MAIT 627 Fast Multipole Methods

Lecture 2
Outline

• **Factorization – One of key parts of the FMM**
  – Extensions of our trick for fast summation
  – “Middleman” scheme
  – Singular and regular fields
  – Far field and near field

• **Local Expansions (or R-expansions)**
  – Local expansions of regular and singular potentials
  – Power series
  – Taylor series

• **Far Field Expansions (or S-expansions)**
  – Far field expansions of regular and singular potentials
  – Asymptotic series
Matrix-Vector Multiplication

Compute matrix vector product

\[ v = \Phi u \]

or

\[ v_j = \sum_{i=1}^{N} \Phi_{ji} u_i, \quad j = 1, \ldots, M, \]

where

\[ \Phi_{ji} = \Phi(y_j, x_i), \quad j = 1, \ldots, M, \quad i = 1, \ldots, N, \]

or

\[
\Phi = \begin{pmatrix}
\Phi_{11} & \Phi_{12} & \ldots & \Phi_{1M} \\
\Phi_{21} & \Phi_{22} & \ldots & \Phi_{2M} \\
\cdots & \cdots & \cdots & \cdots \\
\Phi_{M1} & \Phi_{M2} & \ldots & \Phi_{MM}
\end{pmatrix} = \begin{pmatrix}
\Phi(y_1, x_1) & \Phi(y_1, x_2) & \ldots & \Phi(y_1, x_M) \\
\Phi(y_2, x_1) & \Phi(y_2, x_2) & \ldots & \Phi(y_2, x_M) \\
\cdots & \cdots & \cdots & \cdots \\
\Phi(y_M, x_1) & \Phi(y_M, x_2) & \ldots & \Phi(y_M, x_N)
\end{pmatrix}.
\]

Generally we have two sets of points in \(d\)-dimensions:

**Sources:** \( \mathbf{X} = \{x_1, \ldots, x_N\}, \quad x_i \in \mathbb{R}^d, \quad i = 1, \ldots, N, \)

**Receivers:** \( \mathbf{Y} = \{y_1, \ldots, y_M\}, \quad y_j \in \mathbb{R}^d, \quad j = 1, \ldots, M, \)

The receivers also can be called “targets” or “evaluation points”.
Why $\mathbb{R}^d$?

- $d = 1$
  - Scalar functions, interpolation, etc.
- $d = 2, 3$
  - Physical problems in 2 and 3 dimensional space
- $d = 4$
  - 3D Space + time, 3D grayscale images
- $d = 5$
  - Color 2D images, Motion of 3D grayscale images
- $d = 6$
  - Color 3D images
- $d = 7$
  - Motion of 3D color images
- $d = \text{arbitrary}$
  - d-parametric spaces, statistics, database search procedures
Fields (Potentials)

Field (Potential) of a single ($i$th) unit source

Field (Potential) of the set of sources of intensities $\{u_i\}$

$$\varphi(y) = \sum_{i=1}^{N} u_i \Phi(y, x_i), \quad y \in \mathbb{R}^d,$$

$$\nu_j = \varphi(y_j), \quad j = 1, \ldots, M.$$
Examples of Fields

• There can be vector or scalar fields (we focus mostly on scalar fields)
• Fields can be regular or singular

Scalar Fields:
- Gravity
  \( \Phi(y, x_i) = \frac{1}{|y - x_i|} \)
  (singular at \( y = x_i \))
- Monochromatic Wave (\( k \) is the wavenumber)
  \( \Phi(y, x_i) = \frac{\exp\{ik|y - x_i|\}}{|y - x_i|} \)
  (singular at \( y = x_i \))
- Gaussian
  \( \Phi(y, x_i) = \exp\{-|y - x_i|^2/\sigma\} \)
  (regular everywhere)

Vector Field:
- 3D Velocity field:
  \( \Phi(y, x_i) = \nabla_y \frac{1}{|y - x_i|} = i_1 \frac{\partial}{\partial y_1} \frac{1}{|y - x_i|} + i_2 \frac{\partial}{\partial y_2} \frac{1}{|y - x_i|} + i_3 \frac{\partial}{\partial y_3} \frac{1}{|y - x_i|}, \)
  \( y = (y_1, y_2, y_3) \in \mathbb{R}^3. \)
Straightforward Computational Complexity:

\[ O(MN) \quad \text{Error: 0 ("machine" precision)} \]

The Fast Multipole Methods look for computation of the same problem with complexity \( o(MN) \) and error \( < \) prescribed error.

In the case when the error of the FMM does not exceed the machine precision error (for given number of bits) there is no difference between the “exact” and “approximate” solution.
Factorization
“Middleman Method”
Global Factorization

\[ \forall x_i, y_j \in \Omega \subseteq \mathbb{R}^d : \]

\[ \Phi(y_j, x_i) = \sum_{m=0}^{\infty} a_m(x_i - x_\star) f_m(y_j - x_\star) = \sum_{m=0}^{p-1} a_m(x_i - x_\star) f_m(y_j - x_\star) + \text{Error}(p, x_i, y_j) \]
Factorization Trick

\[ v_j = \sum_{i=1}^{N} \Phi(y_j, x_i) u_i \]

\[ = \sum_{i=1}^{N} \left[ \sum_{m=0}^{p-1} a_m (x_i - x_*) f_m (y_j - x_*) + \text{Error}(p, x_i, y_j) \right] u_i \]

\[ = \sum_{m=0}^{p-1} f_m (y_j - x_*) \sum_{i=1}^{N} a_m (x_i - x_*) u_i + \sum_{i=1}^{N} \text{Error}(p, x_i, y_j) u_i \]

\[ = \sum_{m=0}^{p-1} c_m f_m (y_j - x_*) + \text{Error}(N, p), \]

where

\[ c_m = \sum_{i=1}^{N} a_m (x_i - x_*) u_i. \]
Reduction of Complexity

Straightforward (nested loops):

\[
\begin{align*}
&\text{for } j = 1, \ldots, M \\
&\quad v_j = 0; \\
&\text{for } i = 1, \ldots, N \\
&\quad v_j = v_j + \Phi(y_j, x_i)u_i; \\
&\text{end;}
\end{align*}
\]

