MAIT 627 Fast Multipole Methods

Lecture 4
Outline

• Representation of functions and operators
• Translation operator
• $R|R$, $S|S$, and $S|R$ translation operators
• Properties of translation operators
• Summary of requirements for functions (potentials) that can be used in FMM
• SLFMM algorithm
• Asymptotic complexity of SLFMM
• Optimization of SLFMM
Outline

- Representation of functions in the space of coefficients
- Matrix representation of operators
- Truncation and truncated operators
- Translation operator
- Reexpansion coefficients
- R|R and S|S translation operators
- Examples
- S|R and R|S translation operators
- Properties of translation operators
Why do we need represent functions in different spaces?

- Functions should be efficiently summed up;
- Sums of functions should be compressed;
- Error bounds should be established;
- Functions should be translated and expanded over different bases;
- For computations we need discrete and finite function representations.
- Some functions measured experimentally or approximated by splines, and there is no explicit analytical representation in the whole space.
Linear Spaces

\[ a, b, c \in \mathcal{U} \]

1). \[ a + b \in \mathcal{U}; \]
2). \[ a + b = b + a, a + (b + c) = (a + b) + c; \]
3). \[ \exists 0, \quad a + 0 = a, \quad a + (-a) = a - a = 0; \]
4). \[ \forall \alpha \in \mathbb{C}, \quad \alpha a \in \mathcal{U}; \]
5). \[ \forall \alpha, \beta \in \mathbb{C}, \quad (\alpha \beta)a = \alpha(\beta)a, \quad 1a = a, \]
\[ \alpha(a + b) = \alpha a + \alpha b, \quad (\alpha + \beta)a = \alpha a + \beta a. \]
Linear Operators

Linear Spaces

\[ \psi \in \mathcal{F}(\Omega), \quad \psi' \in \mathcal{F}(\Omega'), \quad \Omega, \Omega' \subset \mathbb{R}^d, \]

Operator

\[ \psi' = \mathcal{A}[\psi], \]

Linear Operator

\[ \mathcal{A}[\alpha \psi_1 + \beta \psi_2] = \alpha \mathcal{A}[\psi_1] + \beta \mathcal{A}[\psi_2], \quad \alpha, \beta \in \mathbb{C}. \]

An example of linear operator: Differential Operator.
Representation of Functions and Bases

\[ \psi \in \mathcal{F}(\Omega), \quad \psi' \in \mathcal{F}(\Omega'), \quad \Omega, \Omega' \subset \mathbb{R}^d. \]

\[ F_n \in \mathcal{F}(\Omega), \quad F'_n \in \mathcal{F}(\Omega'), \]

\[ \psi = \sum_n c_n F_n, \quad \psi' = \sum_{n'} c'_{n'} F'_{n'}. \]

\[ \mathcal{A}[F_n] = \sum_{n'} (F|F')_{n'n} F'_{n'}. \]

\[ \mathcal{A}[\psi] = \mathcal{A}\left[ \sum_n c_n F_n \right] = \sum_n c_n \mathcal{A}[F_n] = \]

\[ = \sum_n c_n \sum_{n'} (F|F')_{n'n} F'_{n'} = \sum_{n'} \left[ \sum_n (F|F')_{n'n} c_n \right] F'_{n'} = \sum_{n'} c'_{n'} F'_{n'} = \psi'. \]

\[ c'_{n'} = \sum_n (F|F')_{n'n} c_n. \]

Reexpansion Coefficients

Matrix Representation of operator \( A \)
Function Representation in the Space of Coefficients

Let $\mathbb{F}(\Omega) \subset C(\Omega), \Omega \subset \mathbb{R}^d$, be a normed space of continuous functions with norm

$$\| \Phi(y) \| = \max_{y \in \Omega} |\Phi(y)|.$$

Let also $\{F_n(y)\}$ be a complete basis in $\mathbb{F}(\Omega)$, so

$$\Phi(y) = \sum_{n=0}^{\infty} A_n F_n(y), \quad y \in \Omega \subset \mathbb{R}^d, \quad \Phi(y), F_n(y) \in \mathbb{F}(\Omega),$$

absolutely and uniformly converges in $\Omega \subset \mathbb{R}^d$. This means that

$$\forall \epsilon > 0, \exists p(\epsilon), \quad |\Phi(y) - \Phi^p(y)| < \epsilon, \quad \forall y \in \Omega,$$

$$\forall \epsilon > 0, \exists p(\epsilon), \quad \sum_{n=p}^{\infty} |A_n F_n(y)| < \epsilon, \quad \forall y \in \Omega,$$

$$\Phi^p(y) = \sum_{n=0}^{p-1} A_n F_n(y).$$
Function Representation in the Space of Coefficients (2)

Expansion coefficients can be stacked in an infinite vector

\[
A = \begin{pmatrix}
A_0 \\
A_1 \\
\vdots \\
A_n \\
\vdots
\end{pmatrix}.
\]

