CMSC 858M/AMSC 698R
Fast Multipole Methods
Nail A. Gumerov & Ramani Duraiswami
Lecture 6

Outline

• Spatial Grouping: One of key stones of the FMM
• Natural spatial grouping. Well separated sets.
• Problem of “outliers”. Modifications of “Middleman”.
• “Pre-FMM”- universal fast algorithm
• Space partitioning with respect to the target Set
• Optimization of the “Pre-FMM”
• Space partitioning with respect to the source set
**Well separated sets**

*Definition:* Two sets of points in $\mathbb{R}^d$, $X$ and $Y$, are called well separated, if there exist two co-centric spheres of radii $r$ and $R$, $r < R$, such that all points of $Y$ are located inside the smaller sphere, and there are no points of $X$ located inside the larger sphere. (In this definition sets $X$ and $Y$ can be exchanged).

**Well separated sets (examples)**

![Diagram of well separated sets](image-url)
Can we prove that…

• For singular factorizable kernel and well separated sets of the sources and targets, the matrix-vector multiplication can be performed using the "Middleman" algorithm?
Peculiarities of "Middleman" for singular kernels

- Separation of sets is crucial;
- Type of factorization (S or R) depends on the type of source/receiver distribution;
- Separation parameter, $r/R$ controls the convergence of the series and for given accuracy the truncation number substantially depends on this parameter (so the efficiency of the fast summation method).

Example of the error bound

\[ \Phi(y, x) = \frac{1}{y-x}, \quad |y-x_*| < r, \quad |x-x_*| > R. \]

We have

\[ \Phi(y, x) = -\frac{1}{x-x_*} \sum_{n=0}^{\infty} \frac{(y-x_*)^n}{(x-x_*)^n} = -\frac{1}{x-x_*} \sum_{n=0}^{p-1} \frac{(y-x_*)^n}{(x-x_*)^n} + \epsilon_p. \]

The residual can be computed exactly:

\[ \epsilon_p = -\frac{1}{x-x_*} \sum_{n=p}^{\infty} \frac{(y-x_*)^n}{(x-x_*)^n} = \frac{(y-x_*)^p}{(x-x_*)^p} \left[ \frac{1}{x-x_*} \sum_{n=0}^{p-1} \frac{(y-x_*)^n}{(x-x_*)^n} \right] = \frac{(y-x_*)^p}{(x-x_*)^p} \Phi(y, x). \]

\[ |\Phi(y, x) - \Phi^{(p)}(y, x)| \leq |\epsilon_p| = \frac{|y-x_*|^p}{|x-x_*|^p} |\Phi(y, x)| \leq \left( \frac{r}{R} \right)^p |\Phi(y, x)|. \]

Relative error is bounded by $(r/R)^p$ and absolute error is bounded by

\[ |\epsilon_p| \leq \left( \frac{r}{R} \right)^p \frac{1}{|y-x|} \leq \frac{1}{R-r} \left( \frac{r}{R} \right)^p. \]
Model of geometric error bound for higher dimensionalities

Single source error:

$$|\epsilon_p| \leq A \left( \frac{R}{R} \right)^p$$

Error for sum of N-sources (assume $\max_i |u_i| = 1$)

$$|\epsilon| \leq \left| \sum_{i=1}^{N} u_i \epsilon_p \right| \leq \sum_{i=1}^{N} |u_i| |\epsilon_p| = |\epsilon_p| \sum_{i=1}^{N} |u_i| \leq N |\epsilon_p| \max_i |u_i| \leq NA \left( \frac{R}{R} \right)^p.$$ 

Then

$$p \geq \frac{\log \frac{NA}{|\epsilon|}}{\log \left( \frac{R}{R} \right)}.$$ 

If $\max_i |u_i| = 1/N$:

$$p \geq \frac{\log \frac{A}{|\epsilon|}}{\log \left( \frac{R}{R} \right)}.$$ 

Actual complexity of “Middleman”