Complexity: \( O(MN) \)

Factoized:

\[
\begin{align*}
&\text{for } m = 0, \ldots, p - 1 \\
&\quad c_m = 0; \\
&\text{for } i = 1, \ldots, N \\
&\quad c_m = c_m + a_m(x_i - x_*)u_i; \\
&\text{end;}
\end{align*}
\]

\[
\begin{align*}
&\text{for } j = 1, \ldots, M \\
&\quad v_j = 0; \\
&\text{for } m = 0, \ldots, p - 1 \\
&\quad v_j = v_j + c_m f_m(y_j - x_*); \\
&\text{end;}
\end{align*}
\]

Complexity: \( O(pN + pM) \)

If \( p \ll \min(M, N) \) then complexity reduces!
Middleman Scheme

Complexity: $O(pN + pM)$

Set of coefficients $\{c_m\}$
Far Field and Near Field

Near Field of the $i$th source:

$|y - x_i| < r_c$. 

Far Field of the $i$th source:

$|y - x_i| > R_c$.

What are these $r_c$ and $R_c$ ?

depends on the potential + some conventions for the terminology.
Local (Regular) Expansion

Do not confuse with the Near Field!

Let

We call expansion local (regular) inside a sphere if the series converges for $\forall \mathbf{y}, |\mathbf{y} - \mathbf{x}_*| < r_*$.

We also call this R-expansion, since basis functions $R_m$ should be regular.

$$\Phi(\mathbf{y}, \mathbf{x}_*) = \sum_{m=0}^{\infty} a_m(\mathbf{x}_i, \mathbf{x}_*) R_m(\mathbf{y} - \mathbf{x}_*)$$

$x_* \in \mathbb{R}^d$. 

$|\mathbf{y} - \mathbf{x}_*| < r_*$.
Local Expansion of a Regular Potential

Can be like this:

\[ |y - x| < r^* < |x_i - x_*| \]

...or like this:

\[ r^* > |y - x| > |x_i - x_*| \]
Local Expansion of a Regular Potential (Example)

Valid for any \( r_* < \infty \), and \( x_i \).

Looking for factorization:

\[
\Phi(y,x_i) = \sum_{m=0}^{\infty} a_m(x_i - x_*)_m R_m(y-x_*)\]

We have

\[
e^{-(y-x_*)^2} = e^{-(y-x_*)^2} e^{-(x_i - x_*)_2} e^{2(x_i - x_*)(y-x_*)}
\]

\[
= e^{-(y-x_*)^2} e^{-(x_i - x_*)_2} \sum_{m=0}^{\infty} \frac{2^m (x_i - x_*)_m (y-x_*)_m}{m!}
\]

Choose

\[
a_m(x_i - x_*) = e^{-(x_i - x_*)^2} \frac{2^m}{m!} (x_i - x_*)^m, \quad m = 0, 1, \ldots,
\]

\[
R_m(y-x_*) = e^{-(y-x_*)^2} \frac{2^m}{m!} (y-x_*)^m, \quad m = 0, 1, \ldots
\]
Local Expansion of a Regular Potential
(The same kernel, Example 2)

\[ e^{-\langle y-x_0 \rangle^2} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} (y-x_0)^{2n}. \]

So

\[ e^{-\langle y-x \rangle^2} = e^{-\langle y-x_0 \rangle^2} e^{-\langle x-x_0 \rangle^2} \sum_{m=0}^{\infty} \frac{2^m (x_0 - x)^m (y-x_0)^m}{m!} = e^{-\langle x-x_0 \rangle^2} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^n 2^m (x - x_0)^m (y-x_0)^{m+2n}}{m!n!}. \]

Rearrange summation:

\[ m + 2n = l \]
\[ m = l - 2n \]

\[ e^{-\langle y-x \rangle^2} = e^{-\langle x-x_0 \rangle^2} \sum_{l=0}^{\infty} \sum_{n=0}^{[l/2]} \frac{(-1)^n 2^{l-2n} (x_0 - x)^{l-2n}}{(l-2n)!n!} (y-x_0)^l = \sum_{l=0}^{\infty} h_l(x-x_0) \frac{(y-x_0)^l}{l!}. \]

Hermit polynomials:

\[ H_l(x) = l! \sum_{n=0}^{[l/2]} \frac{(-1)^n 2^{l-2n} (x)^{l-2n}}{(l-2n)!n!}. \]

Hermit functions:

\[ h_l(x) = e^{-x^2} H_l(x). \]

Choose

\[ a_l(x-x_0) = h_l(x-x_0), \quad R_l(y-x_0) = \frac{1}{l!} (y-x_0)^l, \quad l = 0, 1, \ldots \]
Local Expansion of a Singular Potential

Can be like this:

\[ |y - x_*| < r_* \leq |x_i - x_*| \]

Like this only!

Never ever!

Because \( x_i \) is a singular point!
Local Expansion of a Singular Potential (Example)

Valid for any $|x_i - x_*| > |y - x_*|$

Looking for factorization:

$$\Phi(y, x_i) = \frac{1}{y - x_i}.$$  

We have

$$\Phi(y, x_i) = \sum_{m=0}^{\infty} a_m(x_i - x_*) R_m(y - x_*).$$

Geometric progression:

$$(1 - \alpha)^{-1} = 1 + \alpha + \alpha^2 + \ldots = \sum_{m=0}^{\infty} \alpha^m, \quad |\alpha| < 1.$$