Let us denote \( A(\Omega) \) a subset of \( \mathbb{R}^\infty \) which is an image of \( F(\Omega) \). For any \( A \in A(\Omega) \) we request that there exists one-to-one mapping

\[
\Phi(y) \geq A, \quad \Phi(y) \in F(\Omega), \quad A \in A(\Omega) \subset \mathbb{R}^\infty.
\]
p-Truncated Vectors

\[ \forall A \in \mathbb{R}^p, \exists \Phi^p(y) = \sum_{n=0}^{p-1} A_n F_n(y) \in F^p(\Omega) \subset F(\Omega). \]

\( F^p(\Omega) \) is dense in \( F(\Omega) \):

\[ \forall \Phi(y) \in F(\Omega), \exists p, \Phi^p(y) \in F^p(\Omega), \quad \| \Phi(y) - \Phi^p(y) \| = \sup_{r \in \Omega} \| \Phi(y) - \Phi^p(y) \| < \epsilon. \]
Matrix Representation of Linear Operators

Let $\Omega' \subset \Omega$ and $\mathcal{F}$ is a mapping of $F(\Omega)$ to $F(\Omega')$. Such mapping can be considered as action of operator $\mathcal{F}$ on $\Phi$:

$$\mathcal{F}[\Phi(y)] = \Phi(y), \quad \Phi(y) \in F(\Omega), \quad \Phi(y) \in F(\Omega') \subset F(\Omega)$$

Respectively, operator $\mathcal{F}$ generates operator $F$ that maps the space of expansion coefficients $A(\Omega) \rightarrow A(\Omega')$, which can be considered as *representation* of the operator $\mathcal{F}$ in the space of expansion coefficients:

$$FA = \tilde{A}, \quad A \in A(\Omega), \quad \tilde{A} \in A(\Omega') \subset A(\Omega).$$

Inversely, if we introduce any transform of expansion coefficients $FA = \tilde{A}$ which provides uniform convergence of function $\Phi(y)$ corresponding to these coefficients in $\Omega' \subset \Omega$ then such transform can be treated as operator $\mathcal{F}$ that convert one function from $F(\Omega)$ to another.

![Diagram](image)

**Representation of a Linear Operator**
p-Truncation (Projection) Operator

\[ \text{Pr}(p)A = \tilde{A}, \quad A \in A(\Omega), \quad \tilde{A} \in A^p(\Omega). \]

\[ A = \begin{pmatrix} A_0 \\ A_1 \\ \vdots \\ A_{p-1} \\ A_p \\ A_{p+1} \\ \vdots \end{pmatrix} \quad \rightarrow \quad \tilde{A} = \begin{pmatrix} A_0 \\ A_1 \\ \vdots \\ A_{p-1} \\ 0 \\ 0 \\ \vdots \end{pmatrix}, \quad \tilde{A} = \begin{pmatrix} 1 & 0 & \ldots & 0 & 0 & 0 & \ldots \\ 0 & 1 & \ldots & 0 & 0 & 0 & \ldots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & 0 & 0 & \ldots \\ 0 & 0 & \ldots & 0 & 0 & 0 & \ldots \\ 0 & 0 & \ldots & 0 & 0 & 0 & \ldots \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \cdot A \]

In space \( F(\Omega) \):

\[ \text{Pr}(p)[\Phi(y)] = \Phi^p(y), \quad \Phi(y) \in F(\Omega), \quad \Phi^p(y) \in F^p(\Omega), \]

\[ \lim_{p \to \infty} \| \Phi(y) - \text{Pr}(p)[\Phi(y)] \| = 0. \]
Norm of p-Truncation Operator
(important for error bounds)

Norm:

$$\|Pr(p)\| = \frac{\sup_{y \in \Omega} |Pr(p)[\Phi(y)]|}{\sup_{y \in \Omega} \|\Phi(y)\|}.$$ 

Triangle inequality:

$$\|I\| - \|I - Pr(p)\| \leq \|Pr(p)\| \leq \|I\| + \|I - Pr(p)\| = 1 + \|I - Pr(p)\|$$

$$\forall \epsilon > 0, \ \exists p, \ \|I - Pr(p)\| < \epsilon,$$

so

$$\forall \epsilon > 0, \ \exists p, \ 1 - \epsilon < \|Pr(p)\| < 1 + \epsilon,$$
p-Truncated Operator

Let $H : F(\Omega) \to F(\Omega)$ be an operator, that is represented by infinite matrix

$$H = \begin{pmatrix}
    h_{00} & h_{01} & \ldots & h_{0,p-1} & h_{0p} & \ldots \\
    h_{10} & h_{11} & \ldots & h_{1,p-1} & h_{1p} & \ldots \\
    \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\
    h_{p-1,0} & h_{p-1,1} & \ldots & h_{p-1,p-1} & h_{p-1,p} & \ldots \\
    h_{p0} & h_{p1} & \ldots & h_{p-1,p} & h_{pp} & \ldots \\
    \vdots & \vdots & \ddots & \vdots & \vdots & \ddots
\end{pmatrix}.$$ 

