Chapter 4
Fast multipole method

Originally designed for particle simulations. One of the most well known way to take advantage of the low-rank properties. Applications include

1. Simulation of physical systems
   (a) Gravitational potential due to a distribution of masses
   (b) Electrostatic potential due to a distribution of charges. Electromagnetics of complex systems
   (c) Stellar clusters
   (d) Protein folding
   (e) Acoustics
   (f) Turbulence

2. Grand challenge problems in large numbers of variables

3. Learning theory
   (a) Kernel methods
   (b) Support Vector Machines


Introduced by Rokhlin & Greengard in 1987. One of the 10 most significant advances in computing of the 20th century. Approximation result with $O(m + n)$ cost.

- Use analytical manipulation of series to achieve faster summation
- Approximate result with arbitrary accuracy

This section is mainly based on [4].
4.0.1 A basic idea

$m$ source particle $i$ with charge $q_i$ at position $s_i$.

By Coulomb's law, the potential at target $j$ located at $t_j$ for $n$ targets:

$$\phi(t_j) = \sum_{i=1}^{m} q_i K(s_i, t_j), \text{ } j = 1 : n,$$

where, for example, $K(s, t) = \frac{1}{|s-t|}$. Write

$$K = (K(s_i, t_j)), \text{ } q = (q_i), \text{ } \Phi = (\phi(t_j))$$

Then

$$\Phi = K q$$

This usually costs $O(mn)$.

However, this cost can be reduced if $K$ is separable. Assume

$$K(x, y) = \sum_{k=1}^{r} f_k(x) g_k(y) = \left( f_1(x) \cdots f_p(x) \right) \left( \begin{array}{c} g_1(y) \\ \vdots \\ g_p(y) \end{array} \right)$$

Then

$$K = \left( \begin{array}{ccc} f_1(s_1) & \cdots & f_r(s_1) \\ f_1(s_2) & \cdots & f_r(s_2) \\ \vdots & \vdots & \vdots \\ f_1(s_m) & \cdots & f_r(s_m) \end{array} \right) \left( \begin{array}{ccc} g_1(t_1) & g_1(t_2) & \cdots & g_1(t_n) \\ \vdots & \vdots & \vdots & \vdots \\ g_r(t_1) & g_r(t_2) & \cdots & g_r(t_n) \end{array} \right) = F G^T$$

$$= \sum_{k=1}^{r} f_k g_k^T, \text{ } (f_k = (f_k(x_i)))_i, \text{ } (g_k = (g_k(x_j)))_j.$$ 

Consider a special $K$ as an example.

\textbf{Theorem 4.1.} $\delta \in (0,1), \text{ } z \in [0,1)$. For any $x, y \in [0,1)$ satisfying $\frac{x-z}{y-z} < \delta$ we have

$$K(x, y) = \frac{1}{(x-y)^2} = \sum_{k=1}^{r} f_k(x) g_k(y) + R_r,$$

$$f_k(x) = k(x-z)^{k-1}, \text{ } g_k(y) = \frac{1}{(y-z)^{k+1}},$$

$$R_r \leq (r+1)\delta^r.$$
Proof. \[
\frac{1}{(x-y)^2} = \frac{1}{((y-z)-(x-z))^2} = \frac{1}{(y-z)^2(1 - \frac{x-z}{y-z})^2}.
\]
Then use \[
\frac{1}{(1-t)^2} = \sum_{k=1}^{r} kt^{k-1} + R_r, \quad |t| \leq \delta < 1.
\]
Note that, to reach a given tolerance \(\tau\),
\[(r+1)\delta^r < \tau,
\]
we need \(r = O(|\log \tau|).\)

\[\square\]

Definition 4.2. Two sets \(\{x_i\}, \{y_j\}\) are well separated if there exist points \(x_0, y_0\) and \(d > 0\) s.t.
\[
|x_i - x_0| < d,
|y_i - y_0| < d,
|x_0 - y_0| > \alpha d,
\]
where \(\alpha > 2\) is a constant.

