/k\sum_j y_j^k f_j) + O(\varepsilon)$$

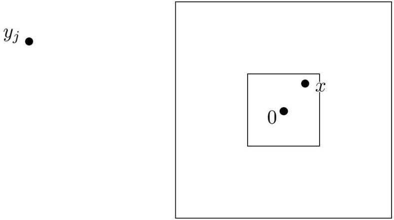
where $p = O(\log(1/\varepsilon))$ because $|y_j/x| < \sqrt{2}/3$.

Hence the far field representation is

$$a_0 = \sum_j f_j, \quad a_k = -1/k\sum_j y_j^k f_j \quad (1 \leq k \leq p).$$

This is called the multipole expansion.

Local field representation



$$G(x,y) = \ln(x-y) = \ln(-y) + \ln(1 - x/y) = \ln(y) + \sum_{k=1}^{\infty} (-1/k)(x/y)^k.$$

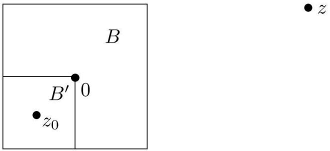
$$u(x) = \sum_j G(x, y_j) f_j = \sum_j \ln(-y_j) f_j + \sum_{k=1}^{p} x^k (-1/k \sum_j 1/y_j^k f_j) + O(\varepsilon)$$

where $p = O(\log(1/\varepsilon))$ because $|x/y_j| < \sqrt{2}/3$.

Hence the local field representation is

$$a_0 = \sum_j \ln(-y_j) f_j, \quad a_k = -1/k \sum_j y_j^k f_j \quad (1 \le k \le p).$$

F2F (far rep of B' to far rep of B)



If the multipole expansion of child B' is $\{a_k\}$, i.e.,

$$u(z) = a_0 \ln(z - z_0) + \sum_{k=1}^{p} a_k/(z - z_0)^k + O(\varepsilon)$$

then the multipole expansion of the parent B is $\{b_l\}$ with

$$b_0 = a_0, \quad b_l = -a_0 \frac{z_0^l}{l} + \sum_{k=1}^{l} a_k \binom{l-1}{k-1} z_0^{l-k} \quad (1 \leq l \leq p).$$

$$u(z) = b_0 \ln(z) + \sum_{l=1}^{p} b_l/z^l + O(\varepsilon).$$

The complexity of F2F is $O(p^2)$.

F2L (far rep of B to local rep of A)

If the multipole representation at B is $\{a_k\}$, i.e.,

$$u(z) = a_0 \ln(z - z_0) + \sum_{k=1}^{p} a_k/(z - z_0)^k + O(\varepsilon)$$

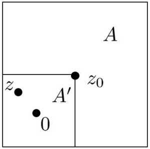
then the local representation at A is $\{b_l\}$ with with

$$b_0 = a_0 \ln(-z_0) + \sum_{k=1}^{p} a_k/(-z_0)^k \quad b_l = -\frac{a_0}{l z_0^l} + 1/z_0^l \sum_{k=1}^{p} a_k(-z_0)^{-k} \binom{l+k-1}{k-1}.$$

$$u(z) = \sum_{l=0}^{p} b_l z^l + O(\varepsilon)$$

The complexity of F2L is $O(p^2)$.

L2L (local rep of A to local rep of A')



If the local representation at A is $\{a_k\}$, i.e.,

$$u(z) = \sum_{k=0}^{p} a_k (z - z_0)^k + O(\varepsilon)$$

then the local representation at A' is $\{b_l\}$ with

$$b_l = \sum_{k=l}^{p} a_k \binom{k}{l} (-z_0)^{k-l}.$$

$$u(z) = \sum_{l=0}^{p} b_l (z)^l + O(\varepsilon).$$

The complexity of L2L is $O(p^2)$.

For a fixed ε,

- both representations are of size $O(p) = O(\log(1/\varepsilon))$,
- all translations are of complexity $O(p^2) = O(\log^2(1/\varepsilon))$,
- the FMM algorithm with these representations and translations still has complexity $O(N)$.