We call operator $H^{(p)} : F(\Omega) \to F(\Omega)$, $p$-truncated if it is represented by matrix

$$H^{(p)} = \begin{pmatrix}
    h_{00} & h_{01} & \ldots & h_{0,p-1} & 0 & \ldots \\
    h_{10} & h_{11} & \ldots & h_{1,p-1} & 0 & \ldots \\
    \vdots & \vdots & \ddots & \vdots & \vdots & \ddots \\
    h_{p-1,0} & h_{p-1,1} & \ldots & h_{p-1,p-1} & 0 & \ldots \\
    0 & 0 & \ldots & 0 & 0 & \ldots \\
    \vdots & \vdots & \ddots & \vdots & \vdots & \ddots
\end{pmatrix}.$$
Norm of $p$-Truncated Operator
(important for error bounds)

**Theorem:** Let $H : F(\Omega) \to F(\Omega)$, such that $0 < \|H\| < \infty$, and $H^{(p)} : F(\Omega) \to F(\Omega)$ is the $p$-truncated operator $H$. Let also $p(\varepsilon)$ be such that $1 - \varepsilon < \|Pr(p)\| < 1 + \varepsilon$. Then

$$(1 - \varepsilon)^2 < \|Pr(p)\| \leq \frac{\|H^{(p)}\|}{\|H\|} = \|Pr(p)\|^2 < (1 + \varepsilon)^2,$$

$$\lim_{p \to \infty} \frac{\|H^{(p)}\|}{\|H\|} = 1.$$ 

**Proof.**
A $p$-truncated operator can be represented in the form

$$H^{(p)} = Pr(p)HPr(p)$$

(check!)
So the norm of $H^{(p)}$ is

$$\|H^{(p)}\| = \|Pr(p)\|\|H\||\|Pr(p)\| = \|H\|\|Pr(p)\|^2.$$ 

End of Proof.
Translation Operator

Operator $T(t) : F(\Omega) \to F(\Omega')$, $\Omega' \subset \mathbb{R}^d$, $\Omega \subset \mathbb{R}^d$ is called translation operator corresponding to translation vector $t$, if

$$T(t)[\Phi(y)] = \Phi(y + t), \quad (y \in \Omega, \quad y + t \in \Omega').$$
Example of Translation Operator

\[ \Phi(y+t) \Rightarrow \mathcal{T}(t) \Rightarrow \Phi(y) \]
$R|R$-reexpansion

Let $y - x_* \in \Omega_r(x_*) \subset \mathbb{R}^d$, $\Omega_r(x_*) : |y - x_*| < r$, and $\{R_{r}(y - x_*)\}$ be a regular basis in $C(\Omega)$. Let $y - x_* + t \in \Omega_r(x_*)$ and

$$R_{r}(y - x_* + t) = \sum_{l=0}^{\infty} (R|R)_{r}^{l}(t)R_{l}(y - x_*).$$

Coefficients $(R|R)_{r}^{l}(t)$ are called $R|R$ – reexpansion coefficients (regular-to-regular),
and infinite matrix

$$(R|R)(t) = \begin{pmatrix}
(R|R)_{00} & (R|R)_{01} & \ldots \\
(R|R)_{10} & (R|R)_{11} & \ldots \\
& \ldots & \ldots & \ldots
\end{pmatrix}$$

is called $R|R$ – reexpansion matrix.
Example of R|R-reexpansion

\[ R_m(x) = x^m, \]
\[ R_m(x + t) = (x + t)^m = x^m + \binom{m}{1}x^{m-1}t + \ldots + \binom{m}{m-1}xt^{m-1} + t^m \]
\[ = \sum_{l=0}^{m} \binom{m}{l}t^lx^{m-l} = \sum_{l=0}^{m} \binom{m}{l}t^{m-l}x^l = \sum_{l=0}^{m} \binom{m}{l}t^{m-l}R_l(x), \]
\[ (R|R)_{l,m} (t) = \begin{cases} \binom{m}{l}t^{m-l}, & l \leq m, \\ 0, & l > m. \end{cases} \]
R|R-translation operator

Translation operator $T(t)$ which is represented in regular basis $\{R_n(y - x_*)\}$ by the $R|R$ – reexpansion matrix is called $R|R$-translation operator.

$$T(t)[\Phi(y)] = \Phi(y + t)$$

$$(R|R)(t) = T(t).$$
Why the same operator named differently?

\[ \mathcal{I}(t)[\Phi(y)] = \Phi(y + t) \]

The first letter shows the basis for \( \Phi(y) \)

\[ \mathcal{I}(t) = \begin{cases} 
\mathcal{R}|\mathcal{R})(t) \\
\mathcal{S}|\mathcal{S})(t) \\
\mathcal{S}|\mathcal{R})(t) \\
\mathcal{R}|\mathcal{S})(t) 
\end{cases} \]