Choose

$$a_m(x_i - x_*) = -\frac{1}{(x_i - x_*)^{m+1}}, \quad m = 0, 1, \ldots,$$

$$R_m(y - x_*) = (y - x_*)^m, \quad m = 0, 1, \ldots$$
Power and Taylor Series

- Power and Taylor Series
  - Power Series in 1D
  - Taylor Series in 1D
- Multidimensional Taylor Series
- Factorization of Scalar Products in $\mathbb{R}^d$
- Compression of Factorized Series
- Factorization of Scalar Products in $\mathbb{R}^d$ (compression)
  - Factorization in 2D.
  - Factorization in 3D.
  - Factorization in $d$D.
  - Multinomial Coefficients.
  - Complexity of Fast Summation.
- General Forms of Factorization for Fast Summation
Power Series

Power series relative to real or complex variable \( y \) is a series of type

\[
f(y - x_\ast) = \sum_{m=0}^{\infty} a_m(y - x_\ast)^m,
\]

where \( a_m \) are real or complex numbers.
Properties of Power Series

1) For any power series there exists \( r_* \), such that the series converges absolutely at \( |y - x_*| < r_* \), and diverges at \( |y-x_*| > r_* \). The number \( r_* \), is called the *convergence radius* of the series, \( 0 \leq r_* \leq \infty \).

For any number \( q \), such that \( 0 < q < r_* \), the power series uniformly converges at \( |y - x_*| < q \).
Properties of Power Series

2) Convergent power series can be summed, multiplied by a scalar, or multiplied according to the Cauchy rule.

For $|y-x_*| < r_*$, the sum of the series is a continuous and infinitely differentiable function of $y$.

The power series can be differentiated term by term at $|y-x_*| < r_*$ and integrated over any closed interval included in $|y-x_*| < r_*$. Differentiated or integrated series (if integration is taken from $x_*$ to $y-x_*$) have the same convergence radius $r_*$.

\[
\sum_{m=0}^{\infty} a_m(y-x_*)^m + \sum_{m=0}^{\infty} b_m(y-x_*)^m = \sum_{m=0}^{\infty} (a_m + b_m)(y-x_*)^m,
\]

\[
a \sum_{m=0}^{\infty} a_m(y-x_*)^m = \sum_{m=0}^{\infty} a a_m(y-x_*)^m,
\]

\[
\left[ \sum_{m=0}^{\infty} a_m(y-x_*)^m \right] \left[ \sum_{m=0}^{\infty} b_m(y-x_*)^m \right] = \sum_{n=0}^{\infty} \left[ \sum_{m=0}^{n} a_m b_{n-m} \right] (y-x_*)^n.
\]
Properties of Power Series

3) Uniqueness. If there exists such positive $r$ that at any $y$ satisfying $|y-x_*|<r$ two power series have the same sum, then the coefficients of these series are the same.
For those who love proofs

Prove the above properties!

(Not the course formal requirement, but a good exercise)
Taylor Series (Finite)

Let $f(y)$ be a real function, $f(y) \in D^n[x_*, x_* + r_*]$ (so the $n$-th derivative $f^{(n)}(y)$ exists for $x_* \leq y < x_* + r_*$). Then

$$f(y) = f(x_*) + f'(x_*)(y - x_*) + \frac{1}{2!}f''(x_*)(y - x_*)^2 + \ldots + \frac{1}{(n-1)!}f^{(n-1)}(x_*)(y - x_*)^{n-1} + \text{Residual}_n(y).$$

Cauchy's evaluation:

$$|\text{Residual}_n(y)| \leq \frac{|y - x_*|^n}{n!} \sup_{x_* \leq x < x_* + r_*} |f^{(n)}(y)|.$$

Lagrange evaluation:

$$\text{Residual}_n(y) = \int_{x_*}^{y} dx \int_{x_*}^{x} dx \ldots \int_{x_*}^{x} f^{(n)}(x)dx = \frac{1}{n!}f^{(n)}(X)(y - x_*)^n,$$

where $X \in (x_*, x_* + r_*)$.

We have similar formulae for $x_* - r_* \leq y < x_*$. 

Taylor Series (Infinite)

Let \( f(y) \in D^\infty(x_*, r_*, x_* + r_*) \) and let

\[
\lim_{n \to \infty} \text{Residual}_n(y) = 0,
\]

then

\[
f(y) = \sum_{m=0}^{\infty} \frac{1}{m!} f^{(m)}(x_*) (y - x_*)^m, \quad |y - x_*| < r_*,
\]

and the series uniformly converges to \( f(y) \) for any \( |y - x_*| \leq q, \) where \( 0 \leq q \leq r. \)
Local 1D Taylor Expansion

Looking for local expansion:

\[ \Phi(y, x_i) = \sum_{m=0}^{\infty} a_m(x_i, x_*) R_m(y-x_*), \]

\[ \Phi(y, x_i) = \sum_{m=0}^{\infty} \frac{1}{m!} \frac{\partial^m \Phi}{\partial y^m}(x_*, x_i)(y-x_*)^m. \]

\[ a_m(x_i, x_*) = \frac{1}{m!} \frac{\partial^m \Phi}{\partial y^m}(x_*, x_i), \quad m = 0, 1, \ldots \]

\[ R_m(y-x_*) = (y-x_*)^m, \quad m = 0, 1, \ldots \]
Local 1D Taylor Expansion
(Example)

\[ \Phi(y, x_i) = e^{x_i y}. \]

\[ \frac{\partial^m \Phi}{\partial y^m}(y, x_i) = x_i^m e^{x_i y}, \quad \frac{\partial^m \Phi}{\partial y^m}(x_*, x_i) = x_i^m e^{x_* y}. \]

\[ a_m(x_i, x_*) = \frac{1}{m!} \frac{\partial^m \Phi}{\partial y^m}(x_*, x_i) = \frac{x_i^m}{m!} e^{x_* y}. \]

\[ \Phi(y, x_i) = e^{x_* y} \sum_{m=0}^{\infty} \frac{x_i^m}{m!} (y-x_*)^m. \]

Residual for \(|y-x_*| < \alpha\) (assume \(x_i > 0, x_* > 0\)):

\[ |\text{Residual}_{n}(y)| \leq \frac{|y-x_*|^n}{n!} \sup_{x_* - \alpha < y < x_* + \alpha} \left| \frac{\partial^n \Phi}{\partial y^n}(y, x_i) \right| < \frac{\alpha^n}{n!} x_i^n e^{x_i(y+x*)}. \]