Corollary 4.3. If \(K\) is formed for all the subsets of a total of \(n\) points, then any off-diag block of \(K\) has numerical rank \(O(\log n)\).

\[\text{Proof.}\] The interval can be repeatedly partitioned. \[\square\]

4.0.2 • Math preliminaries

Multipole expansion

Consider
\[K(z, z_0) = \log(z - z_0).\]
Lemma 4.4. A point change is located at $z_0$. Then for any $z$ s.t. $|z| > |z_0|

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

Proof. $\log(z - z_0) - \log z = \log(1 - t)$. Taylor. \qed

Theorem 4.5. (Multipole expansion (with center 0))

$q_i, i = 1 : m$ at points $z_i, i = 1 : m$ with $|z_i| < d$. Then for any $z \in \mathbb{C}$ with $|z| > d$, the potential is

$$
\phi(z) = \hat{q} \log z + \sum_{k=1}^{\infty} \frac{a_k}{z^k}
$$

$$
\hat{q} = \sum_{i=1}^{m} q_i, \quad a_k = \sum_{i=1}^{m} \frac{-q_i z_i^k}{k}
$$

Furthermore, with truncation

$$
\phi(z) = M_p(z, z_0) + R_r
$$

$$
M_p(z, z_0) = \hat{q} \log z + \sum_{k=1}^{r} \frac{a_k}{z^k}
$$

$$
|R_r| \leq \alpha \left( \frac{1}{c} \right)^{r+1} \leq \left( \frac{A}{c - 1} \right) \left( \frac{1}{c} \right)^r
$$

$$
c = \frac{|z|}{d}, \quad \bar{Q} = \sum_{i=1}^{m} |q_i|, \quad \alpha = \frac{A}{1 - 1/c}
$$

Proof. The previous lemma gives the expansion:

$$
\phi(z) = \sum_{i=1}^{m} q_i K(z_i, z) = \sum_{i=1}^{m} q_i \left[ \log z - \sum_{k=1}^{\infty} \frac{1}{k} \left( \frac{z_i}{z} \right)^k \right]
$$

$$
= \left( \sum_{i=1}^{m} q_i \right) \log z - \sum_{i=1}^{m} q_i \sum_{k=1}^{\infty} \frac{1}{k} \left( \frac{z_i}{z} \right)^k
$$

$$
= Q \log z + \sum_{k=1}^{\infty} \left( \sum_{i=1}^{m} \frac{-q_i z_i^k}{k} \right) \frac{1}{z^k}
$$

$$
\left| \sum_{k=r+1}^{\infty} \frac{a_k}{z^k} \right| \leq \bar{q} \sum_{k=r+1}^{\infty} \frac{d^k}{k|z|^k} \leq \bar{q} \sum_{k=r+1}^{\infty} \left( \frac{1}{c} \right)^k.
$$

\qed

In particular, if $c \geq 2$ or $|z| \geq 2d$,

$$
|R_r| \leq \bar{q} \left( \frac{1}{2} \right)^r
$$
By the theorem
\[ \left| \sum_{i=1}^{m} \phi_{x_i}(y_j) - M_p(y_j, x_0) \right| \leq q \left( \frac{1}{2} \right)^r \]

The coefficients of a multipole expansion costs \( mp \), once for all \( y_i \).

To compute the potential (force) at \( f_j \) due to the charges at \( f_i \), we need \( \sum_{i=1}^{m} \phi_{x_i}(y_j) \) for all \( j \). The evaluation of the expansion at \( f_j \) is \( nr \). Total cost \( mr + nr \)

**Translation/shift**

**Theorem 4.6.** *(Shifting center to 0)*

Suppose
\[ \phi(z) = a_0 \log(z - z_0) + \sum_{k=1}^{\infty} \frac{a_k}{(z - z_0)^k} \]  

(4.1)

is a ME of the potential due to \( q_i, i = 1 : m \) located inside the circle \( D \) of radius \( R \) with center \( z_0 \). Then for \( z \) outside the circle \( D_1 \) of radius \( R + |z_0| \) and centered at the origin,

\[ \phi(z) = a_0 \log z + \sum_{l=1}^{\infty} \frac{b_l}{z^l} \]

\[ b_l = \sum_{k=1}^{l} a_k z_0^{-k} \left( \frac{l-k}{k} \right) - a_0 \frac{z_0^l}{l} \]

With truncation, the error is bounded by

\[ \frac{A}{1 - \left| \frac{z_0 + R}{z} \right|} \left| \frac{z_0 + R}{z} \right|^{r+1} \]

**Proof.** \( \log(z - z_0) - \log z = \log(1 - t) \), etc. Taylor expansion at \( z_0 \).

This means we can shift the center without loss of accuracy.