The second letter shows the basis for \( \Phi(y + t) \)

Needed only to show the expansion basis (for operator representation)
Matrix representation of $R|R$-translation operator

Consider

$$
\Phi(y) = \sum_{n=0}^{\infty} A_n(x_*) R_n(y - x_*) .
$$

$$
\Phi(y + t) = (R|R)(t)[\Phi(y)] = \sum_{n=0}^{\infty} A_n(x_*) (R|R)(t)[R_n(y - x_*)] .
$$

$$
= \sum_{n=0}^{\infty} A_n(x_*) R_{2n}(y - x_* + t) .
$$

$$
= \sum_{n=0}^{\infty} A_n(x_*) \sum_{l=0}^{\infty} (R|R)_{ln}(t) R_l(y - x_*) .
$$

$$
= \sum_{l=0}^{\infty} \left[ \sum_{n=0}^{\infty} (R|R)_{ln}(t) A_n(x_*) \right] R_l(y - x_*) .
$$

$$
= \sum_{l=0}^{\infty} \tilde{A}_l(x_*, t) R_l(y - x_*) ,
$$

$$
\tilde{A}_l(x_*, t) = \sum_{n=0}^{\infty} (R|R)_{ln}(t) A_n(x_*) , \quad \tilde{A}(x_*, t) = (R|R)(t) A(x_*) .
$$
Reexpansion of the same function over shifted basis

Compact notation:

\[ \Phi(y) = \sum_{n=0}^{\infty} A_n(x_*) R_n(y - x_*) = A(x_*) \circ R(y - x_*), \]

\[ \Phi(y + t) = \sum_{l=0}^{\infty} \tilde{A}_l(x_*, t) R_l(y - x_*) = \tilde{A}(x_*, t) \circ R(y - x_*), \]

We have:

\[ \Phi(y) = \Phi((y - t) + t) = \tilde{A}(x_*, t) \circ R((y - t) - x_*) \]

\[ = \tilde{A}(x_*, t) \circ R(y - x_* - t). \]

Also

\[ \Phi(y) = A(x_*) \circ R(y - x_*) = A(x_* + t) \circ R(y - x_* - t), \]

so

\[ A(x_* + t) = \tilde{A}(x_*, t) = (R \circ R)(t) A(x_*). \]
R|R-reexpansion of the same function over shifted basis (2)

Since $\Omega_{r_1}(x_*+t) \subset \Omega_r(t)\!$!
Example of power series reexpansion

\[ R_{\eta\eta}(x) = x^{\eta\eta} \]

\[ \Phi(y \cdot x_i) = \sum_{\eta\eta=0}^{\infty} A_{m}(x_{*1}, x_{i}) R_{m}(y - x_{*1}) = \sum_{\eta\eta=0}^{\infty} A_{m}(x_{*2}, x_{i}) R_{m}(y - x_{*2}) \]

\[ A(x_{*2}, x_{i}) = (R|R)(x_{*2} - x_{*1}) \cdot A(x_{*1}, x_{i}) \cdot \]

\[
\begin{pmatrix}
A_0(x_{*2}, x_{i}) \\
A_1(x_{*2}, x_{i}) \\
A_2(x_{*2}, x_{i}) \\
\vdots
\end{pmatrix}
= 
\begin{pmatrix}
1 & \begin{pmatrix} 1 \\
0 \end{pmatrix} (x_{*2} - x_{*1}) & \begin{pmatrix} 2 \\
0 \end{pmatrix} (x_{*2} - x_{*1})^2 & \cdots \\
0 & 1 & \begin{pmatrix} 2 \\
1 \end{pmatrix} (x_{*2} - x_{*1}) & \cdots \\
0 & 0 & 1 & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\begin{pmatrix}
A_0(x_{*1}, x_{i}) \\
A_1(x_{*1}, x_{i}) \\
A_2(x_{*1}, x_{i}) \\
\vdots
\end{pmatrix}
\]
Let \( y - x_* \in \Omega_r(x_*) \subseteq \mathbb{R}^d \), \( \Omega_r(x_*) : |y - x_*| > r \), and \( \{S_n(y - x_*)\} \) be a singular basis in \( C(\Omega) \). Let \( y - x_* + t \in \Omega_r(x_*) \) and

\[
S_n(y - x_* + t) = \sum_{l=0}^{\infty} (S|S)_{ln}(t) S_l(y - x_*).
\]

Coefficients \( (S|S)_{ln}(t) \) are called \( S|S - \text{reexpansion coefficients} \) (singular-to-singular), and infinite matrix

\[
(S|S)(t) = \begin{pmatrix}
(S|S)_{00} & (S|S)_{01} & \cdots \\
(S|S)_{10} & (S|S)_{11} & \cdots \\
\vdots & \vdots & \ddots \\
\end{pmatrix}
\]

is called \( S|S - \text{reexpansion matrix} \).
S|S-translation operator

Translation operator $\mathcal{T}(t)$ which is represented in singular basis $\{S_n(y - x_*)\}$ by the $S|S − \text{reexpansion matrix}$ is called $S|S$-translation operator.