For \(n = 5, \alpha = 0.5, x_i = 1, x_* = 0.5\) we have

\[ |\text{Residual}_{5}(y)| < \frac{e}{2^5 5!} < \frac{3}{32 \cdot 120} = \frac{1}{1280} < 10^{-3}. \]
Multidimensional Taylor Series

Let $f(y)$ be a real function,

$$f(y) \in D^\infty(U_x), \quad y = (y_1, \ldots, y_d) \in U_x \subset \mathbb{R}^d, \quad x_+ = (x_{*1}, \ldots, x_{*d}) \subset \mathbb{R}^d$$

Then we can write

$$f(y) = f(y_1, y_2, \ldots, y_d)$$

$$f(y_1, y_2, \ldots, y_d) = \sum_{m_1=0}^{\infty} \frac{1}{m_1!} \frac{\partial^{m_1} f(x_{*1}, y_2, \ldots, y_d)}{\partial y_1^{m_1}} (y_1 - x_{*1})^{m_1}$$

$$= \sum_{m_1=0}^{\infty} \frac{1}{m_1!} \sum_{m_2=0}^{\infty} \frac{1}{m_2!} \frac{\partial^{m_2} f(x_{*1}, x_{*2}, \ldots, y_d)}{\partial y_1^{m_2}} (y_1 - x_{*1})^{m_1} (y_2 - x_{*2})^{m_2}$$

$$= \ldots$$

$$= \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \ldots \sum_{m_d=0}^{\infty} \frac{\partial^{m_1}}{\partial y_1^{m_1}} \frac{\partial^{m_2}}{\partial y_2^{m_2}} \ldots \frac{\partial^{m_d}}{\partial y_d^{m_d}} f(x_{*1}, x_{*2}, \ldots, x_{*d}) \prod_{i=1}^{d} \frac{1}{m_i!} (y_i - x_{*i})^{m_i}.$$
Multidimensional Taylor Series
(using some vector algebra)

Operator $\nabla$:

$$\nabla = i_1 \frac{\partial}{\partial y_1} + \ldots + i_d \frac{\partial}{\partial y_d}.$$

Differential along direction $s$:

$$\frac{d^n f(y)}{ds^n} = (s \cdot \nabla)^n f(y), \quad |s| = 1.$$

Taylor series (let $s = (y - x_*)/|y - x_*|$)

$$f(y) = f(x_*) + \frac{df(x_*)}{ds} |y - x_*| + \frac{1}{2!} \frac{d^2 f(x_*)}{ds^2} |y - x_*|^2 + \ldots$$

$$= f(x_*) + [(y - x_*) \cdot \nabla] f(x_*) + \frac{1}{2!} [(y - x_*) \cdot \nabla]^2 f(x_*) + \ldots$$

$$= \sum_{m=0}^{\infty} \frac{1}{m!} [(y - x_*) \cdot \nabla]^m f(x_*).$$
Example

\[ \Phi(y, x_i) = e^{y \cdot x_i} = \sum_{m=0}^{\infty} \frac{1}{m!} [(y - x_*) \cdot \nabla x_*]^m \Phi(x_*, x_i), \]

Fix \((y - x_*)\):

\[ \Phi(x_*, x_i) = e^{x_* \cdot x_i}, \]

\[ \nabla_{x_*} \Phi(x_*, x_i) = x_i e^{x_* \cdot x_i} = x_i \Phi(x_*, x_i), \]

\[ [(y - x_*) \cdot \nabla x_*] \Phi(x_*, x_i) = [(y - x_*) \cdot x_i] \Phi(x_*, x_i), \]

\[ [(y - x_*) \cdot \nabla x_*]^m \Phi(x_*, x_i) = [(y - x_*) \cdot x_i]^m \Phi(x_*, x_i), \]

\[ \Phi(y, x_i) = \sum_{m=0}^{\infty} \frac{1}{m!} [(y - x_*) \cdot x_i]^m \Phi(x_*, x_i) = e^{x_* \cdot x_i} \sum_{m=0}^{\infty} \frac{1}{m!} [(y - x_*) \cdot x_i]^m. \]

Check: \(e^{y \cdot x_i} = e^{x_* \cdot x_i} e^{(y - x_*) \cdot x_i} = e^{x_* \cdot x_i} \sum_{m=0}^{\infty} \frac{1}{m!} [(y - x_*) \cdot x_i]^m.\)
Is That a Factorization?

\[ e^{y \cdot x_i} = e^{x^* \cdot x_i} \sum_{m=0}^{\infty} \frac{1}{m!} [(y - x^*) \cdot x_i]^m \]
Scalar Product in d-Dimensional Space

Definition of scalar product:

\[ \mathbf{a} = (a_1, \ldots, a_d), \quad \mathbf{b} = (b_1, \ldots, b_d), \]

\[ \mathbf{a} \cdot \mathbf{b} = a_1 b_1 + \ldots + a_d b_d = \sum_{k=1}^{d} a_k b_k. \]

\[ \mathbf{a} \cdot \mathbf{b} = |\mathbf{a}| |\mathbf{b}| \cos \theta, \]

\[ |\mathbf{a}| = \sqrt{\mathbf{a} \cdot \mathbf{a}}. \]

What if

\[ a_1, \ldots, a_d, b_1, \ldots, b_d \in \mathbb{C} \quad ? \]

Definition:

\[ \mathbf{a} \cdot \mathbf{b} = \overline{\mathbf{a}} \cdot \mathbf{b} = \overline{a_1} b_1 + \ldots + \overline{a_d} b_d = \sum_{k=1}^{d} \overline{a_k} b_k. \]
Properties of Scalar Product

Commutativity:

\[ a \cdot b = b \cdot a \]

Scaling:

\[ (\lambda a) \cdot b = a \cdot (\lambda b) = \lambda (a \cdot b), \quad \lambda \in \mathbb{R} \]