**Theorem 4.7.** *(Multipole to local expansion (for the purpose of later evaluation))*

\( q_i, i = 1 : m \) located inside the circle \( D_1 \) with radius \( R \) and centered at \( z_0 \), \( |z_0| > (c + 1)R, c > 1 \). Then (4.1) converges inside the circle \( D_2 \) of radius \( R \) about the origin. Inside \( D_2 \),

\[ \phi(z) = \sum_{l=1}^{\infty} b_l z^l \]

\[ b_0 = \sum_{k=1}^{\infty} a_k (-1)^k + a_0 \log(-z_0) \]

\[ b_l = \sum_{k=0}^{l} \frac{a_k (l-k-1)^{k+l}}{k^{k+l}} (-1)^k - \frac{a_0}{lz_0^l}, \ l \geq 1 \]
For $r \geq \text{max}(2, 2c/(c-1))$, error bound

$$\frac{A(4e(r+c)(c+1)+c^2)}{e(c-1)} \left(\frac{1}{c}\right)^{r+1}$$

\[\sum_{k=0}^{n} a_k (z - z_0)^k = \sum_{l=0}^{n} \left[ \sum_{k=l}^{n} a_k \binom{k}{l} (-z_0)^{k-l} \right] z^l \]

\[\Phi_{li} : r\text{-term multipole expansion} \text{ about the box center of the potential field due to all the particles in box } i \text{ at level } l\]
Figure 4.4. Single-level FMM and multi-level FMM.

- \( \Psi_{li} \): \( r \)-term local expansion about the box center of the potential field due to all the particles outside box \( i \) and its nearest neighbors

- \( \tilde{\Psi}_{li} \): \( r \)-term local expansion about the box center of the potential field due to all the particles outside box \( i \)'s parent and its parent’s nearest neighbors

- \( I_i \): Interaction list: children of the nearest neighbors of \( i \)'s parent which are well separated from \( i \)

Figure 4.5. Computational boxes at different levels.

Main steps:

1. Upward:
   (a) for \( i = 1 : 4^{l_{\text{max}}} \)
      form ME of \( \Phi_{i_{\text{max}},i} \) — coefficients of ME only and NO evaluation!

   (b) for \( l = l_{\text{max}} - 1 : 0 \)
      for \( i = 1 : 4^l \)
      form ME of \( \Phi_{l,i} \) by shifting the center of each child — coefficients of ME only and NO evaluation!
2. Downward:
   for \( l = 1 : l_{\text{max}} \)
   for \( i = 1 : 4^l \)
   for \( j \in \mathcal{I}_i \), \( \Psi_{li} = \tilde{\Psi}_{li} + \Phi_{lj} \) with center of \( \Phi_{lj} \) shifted to that of \( i \)
   if \( l < l_{\text{max}} \)
   for \( i = 1 : 4^l \)
   for \( j \in \mathcal{I}_{ch(i)} \), form \( \tilde{\Psi}_{l+1,i} \) by shifting the center of \( \Psi_{li} \) to \( j \)

3. Sum:
   for \( i = 1 : 4^{l_{\text{max}}} \)
   for \( j \in \text{box } i \), evaluate \( \Psi_{l_{\text{max}},i}(z_j) \), \( \tilde{\Psi}_{l_{\text{max}},ij} \) of \( j \) with \( i \)'s other nodes and \( i \)'s neighbors
   \[
   \sum_i \sum_j \Psi_{l_{\text{max}},i}(z_j) + \tilde{\Psi}_{l_{\text{max}},ij}
   \]
Bibliography