$$\mathcal{T}(t)[\Phi(y)] = \Phi(y + t)$$

$$(S|S)(t) = \mathcal{T}(t).$$
S|S and R|R-translation operators are very similar,

(actually, this is just two representations of the same translation operator in different domains and bases)

\[ \Phi(y) = B(x_*) \circ S(y - x_*), \]
\[ \Phi(y + t) = \tilde{B}(x_*, t) \circ S(y - x_*) \]
\[ \Phi(y) = \tilde{B}(x_*, t) \circ S(y - x_* - t). \]
\[ \tilde{B}(x_*, t) = (S|S)(t)B(x_*) = B(x_* + t). \]
But picture is different...

Original expansion
Is valid only here!

\[ |y - x_\ast - t| > r_1 = r + |t| \]

Since
\[ \Omega_{r_1}(x_\ast + t) \subset \Omega_r(t) \]

Also
\[ |x_i - x_\ast| < r \]

singular point!
$S|\mathbf{R}$-reexpansion

Let $\mathbf{y} - \mathbf{x}_* \in \Omega_r(\mathbf{x}_*) \subset \mathbb{R}^d$, $\Omega_r(\mathbf{x}_*) : |\mathbf{y} - \mathbf{x}_*| < r$, and $\{R_n(\mathbf{y} - \mathbf{x}_*)\}$ be a regular basis in $C(\Omega_r(\mathbf{x}_*))$. Let also $\Omega_{r1}(\mathbf{x}_* - \mathbf{t}) : |\mathbf{y} - \mathbf{x}_* + \mathbf{t}| > R > r$, and $\{S_n(\mathbf{y} - \mathbf{x}_* + \mathbf{t})\}$ be a singular basis in $C(\Omega_{r1}(\mathbf{x}_*))$, then

$$S_n(\mathbf{y} - \mathbf{x}_* + \mathbf{t}) = \sum_{i=0}^{\infty} (S|R)_{in}(\mathbf{t})R_i(\mathbf{y} - \mathbf{x}_*).$$

Coefficients $(S|R)_{in}(\mathbf{t})$ are called $S|R$ – reexpansion coefficients (singular-to-regular), and infinite matrix

$$\begin{pmatrix}
(S|R)_{00} & (S|R)_{01} & \cdots \\
(S|R)_{10} & (S|R)_{11} & \cdots \\
\vdots & \vdots & \ddots
\end{pmatrix}$$

is called $S|R$ – reexpansion matrix.
Does R|S reexpansion exist?

- Theoretically yes (in some cases, e.g. analytical continuation);
- In practice, since the domain of S-expansion is larger than the domain of R-expansion, this either not useful (due to error bounds), or can be avoided in algorithms;
- We will not use R|S-reexpansions in the FMM algorithms.
Translation operator $T(t)$ which is represented in singular basis by the $S|R$ - reexpansion matrix is called $S|R$-translation operator if the basis of expansion is changed with the translation operation from singular $\{S_n(y - x_*)\}$ to regular $\{R_n(y - x_* + t)\}$

$$T(t)[\Phi(y)] = \Phi(y + t)$$

$$(S|R)(t) = T(t).$$
S|R-operator has almost the same properties as S|S and R|R

\[(t \text{ cannot be zero)}\]

\[
\Phi(y) = B(x_*) \circ S(y - x_*) ,
\]

\[
\Phi(y + t) = \tilde{A}(x_*, t) \circ R(y - x_*)
\]

\[
\Phi(y) = \tilde{A}(x_*, t) \circ R(y - x_* - t).
\]

\[
\tilde{A}(x_*, t) = (S|R)(t)B(x_*) .
\]
Since $\Omega_{r_1}(x_*+t) \subset \Omega_r(t)$!

Original expansion Is valid only here!

Also

$$|y - x_* - t| < r_1 = |t| - r$$

Also

$$|x_i - x_*| < r$$

singular point!
Properties of the translation operator

\[ T(t)[\Phi(y)] = \Phi(y + t) \]

- **T(0) = I (identity operator).** Proof:
  \[ T(0)[\Phi(y)] = \Phi(y). \]

- **T(t_1 + t_2) = T(t_1) \circ T(t_2) = T(t_2) \circ T(t_1).** Proof:
  \[ T(t_1) \circ T(t_2)[\Phi(y)] = \Phi(y + t_2 + t_1) = T(t_2 + t_1)[\Phi(y)] = T(t_1 + t_2)[\Phi(y)]. \]

- **(corollary 1): T^{-1}(t) = T(-t).** Proof:
  \[ I = T(0) = T(t - t) = T(t) \circ T(-t). \]

- **(corollary 2): T^n(t) = T(nt).** Proof (use induction):
  \[ T(nt) = T((n - 1)t) \circ T(t) = T^{n-1}(t) \circ T(t) = T^n(t). \]
Spectrum of the translation operator