Distributivity:

\[ (a + b) \cdot c = a \cdot c + b \cdot c \]
Factorization of Scalar Product Powers

\[(a \cdot b)^n = \left( \sum_{k=1}^{d} a_k b_k \right)^n = \sum_{k_1=1}^{d} a_{k_1} b_{k_1} \sum_{k_2=1}^{d} a_{k_2} b_{k_2} \ldots \sum_{k_n=1}^{d} a_{k_n} b_{k_n} \]

\[= \sum_{k_1=1}^{d} \sum_{k_2=1}^{d} \ldots \sum_{k_n=1}^{d} a_{k_1} a_{k_2} \ldots a_{k_n} b_{k_1} b_{k_2} \ldots b_{k_n} \]

\[= [a \otimes a \otimes \ldots \otimes a] \cdot [b \otimes b \otimes \ldots \otimes b] = a^n \cdot b^n \]

\[a^n \cdot b^n = (a \cdot b)^n = (b \cdot a)^n = b^n \cdot a^n.\]

\[e^{y \cdot x_i} = e^{x_i \cdot x_i} \sum_{m=0}^{\infty} \frac{1}{m!} (y - x_\star) \cdot x_i \, x_i^m = e^{x_i \cdot x_i} \sum_{m=0}^{\infty} \frac{1}{m!} x_i^m \cdot (y - x_\star)^{bn}.\]
Is That Factorization?

1) Truncation:

\[ \Phi(y, x_i) = e^{y^* x_i} = e^{x_i^* x_i} \left[ \sum_{m=0}^{p-1} \frac{1}{m!} x_i^m \cdot (y - x_*)^m + \text{Residual}_p \right] \]

2) Fast summation:

\[ v_j = \sum_{i=1}^{N} u_i \Phi(y_j, x_i) = \sum_{i=1}^{N} u_i e^{x_i^* x_i} \left[ \sum_{m=0}^{p-1} \frac{1}{m!} x_i^m \cdot (y_j - x_*)^m + \text{Residual}_p \right] \]

\[ = \sum_{i=1}^{N} u_i e^{x_i^* x_i} \sum_{m=0}^{p-1} \frac{1}{m!} x_i^m \cdot (y_j - x_*)^m + N \max_i \left( u_i e^{x_i^* x_i} \right) \text{Residual}_p \]

\[ = \sum_{m=0}^{p-1} \frac{1}{m!} \left( \sum_{i=1}^{N} u_i e^{x_i^* x_i} x_i^m \right) \cdot (y_j - x_*)^m + \text{Residual} \]

\[ = \sum_{m=0}^{p-1} c_m \cdot (y_j - x_*)^m + \text{Residual}, \quad c_m = \frac{1}{m!} \sum_{i=1}^{N} u_i e^{x_i^* x_i} x_i^m. \]

Yes! It is!
Example (Let’s Try To Get Explicit Forms in 2D)

\[ \mathbf{a} = (\alpha_1, \alpha_2), \]
\[ \mathbf{a}^2 = (\alpha_1(\alpha_1, \alpha_2), \alpha_2(\alpha_1, \alpha_2)) = (\alpha_1^2, \alpha_1 \alpha_2, \alpha_2 \alpha_1, \alpha_2^2), \]
\[ \mathbf{a}^3 = (\alpha_1^2(\alpha_1, \alpha_2), \alpha_1 \alpha_2(\alpha_1, \alpha_2), \alpha_2 \alpha_1(\alpha_1, \alpha_2), \alpha_2^2(\alpha_1, \alpha_2)) \]
\[ = (\alpha_1^3, \alpha_1^2 \alpha_2, \alpha_1 \alpha_2^2, \alpha_2 \alpha_1^2, \alpha_2 \alpha_2 \alpha_1, \alpha_2^2 \alpha_1, \alpha_2^3), \ldots \]

The length of \( \mathbf{a}^n \) is \( 2^n \)! This is not factorial!

In \( d \) dimensions the length of \( \mathbf{a}^n \) is even \( d^n \)

What to do in practical problems?
Use Compression!

Compression operator:

\[ A^n = \text{Compress}(a^n) \]

Required Property:

\[ a^n \cdot b^n = \text{Compress}(a^n) \cdot \text{Compress}(b^n). \]

Consider \( \mathbb{R}^2 \):

\[ a^n \cdot b^n = (a \cdot b)^n = (a_1 b_1 + a_2 b_2)^n \]

\[ = a_1^n b_1^n + \binom{n}{1} a_1^{n-1} b_1^{n-1} a_2 b_2 + \binom{n}{2} a_1^{n-2} b_1^{n-2} a_2^2 b_2^2 + \ldots + a_2^n b_2^n \]

The length is only \((n +1), \text{not } 2^n\)

Let us define:

\[ A^n = \text{Compress}(a^n) = \left( \begin{array}{c}
\alpha_1^n, \\
\alpha_1^{n-1} \alpha_2, \\
\alpha_1^{n-2} \alpha_2^2, \ldots, \\
\alpha_2^n
\end{array} \right) \]

\[ B^n = \text{Compress}(b^n) = \left( \begin{array}{c}
b_1^n, \\
b_1^{n-1} b_2, \\
b_1^{n-2} b_2^2, \ldots, \\
b_2^n
\end{array} \right) \]
Example of Fast Computation

\[ v_j = \sum_{i=1}^{N} u_i \Phi(y_j, x_i) = \sum_{m=0}^{p-1} c_m \cdot (y_j - x_*)^m + \text{Residual}, \quad c_m = \frac{1}{m!} \sum_{i=1}^{N} u_i e^{x_\ast \cdot x_i} x_i^m. \]

Equivalent to:

\[ v_j = \sum_{m=0}^{p-1} C_m \cdot \text{Compress}((y_j - x_*)^m) + \text{Residual}, \quad C_m = \frac{1}{m!} \sum_{i=1}^{N} u_i e^{x_\ast \cdot x_i} \text{Compress}(x_i^m). \]