Assume $M \sim N$ and $p \sim \log N + \log \frac{1}{\epsilon}$. Then complexity of the “Middleman” is

$$C = O(pN) = O(N \log N + N \log \frac{1}{\epsilon}).$$

For $p \sim \log \frac{1}{\epsilon}$ we have

$$C = O(pN) = O(N \log \frac{1}{\epsilon}).$$
One point that spoils algorithm…

“bad point”, “outlier”

Modification of the “Middleman” for outliers

Complexity: $O(NM)$

Complexity: $O(pN+pM)$

Complexity: $O(p(N-q)+pM+qM)$
Natural spatial grouping (grouping with respect to the target set)

Natural spatial grouping (continuation)

R-expansions near the group centers
Natural spatial grouping (continuation)

Asymptotic Complexity:

1) Let the R-expansion has p-terms;
2) To build them for K groups we need $O(pNK)$ operations.
3) To evaluate them we need $O(pM)$ operations.
4) Total complexity: $O(p(NK+M))$.
5) Better than the Straightforward method, if $pK<<M$. In this case $p(NK+M)<<NM$.
Natural spatial grouping (continuation)

\[ S\text{-expansions near the group centers} \]

\[ N \rightarrow \begin{array}{c} \text{Sources} \\ \vdots \end{array} \]

\[ M \rightarrow \begin{array}{c} \text{Targets} \\ \vdots \end{array} \]

\[ K \rightarrow \text{Groups} \]

Outliers (an example from room acoustics)

``Bad'' points

Room (a set of targets)

Image Sources

Actual Source

Comparison of Straightforward and Fast Solutions

Outliers (continued)

*Universal Recipe:* If the number of the outliers is small, then compute their contribution directly.

E.g. if this number is smaller than \( p \), then the outliers do not change the algorithm complexity.

Examples of natural spatial grouping

- Stars (form galaxies, gravity);
- Flow past a body (vortices are grouped in a wake);
- Statistics (clusters of statistical data points);
- People (Organized in groups, cities, etc.);
- Create your own example!
Deficiencies

• Data points may be not naturally grouped;
• Need intelligence to identify the groups: Problem with the algorithms (Artificial Intelligence?)
• Problem dependent.

The Answer is: Space Partitioning
Space partitioning with respect to the target set

An algorithm for computation with space partitioning (Pre-FMM)

- **Decomposition of the sum:**
  \[ v(y_j) = \sum_{x_i \in R^*_T} u_i \Phi(y_j - x_i) + \sum_{y_j \in R_Y} u_i \Phi(y_j - x_i), \quad y_j \in R_Y. \]

  - **Singular Part** (sources in the neighborhood)
  - **Regular Part** (sources outside the neighborhood)

- **Factorization of the regular part**
  \[ \Phi(y_j - x_i) = \sum_{m=0}^{p-1} a_m(x_i, x_{ss}) R_m(y_j - x_{ss}) + Error_p, \quad y_j, x_{ss} \in R_g, \quad x_i \in R_g. \]

- **Fast computation of the regular part**
  \[ \sum_{x_i \in R^*_T} u_i \Phi(y_j - x_i) = \sum_{m=0}^{p-1} \left[ \sum_{x_i \in R_g} u_i a_m(x_i, x_{ss}) \right] R_m(y_j - x_{ss}). \]

- **Direct summation of the singular part,** \[ \sum_{x_i \in R^*_T} u_i \Phi(y_j - x_i) \]
Asymptotic complexity of the Pre-FMM

Let $N$ be the number of sources, $M$ the number of targets, and $K$ the number of target boxes.

Each target box, $R_n$, $M_n$ targets, $n = 1, ..., K$.

The neighborhood of each target box contains $N_n$ sources, $n = 1, ..., K$.

Computation of the expansion coefficients for the regular part for the $n$th box requires $O((N - N_n)p)$ operations.

Evaluation of the regular expansion for the $n$th box requires $O(M_np)$ operations.

Direct computation of the singular part requires $O(M_n N_n)$ operations.