**eigen value** \( \Psi(y) \)

**eigen function** \( T(t)[\Psi(y)] = \lambda \Psi(y), \quad y \in \mathbb{R}^d. \)

Any function of type

\[ \forall a \in \mathbb{R}^d, \quad \Psi(y) = e^{ay}, \quad \lambda = e^{at}. \]

Check:

\[ T(t)[\Psi(y)] = \Psi(y + t) = e^{a(y + t)} = e^{at}e^{ay} = \lambda \Psi(y). \]

Relation to differential operator:

\[ \frac{d \Phi(y)}{ds} = \lim_{|t| \to 0} \frac{\Phi(y + t) - \Phi(y)}{|t|} = \lim_{|t| \to 0} \frac{T(t)[\Phi(y)] - \Phi(y)}{|t|} = \lim_{|t| \to 0} \frac{T(t) - T}{|t|} [\Phi(y)], \quad s = \frac{t}{|t|}. \]

derivative in direction \( s \)
Outline

• Norm of the translation operator
• Example of S|R-translation
• Summary of requirements for functions (potentials) that can be used in FMM
• Idea of a Single Level FMM (SLFMM)
• Space division and expansion domains
• SLFMM algorithm
• Asymptotic complexity of SLFMM
• Optimization of SLFMM
Example from previous lectures

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

\(|y - x_*| < |x_i - x_*| : \]

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

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

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

\(|y - x_*| > |x_i - x_*| : \]

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

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

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

\[ |y - x_* | < |t| \]

\[
S_n(y - x_* + t) = (t + y)^{-n-1} = \sum_{m=0}^{\infty} \frac{1}{m!} \frac{d^m S_n(t)}{dt^m} (y-x_*)^m
\]

\[
= \sum_{m=0}^{\infty} \frac{1}{m!} \frac{d^m S_n(t)}{dt^m} R_m(y-x_*) = \sum_{m=0}^{\infty} (S|R)_{mn}(t) R_m(y-x_*)
\]

So

\[
(S|R)_{mn}(t) = \frac{1}{m!} \frac{d^m S_n(t)}{dt^m} = \frac{(-1)^m (m+n)!}{m! n! t^{n+m+1}}
\]

\[
(S|R)(t) = \begin{pmatrix}
\frac{1}{t} & \frac{1}{t^2} & \frac{1}{t^3} & \cdots \\
-t^2 & -2t^3 & -3t^4 & \cdots \\
t^3 & 3t^4 & 6t^5 & \cdots \\
\vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\]
Norm of the Translation Operator

**Theorem.** Let $F(\Omega)$ be a set of functions bounded in $\mathbb{R}^d$. Then $\|T(t)\| = 1$.

**Proof.**

$$\|T(t)\| = \frac{\|T(t)\Phi(y)\|}{\Phi(y)} = \frac{\|\Phi(y + t)\|}{\Phi(y)} = \frac{\sup_{y \in \mathbb{R}^d} |\Phi(y + t)|}{\sup_{y \in \mathbb{R}^d} |\Phi(y)|} = 1.$$
Active and Passive points of view on translation operator

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Norms of $R|R$, $S|S$, and $S|R$-operators (1)

\[ \Phi(y) \]

\[ \Omega \]

\[ \Omega' \]

\[ \Phi(y) \]

\[ x_i \]

\[ t \]

\[ y \]

\[ \| \Phi(y) \|_{\Omega'} = \sup_{y \in \Omega'} |\Phi(y)| < \sup_{y \in \Omega} |\Phi(y)| = \| \Phi(y) \|_{\Omega} \]

\( \Phi(y) \) is bounded in \( \Omega \).
\( \Omega' \subset \Omega \).

Therefore \( \Phi(y) \) is bounded in \( \Omega' \), and
Norms of $R|R$, $S|S$, and $S|R$-operators (2)

From the passive point of view, the translation operator does nothing, but just changes the reference frame. So if we consider that $R|R$, $S|S$, and $S|R$ do just change of the reference frame PLUS they shrink the domain, where the function is bounded, then their norms do not exceed 1.

\[
\Omega' \subset \Omega
\]

\[
\| (R|R)(t) \| = \frac{\sup_{y \in \Omega'} |\Phi(y)|}{\sup_{y \in \Omega} |\Phi(y)|} \leq 1,
\]

\[
\| (S|S)(t) \| = \frac{\sup_{y \in \Omega'} |\Phi(y)|}{\sup_{y \in \Omega} |\Phi(y)|} \leq 1,
\]

\[
\| (S|R)(t) \| = \frac{\sup_{y \in \Omega'} |\Phi(y)|}{\sup_{y \in \Omega} |\Phi(y)|} \leq 1.
\]

This is the difference between general translation operator and $R|R$, $S|S$, and $S|R$ operators.
Error of exact $R|R$, $S|S$, and $S|R$-translation