Number of multiplications (complexity) to obtain \( v_j \):

\[ \text{Complexity} = 1 + 2 + \ldots + p = \frac{p(p + 1)}{2}. \]
Compression Can be Performed for any Dimensionality (Example for 3D):

\[ a^n \cdot b^n = (a \cdot b)^n = (a_1 b_1 + a_2 b_2 + a_3 b_3)^n \]

\[ = [(a_1 b_1 + a_2 b_2) + a_3 b_3]^n = \sum_{m=0}^{n} \binom{n}{m} (a_1 b_1 + a_2 b_2)^{n-m} a_3^m b_3^m \]

\[ = \sum_{m=0}^{n} \sum_{l=0}^{n-m} \binom{n}{m} \binom{n-m}{l} a_1^{n-m-l} b_1^{n-m-l} a_2^l b_2^l a_3^m b_3^m \]

\[ = a_1^n b_1^n + \binom{n}{1} a_1^{n-1} b_1^{n-1} a_2 b_2 + \binom{n}{2} a_1^{n-2} b_1^{n-2} a_2^2 b_2^2 + \ldots + a_2^n b_2^n \]

\[ + \binom{n}{1} a_1^{n-1} b_1^{n-1} a_3 b_3 + \binom{n}{1} \binom{n-1}{1} a_1^{n-2} b_1^{n-2} a_2 b_2 a_3 b_3 + \ldots + a_3^n b_3^n \]

\[ \text{Compress}(a^n) = \left( a_1^n, \left( \binom{n}{1} a_1^{n-1} a_2, \left( \binom{n}{2} a_1^{n-2} a_2^2, \ldots, \binom{n}{2} a_2^n \right), a_1^{n-1} a_3, \ldots, a_3^n \right) \right) \]

The length of \( a^n \) is \((n+1)+n+\ldots+1=(n+1)(n+2)/2\)
Compression Can be Performed for any Dimensionality (General Case):

\[(a_1 + a_2 + \ldots + a_d)^n = \sum_{n_1 + \ldots + n_d = n} (n, n_1, n_2, \ldots, n_d) a_1^{n_1} a_2^{n_2} \ldots a_d^{n_d}.\]

\[(n, n_1, n_2, \ldots, n_d) = \frac{n!}{n_1! n_2! \ldots n_d!}.\]

\[
\text{Compress}(a^n) = \left( a_1^n, \sqrt{(n, n-1, 1, 0, \ldots, 0)} a_1^{n-1} a_2, \ldots, \sqrt{(n, n_1, n_2, \ldots, n_d)} a_1^{n_1} a_2^{n_2} \ldots a_d^{n_d}, \ldots, a_d^n \right).\]

So we have

\[a^n \cdot b^n = \text{Compress}(a^n) \cdot \text{Compress}(b^n)\]

\[= \sum_{n_1 + \ldots + n_d = n} (n, n_1, n_2, \ldots, n_d) a_1^{n_1} a_2^{n_2} \ldots a_d^{n_d} b_1^{n_1} b_2^{n_2} \ldots b_d^{n_d}\]

\[= (a_1 b_1 + a_2 b_2 + \ldots + a_d b_d)^n = (a \cdot b)^n.\]
What are multinomial coefficients?

\[(n ; n_1, n_2, \ldots, n_d)\] is the number of ways of putting \(n\) different objects into \(d\) different boxes with \(n_k\) in the \(k\)-th box.

\[n_1 + n_2 + \ldots + n_d = n\]
The length of the compressed vector

\begin{align*}
    d = 1 & : \quad 1, \\
    d = 2 & : \quad n + 1, \\
    d = 3 & : \quad \frac{1}{2}(n + 1)(n + 2), \\
    \ldots
\end{align*}

**Theorem:** If \( a \in \mathbb{R}^d \), then the length of compressed vector \( \text{Compress}(a^n) \), is

\[
\binom{n + d - 1}{n} = \frac{(n + 1) \ldots (n + d - 1)}{(d - 1)!}.
\]

**Proof:** We have a basis for induction (see above). Let this holds for \( d \) dimensions. Consider \( d + 1 \) dimensions:

\[
((a_1 + \ldots + a_d) + a_{d+1})^n = \sum_{m=0}^{n} \binom{n}{m} (a_1 + \ldots + a_d)^m a_{d+1}^{n-m}
\]

The number of terms is then

\[
\sum_{m=0}^{n} \binom{m + d - 1}{m} = \binom{d - 1}{0} + \binom{d}{1} + \ldots + \binom{n + d - 1}{n} = \binom{n + d}{n}
\]

This proves the theorem.
Example of Fast Computation

\[ v_j = \sum_{i=1}^{N} u_i \Phi(y_j, x_i) = \sum_{m=0}^{p-1} c_m \cdot (y_j - x_{\ast})^m + \text{Residual}, \quad c_m = \frac{1}{m!} \sum_{i=1}^{N} u_i e^{x_i \cdot x_{\ast} x_i} x_i^m. \]

Equivalent to:

\[ v_j = \sum_{m=0}^{p-1} c_m \cdot \text{Compress}((y_j - x_{\ast})^m) + \text{Residual}, \quad c_m = \frac{1}{m!} \sum_{i=1}^{N} u_i e^{x_i \cdot x_{\ast} x_i} \text{Compress}(x_i^m). \]

Number of multiplications (complexity) to obtain \( v_j \): (in 2D case!)

\[ \text{Complexity} = 1 + 2 + ... + p = \frac{p(p+1)}{2}. \]

\[ C_0 = \sum_{i=1}^{N} u_i e^{x_i \cdot x_i}, \]

\[ C_1 = (C_{11}, C_{12}) = \sum_{i=1}^{N} u_i e^{x_i \cdot x_i} (x_{i1}, x_{i2}), \]

\[ C_2 = (C_{21}, C_{22}, C_{23}) = \sum_{i=1}^{N} u_i e^{x_i \cdot x_i} \left( x_{i1}^2, \sqrt{2} x_{i1} x_{i2}, x_{i2}^2 \right), \]
Complexity of Fast Summation