Total complexity is:

$$\text{Complexity} = O\left( \sum_{n=1}^{K} [(N - N_n)p + M_n p + M_n N_n] \right).$$

Asymptotic Complexity of the Pre-FMM (continued)

We have

$$\sum_{n=1}^{K} M_n = M$$

Consider a uniform distribution, then

$$N_n \sim \text{const} \sim \frac{N \text{Pow}(d)}{K},$$

Power of the neighborhood of dimensionality $d$ (the number of boxes in the neighborhood)

$$F(K) = \sum_{n=1}^{K} [(N - N_n)p + M_n p + M_n N_n] = KNp - Np \text{Pow}(d) + Mp + \frac{MN \text{Pow}(d)}{K}$$

$$= \frac{MN}{K} \text{Pow}(d) + (K - \text{Pow}(d))Np + Mp$$

$$\text{Complexity} = O(F(K))$$
Optimization of the box number

\[ F(K) = \frac{MN}{K} Pow(d) + (K - Pow(d))Np + Mp \]

\[ K_{opt} = \left( \frac{MN Pow(d)}{Np} \right)^{1/2} = \frac{MPow(d)}{p} \]

\[ \text{Complexity} = O(F(K_{opt})) = O\left(Np \left(2\sqrt{\frac{MPow(d)}{p}} - Pow(d)\right) + Mp\right) \]

For \( M \sim N, \ p \ll N \): \n
\[ \text{Complexity} = O\left(N^{3/2}p^{1/2}\right) \]

Actual complexity of “Pre-FMM”

Assume \( M \sim N \) and \( p \sim \log N \). Then complexity of the “Pre-FMM” is

\[ C = O(p^{1/2}N^{3/2}) = O(N^{3/2}\log^{1/2}N) \]

For \( p \sim \log \frac{1}{\epsilon} \) we have

\[ C = O(p^{1/2}N^{3/2}) = O(N^{3/2}\log^{1/2}\frac{1}{\epsilon}) \]
Optimize with error bound constraint

How the complexity changes, if we change the size of the neighborhood and request the same accuracy of the computation?

Complexity \((M \sim N \gg p)\)

\[ C \sim 2N^{3/2}p^{1/2} \sqrt{\text{Pow}(d)}. \]

1). \(d = 1\), Neighborhoods of chess radius 1:

\[ C_1 \sim 2N^{3/2}p_1^{1/2} \sqrt{3}, \quad p_1 \sim \frac{\log \frac{4}{\|x\|}}{\log \left(\frac{R_1}{r}\right)} = \frac{\log 4}{\log 3}; \]

2). \(d = 1\), Neighborhoods of chess radius 2:

\[ C_2 \sim 2N^{3/2}p_2^{1/2} \sqrt{5}, \quad p_2 \sim \frac{\log \frac{4}{\|x\|}}{\log \left(\frac{R_2}{r}\right)} = \frac{\log 4}{\log 5}; \]

Then

\[ \frac{C_2}{C_1} \sim \frac{2N^{3/2}p_2^{1/2} \sqrt{5}}{2N^{3/2}p_1^{1/2} \sqrt{3}} = \frac{\sqrt{5p_2}}{\sqrt{3p_1}} = \frac{\sqrt{5 \log 3}}{\sqrt{3 \log 5}} = \sqrt{\frac{\log 243}{\log 125}} > 1. \]

Chess radius = 1 is better!

Optimize with error bound constraint

\((d = 2)\)

\[ \frac{C_2}{C_1} \sim \sqrt[3]{\frac{25p_2}{9p_1}} = \frac{5}{3} \sqrt[3]{\frac{p_2}{p_1}} = \frac{5}{3} \sqrt[3]{\frac{\log \left(\frac{R_1}{r}\right)}{\log \left(\frac{R_2}{r}\right)}} = \frac{5}{3} \sqrt[3]{\frac{\log \left(\frac{3}{2}\right)}{\log \left(\frac{5}{4}\right)}} \approx 1.29 > 1. \]

Chess radius = 1 is better!