If

$$\|\Phi(y) - \Phi^p(y)\| < \epsilon,$$

then

$$\|(R|R)(t)(\Phi(y) - \Phi^p(y))\| = \|(R|R)(t)\|\|\Phi(y) - \Phi^p(y)\| < \epsilon,$$

$$\|(S|S)(t)(\Phi(y) - \Phi^p(y))\| = \|(S|S)(t)\|\|\Phi(y) - \Phi^p(y)\| < \epsilon,$$

$$\|(S|R)(t)(\Phi(y) - \Phi^p(y))\| = \|(S|R)(t)\|\|\Phi(y) - \Phi^p(y)\| < \epsilon.$$
Four Key Stones of FMM

- Factorization
- Error
- Translation
- Grouping
Summary of formal requirements for functions that can be used in FMM

We have two sets of points:

\[ X = \{x_1, x_2, \ldots, x_N\}, \quad x_i \in \mathbb{R}^d, \quad i = 1, \ldots, N, \]
\[ Y = \{y_1, y_2, \ldots, y_M\}, \quad y_j \in \mathbb{R}^d, \quad j = 1, \ldots, M. \]

We have functions (potentials):

\[ \Phi(x_i, y) : \mathbb{R}^d \to \mathbb{R}, \quad y \in \mathbb{R}^d, \quad i = 1, \ldots, N. \]

These functions can be factorized as (local expansion):

\[ \Phi(x_i, y) = A(x_i, x_*) \circ R(y - x_*), \quad |y - x_*| < r < |x_i - x_*|, \quad i = 1, \ldots, N \]

These functions can be factorized as (far field expansion):

\[ \Phi(x_i, y) = B(x_i, x_*) \circ S(x - x_*), \quad |y - x_*| > R > |x_i - x_*|, \quad i = 1, \ldots, N \]

The product is distributive operation with respect to addition

\[ (u_1 A_1 + u_2 A_2) \circ F = u_1 A_1 \circ F + u_2 A_2 \circ F, \quad F = S, R \]
Summary of formal requirements for functions that can be used in FMM (2)

- R-expansion coefficients can be $R|R$-translated:
  \[ |x - x_{*2}| < |x_i - x_{*1}| - |x_{*1} - x_{*2}| : \]
  \[ A(x_i, x_{*2}) = (R|R)(x_{*2} - x_{*1})A(x_i, x_{*1}) \]

- S-expansion coefficients can be $S|S$-translated:
  \[ |x - x_{*2}| > |x_{*1} - x_{*2}| + |x_i - x_{*1}|, \]
  \[ B(x_i, x_{*2}) = (S|S)(x_{*2} - x_{*1})B(x_i, x_{*1}) \]

- S-expansion coefficients can be $S|R$-translated (converted to $R$-expansion coefficients)
  \[ |x - x_{*2}| < |x_{*1} - x_{*2}| + |x_i - x_{*1}|, \]
  \[ A(x_i, x_{*2}) = (S|R)(x_{*2} - x_{*1})B(x_i, x_{*1}) \]

- And we are looking for sums:
  \[ v_j = \sum_{i=1}^{N} u_i \Phi(y_j, x_i), \quad j = 1, \ldots, M. \]

- Some generalization are possible, say instead of $\Phi(y_j, x_i)$ we can consider $\Phi_i(y_j)$, etc.
Middleman Algorithm

Standard algorithm

Middleman algorithm

Sources

Evaluation Points

Sources

Evaluation Points

Total number of operations: $O(NM)$

Total number of operations: $O(N+M)$
Idea of a Single Level FMM

Standard algorithm

Sources

Evaluation Points

Total number of operations: $O(NM)$

SLFMM

Sources $L$ groups

Points

Kh groups

Total number of operations: $O(N+M+KL)$
Spatial Domains

Potentials due to sources in these spatial domains

\[ \Phi_1^{(n)}(y) \]

\[ \Phi_2^{(n)}(y) \]

\[ \Phi_3^{(n)}(y) \]

\[ I_1(n) = n \]

\[ I_2(n) = \{ \text{Neighbors}(n) \} \cup n \]

\[ I_3(n) = \{ \text{All boxes} \} \setminus I_2(n) \]

Boxes with these numbers belong to these spatial domains
Definition of potentials

\[
\Phi_1^{(n)}(y) = \sum_{x_i \in E_1(n)} u_i \Phi(y, x_i),
\]

\[
\Phi_2^{(n)}(y) = \sum_{x_i \in E_2(n)} u_i \Phi(y, x_i),
\]

\[
\Phi_3^{(n)}(y) = \sum_{x_i \in E_3(n)} u_i \Phi(y, x_i),
\]

Since domains \(E_2(n)\) and \(E_3(n)\) are complimentary:

\[
\Phi(y) = \sum_{i=1}^{N} u_i \Phi(y, x_i) = \sum_{x_i \in E_2(n) \cup E_3(n)} u_i \Phi(y, x_i) = \Phi_2^{(n)}(y) + \Phi_3^{(n)}(y)
\]

for arbitrary \(n\).
SLFMM Algorithm

Step 1. Generate S-expansion coefficients for each box

For $n \in \text{NonEmptySource}$

Get $x_c^{(n)}$, the center of the box;