Let $\circ$ be a scalar product of vectors $A_i$ and $F_j$ of length $P(p)$ ($p$ is the truncation number). Complexity of summation over $i$ is then $O(PN)$. Complexity of scalar product operation is $P$. Complexity of $M$ scalar product operations is $O(PM)$ (for $j = 1, ..., M$). Total complexity is $O(PM + PN)$. Fast Method is more efficient than direct only if $O(PM + PN) < O(MN)$, so we should have

$$P(p) \ll \min(M,N)$$
General Forms of Factorization for Fast Summation (1)

\[ v_j = \sum_{i=1}^{N} u_i \Phi(y_j, x_i), \quad j = 1, ..., M. \]

\[ \Phi(y_j, x_i) = \sum_{m=0}^{p} a_m(x_i, x_*) f_m(y_j - x_*) + \text{Error}(p, x_i, x_*, y_j) \]

Scalar product

\[ = a(x_i, x_*) \cdot f(y_j - x_*) + \text{Error}. \]

How about vectors of length \( p \)

\[ v_j = \sum_{i=1}^{N} u_i e^{-\lambda_i |x_i - y_j|^2} \]

Some parameter depending on \( i \)

More general to have

\[ v_j = \sum_{i=1}^{N} u_i \Phi_i(y_j) \quad \text{or} \quad v(y) = \sum_{i=1}^{N} u_i \Phi_i(y). \]
General Forms of Factorization for Fast Summation (2)

The potential can be factorized as

$$\Phi_i(y) = A_i(x_*) \circ F(y - x_*)$$

Generalized product $\circ$ can be scalar product, contraction, etc. $A_i$ and $F$ can be real or complex vectors, tensors, etc. in $p$-dimensional space.

Requirements to the product (distributivity with respect to addition)

$$(\alpha A_i + \beta A_j) \circ F = \alpha A_i \circ F + \beta A_j \circ F.$$

In this case

$$v(y) = \sum_{i=1}^{N} u_i \Phi_i(y) = \sum_{i=1}^{N} u_i A_i(x_*) \circ F(y - x_*) = A(x_*) \circ F(y - x_*)$$

$$A(x_*) = \sum_{i=1}^{N} u_i A_i(x_*)$$

We do not need commutativity of $\circ$ (i.e. we do not request $A_i \circ F = F \circ A_i$).
General Forms of Factorization for Fast Summation (3)

Actually, we even do need continuous variable \( y \),
The problem is to represent all matrix elements in the form

\[
\Phi_{ji} = A_i \circ F_j
\]

then

\[
v_j = \sum_{i=1}^{N} u_i \Phi_{ji} = \sum_{i=1}^{N} u_i (A_i \circ F_j) = \left( \sum_{i=1}^{N} u_i A_i \right) \circ F_j.
\]
Outline

• Far Field Expansions (or S-expansions)
  – Regular Potential (Convergent Series);
  – Regular Potential (Asymptotic Series);
  – Singular Potential;
• Asymptotic Series
• Approaches for Selection of the Basis Functions
Far Field Expansions (S-expansions)

Let \( x_* \in \mathbb{R}^d \).

We call expansion

\[
\Phi(y, x_i) = \sum_{m=0}^{\infty} b_m(x_i, x_*) S_m(y - x_*)
\]

far field expansion (or S-expansion) outside a sphere

\[|y - x_*| > R_*\]

if the series converges for \( \forall y, |y - x_*| > R_* \).
Far Field Expansion of a Regular Potential

...sometimes like this:

\[ |y - x_*| > R_* > |x_i - x_*| \]

Can be like this:

\[ |y - x_*| > R_* > |x_i - x_*| \]

...sometimes like this:

\[ |x_i - x_*| > |y - x_*| > R_* \]
Local Expansion of a Regular Potential
Can be Far Field Expansion Also

Valid for any $r_* < \infty$, and $x_i$.

\[
\Phi(y, x_i) = e^{-(y-x_i)^2} = \sum_{m=0}^{\infty} a_m(x_i, x_*) S_m(y-x_*).
\]

We have

\[
e^{-(y-x_i)^2} = \sum_{m=0}^{\infty} S_m(x_i - x_*) R_m(y - x_*) = \sum_{m=0}^{\infty} R_m(x_i - x_*) S_m(y - x_*)
\]

\[
R_m(x) = S_m(x) = \sqrt{\frac{2^m}{m!}} e^{-x^2} x^m, \quad m = 0, 1, \ldots
\]
Or may be not…

\[ e^{-(y-x_i)^2} = \sum_{l=0}^{\infty} h_l(x_i - x_*) \frac{(y-x_*)^l}{l!} = \sum_{l=0}^{\infty} \frac{(x_i - x_*)^l}{l!} h_l(y - x_*) \]

Decays at large y

Local

Far
Asymptotic Series

\[ f(x, \epsilon) = f_0(x) \varphi_0(\epsilon) + f_1(x) \varphi_1(\epsilon) + f_2(x) \varphi_2(\epsilon) + \ldots = \sum_{n=0}^{\infty} f_n(x) \varphi_n(\epsilon) \]

\[ \lim_{\epsilon \to 0} \frac{\varphi_n(\epsilon)}{\varphi_{n+1}(\epsilon)} = 0. \]

Gauge functions

\[ f(x, \epsilon) - \sum_{n=0}^{p-1} f_n(x) \varphi_n(\epsilon) = O(f_p(x) \varphi_p(\epsilon)) \]

The asymptotic expansion is *uniform* in domain \( x \in \Omega \) if

\[ \forall x \in \Omega, \quad \left| f(x, \epsilon) - \sum_{n=0}^{p-1} f_n(x) \varphi_n(\epsilon) \right| = O(\varphi_p(\epsilon)). \]

Otherwise the asymptotic expansion is not uniform.
Examples of Uniform and Non-Uniform Expansions