$C^{(n)} = 0$;

For $x_i \in E_1(n)$

Get $B(x_i, x_c^{(n)})$, the S-expansion coefficients near the center of the box;

$C^{(n)} = C^{(n)} + u_i B(x_i, x_c^{(n)})$;

End;

End;

Implementation can be different!
All we need is to get $C^{(n)}$. 

\[
\Phi_1^{(n)}(x) = C^{(n)} \circ S(x - x_c^{(n)}),
\]

\[
C^{(n)} = \sum_{x_i \in E_1(n)} u_i B(x_i, x_c^{(n)}).
\]
SLFMM Algorithm

Step 2. (S|R)-translate expansion coefficients

\[ \Phi_3^{(n)}(y) = D^{(n)} \circ R(y - x_c^{(n)}) , \]
\[ D^{(n)} = \sum_{m \in I_3(n)} (S|R)(x_c^{(n)} - x_c^{(m)}) C^{(m)} . \]

For \( n \in \text{NonEmptyEvaluation} \)

Get \( x_c^{(n)} \), the center of the box;
\( D^{(n)} = 0 ; \)

For \( m \in I_3(n) \)

Get \( x_c^{(m)} \), the center of the box;
\[ D^{(n)} = D^{(n)} + (S|R)(x_c^{(n)} - x_c^{(m)}) C^{(m)} ; \]

End;

Implementation can be different!
All we need is to get \( D^{(n)} \).
S|R-translation
SLFMM Algorithm

Step 3. Final Summation

\[ v_j = \Phi(y_j) = \sum_{x_i \in E_2(n)} \Phi(y_j, x_i) + D^{(n)} \circ R(y_j - x_c^{(n)}), \quad y_j \in E_1(n). \]

For \( n \in \text{NonEmptyEvaluation} \)

Get \( x_c^{(n)} \), the center of the box;

For \( y_j \in E_1(n) \)

\[ v_j = D^{(n)} \circ R(y_j - x_c^{(n)}); \]

For \( x_i \in E_2(n) \)

\[ v_j = v_j + \Phi(y_j, x_i); \]

End;

End;

End;

Implementation can be different!
All we need is to get \( v_j \).
Asymptotic Complexity of SLFMM

Assume that:

- By some magic we can easily find neighbors, and lists of points in each box.
- Translation is performed by straightforward $P \times P$ matrix-vector multiplication, where $P(p)$ is the total length of the translation vector. So the complexity of a single translation is $O(P^2)$.
- The source and evaluation points are distributed uniformly, and there are $K$ boxes, with $s$ source points in each box ($s=N/K$). We call $s$ the grouping (or clustering) parameter.
- The number of neighbors for each box is $O(1)$. 
Then Complexity is:

- For Step 1: \( O(PN) \)
- For Step 2: \( O(P^2K^2) \)
- For Step 3: \( O(PM+Ms) \)
- Total: \( O(PN+ P^2K^2 +PM+Ms) = O(PN+ P^2K^2 +PM+MN/K) \)
Selection of Optimal $K$ (or $s$)

$$F(K) = PN + P^2K^2 + PM + PMN/K.$$ 

$$F'(K) = 2P^2K - PMN/K^2 = 0.$$ 

$$K_{opt} = \left( \frac{MN}{2P} \right)^{1/3} = O\left( \left( \frac{MN}{P} \right)^{1/3} \right).$$ 

$$s_{opt} = \frac{N}{K_{opt}} = \left( \frac{2PN^2}{M} \right)^{1/3} = O\left( \frac{PN^2}{M} \right)^{1/3}.$$
Complexity of Optimized SLFMM

\[ F(K_{opt}) = PN + P^2 \left( \frac{MN}{2P} \right)^{2/3} + PM + PMN \left( \frac{MN}{2P} \right)^{-1/3} \]

\[ = P(M + N) + (MN)^{2/3} O(P^{4/3}). \]

At \( K = K_{opt}, \) and \( M = O(N), \) the complexity of SLFMM is:

\[ O(PN + P^{4/3} N^{4/3}) = O(P^{4/3} N^{4/3}). \]
Example of Complexity:

\[ P = 10, \; N = 10^5 \]

Straightforward \( O(N^2) \): Complexity \( \sim 10^{10} \)
SLFMM \( O((PN)^{4/3}) \): Complexity \( \sim 10^8 \)

100 Times CPU savings!

\[ P = 10, \; N = 10^8 \]

Straightforward \( O(N^2) \): Complexity \( \sim 10^{16} \)
SLFMM \( O((PN)^{4/3}) \): Complexity \( \sim 10^{12} \)

100000 Times CPU savings!

Sorry, but my PC cannot solve such a problem!