Example of uniform expansion:

\[ f(x; \varepsilon) = \frac{1}{x + \varepsilon}, \quad x > 10 \]

\[ f(x; \varepsilon) = \frac{1}{x} \left( 1 + \frac{\varepsilon}{x} \right)^{-1} = \frac{1}{x} \sum_{n=0}^{\infty} \frac{(-1)^n \varepsilon^n}{x^n} \]

Example of non-uniform expansion:

\[ f(x; \varepsilon) = e^{\varepsilon x}, \quad x \in \mathbb{R}^1 \]

\[ e^{\varepsilon x} = \sum_{n=0}^{\infty} \frac{\varepsilon^n x^n}{n!}. \]

Prove that! (Hint: consider \( x \gg \varepsilon^{-1} \)).
Example of Far Field Expansion of a Regular Function (Using Asymptotic Series)

\[
\Phi(y, x_i) = \frac{1}{1 + (y - x_i)^2} = \frac{1}{1 + [y - x_\ast - (x_i - x_\ast)]^2} = \frac{1}{(y - x_\ast)^2} \frac{(y - x_\ast)^2}{1 + [y - x_\ast - (x_i - x_\ast)]^2}.
\]

Let

\[
\epsilon = \frac{1}{y - x_\ast}
\]

\[
\Phi(\epsilon, x_i - x_\ast) = \epsilon^2 \frac{1}{1 \left[ \frac{1}{\epsilon} - (x_i - x_\ast) \right]^2} = \frac{1}{\epsilon^2 + (1 - \epsilon x)^2} = \epsilon^2 f(x, \epsilon), \quad x = x_i - x_\ast
\]

\[
f(x, \epsilon) = \frac{1}{\epsilon^2 + (1 - \epsilon x)^2} = \sum_{n=0}^{\infty} f_n(x) \epsilon^n
\]

\[
f_n(x) = \frac{1}{n!} \left. \frac{\partial^n f(x, \epsilon)}{\partial \epsilon^n} \right|_{\epsilon=0}
\]
Example of Far Field Expansion of a Regular Function (continuation)

\[ f_0(x) = 1, \]
\[ f_1(x) = \left. \frac{\partial f(x, \varepsilon)}{\partial \varepsilon} \right|_{\varepsilon=0} = 2x, \]
\[ f_2(x) = \left. \frac{1}{2!} \frac{\partial^2 f(x, \varepsilon)}{\partial \varepsilon^2} \right|_{\varepsilon=0} = 3x^2 - 1, \]

\[ \Phi(y, x_i) = \frac{1}{(y - x_*)^2} \sum_{n=0}^{\infty} f_n(x_i - x_*) \frac{1}{(y - x_*)^n} \]

\[ y \geq 100, \quad x_i = 1, \quad x_* = 0, \]
\[ \varepsilon = 10^{-2}, \quad x = 1 \]

\[ \left| \Phi(y, x_i) - \frac{1}{(y - x_*)^2} \left[ 1 + \frac{2(x_i - x_*)}{(y - x_*)} \right] \right| \leq \varepsilon^4 (3x^2 - 1) = 2 \cdot 10^{-8}. \]
Far Field Expansion of a Singular Potential

\[ |y - x_*| > R_* > |x_i - x_*| \]

This case only!
Example For S-expansion of Singular Potential

\[ \Phi(y, x_i) = \frac{1}{y - x_i}. \]

\[ \frac{1}{y - x_i} = \frac{1}{y - x_* - (x_i - x_*)} = \frac{1}{(y - x_*) \left[ 1 - \frac{x_i - x_*}{y - x_*} \right]} = \frac{1}{(y - x_*) \left[ 1 - \frac{x_i - x_*}{y - x_*} \right]^{-1}}. \]

\[ \left[ 1 - \frac{x_i - x_*}{y - x_*} \right]^{-1} = \sum_{m=0}^{\infty} \frac{(x_i - x_*)^m}{(y - x_*)^m}, \quad |y - x_*| > |x_i - x_*|. \]

\[ \Phi(y, x_i) = \sum_{m=0}^{\infty} b_m(x_i, x_*) S_m(y - x_*), \]

\[ b_m(x_i, x_*) = (x_i - x_*)^m, \quad m = 0, 1, ..., \]

\[ S_m(y - x_*) = (y - x_*)^{-m-1}, \quad m = 0, 1, ... \]
Let us compare with the R-expansion of the same function

\[
\Phi(y, x_i) = \sum_{m=0}^{\infty} a_m(x_i, x_*) R_m(y-x_*),
\]

\[
a_m(x_i, x_*) = -(x_i - x_*)^{-m-1}, \quad m = 0, 1, \ldots,
\]

\[
R_m(y-x_*) = (y-x_*)^m, \quad m = 0, 1, \ldots
\]

\[
|y - x_*| < |x_i - x_*| : \quad \text{R-expansion}
\]

|y - x_*| > |x_i - x_*| : \quad \text{S-expansion}

\[
\Phi(y, x_i) = \sum_{m=0}^{\infty} b_m(x_i, x_*) S_m(y-x_*),
\]

\[
b_m(x_i, x_*) = (x_i - x_*)^m, \quad m = 0, 1, \ldots,
\]

\[
S_m(y-x_*) = (y-x_*)^{-m-1}, \quad m = 0, 1, \ldots
\]

Singular Point is located at the Boundary of regions for the R- and S-expansions!
What Do We Need For Real FMM (that provides spatial grouping)

We need S-expansion for \( |y - x_\star| > R_\star > |x_i - x_\star| \)
We need R-expansion for \( |y - x_\star| < r_\star < |x_i - x_\star| \)
Basis Functions

• Power series are great, but do they provide the best approximation? (sometimes yes!)

• Other approaches to factorization:
  – Asymptotic Series (Can be divergent!);
  – Orthogonal Bases in $L_2$;
  – Eigen Functions of Differential Operators;
  – Functions Generated by Differentiation or Other Linear Operators.

• Some of this approaches will be considered in this course.