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

$$\mathbf{a}, \mathbf{b}, \mathbf{c} \in \mathcal{U}$$

$$1). \quad \mathbf{a} + \mathbf{b} \in \mathcal{U};$$

$$2). \quad \mathbf{a} + \mathbf{b} = \mathbf{b} + \mathbf{a}, \mathbf{a} + (\mathbf{b} + \mathbf{c}) = (\mathbf{a} + \mathbf{b}) + \mathbf{c};$$

$$3). \quad \exists \mathbf{0}, \quad \mathbf{a} + \mathbf{0} = \mathbf{a}, \quad \mathbf{a} + (-\mathbf{a}) = \mathbf{a} - \mathbf{a} = \mathbf{0};$$

$$4). \quad \forall \alpha \in \mathbb{C}, \quad \alpha \mathbf{a} \in \mathcal{U};$$

$$5). \quad \forall \alpha, \beta \in \mathbb{C}, \quad (\alpha\beta)\mathbf{a} = \alpha(\beta)\mathbf{a}, \quad 1\mathbf{a} = \mathbf{a},$$

$$\alpha(\mathbf{a} + \mathbf{b}) = \alpha\mathbf{a} + \alpha\mathbf{b}, \quad (\alpha + \beta)\mathbf{a} = \alpha\mathbf{a} + \beta\mathbf{a}.$$

Linear Operators

Linear Spaces

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

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

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

Bases → $F_n \in \mathbb{F}(\Omega), \quad F'_n \in \mathbb{F}(\Omega'),$

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

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

Reexpansion Coefficients

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

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

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

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 continous functions with norm

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

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

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

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

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

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

$$\Phi^p(\mathbf{y}) = \sum_{n=0}^{p-1} A_n F_n(\mathbf{y}).$$

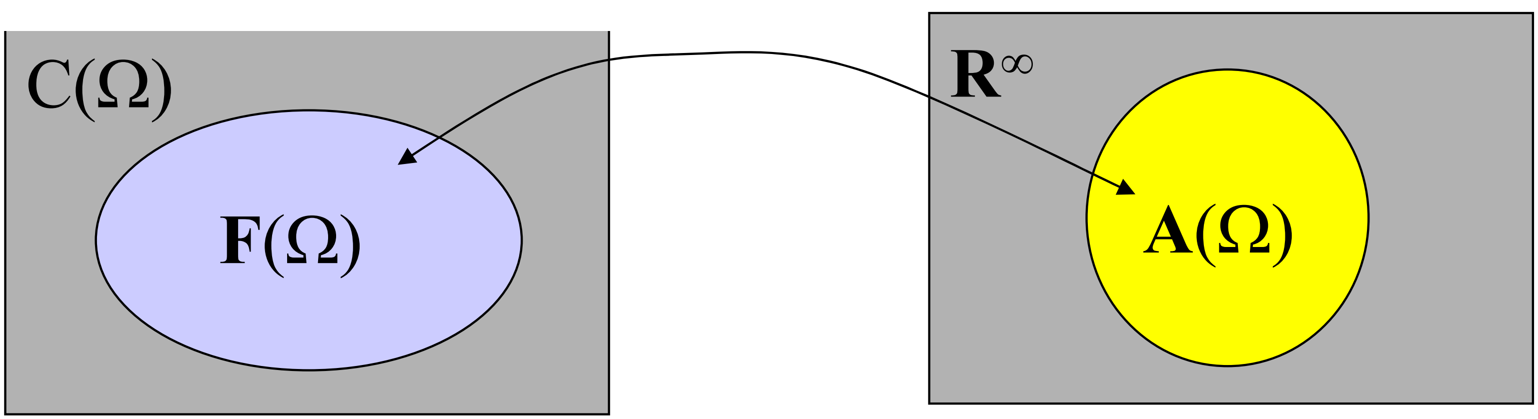
Function Representation in the Space of Coefficients (2)

Expansion coefficients can be stacked in an infinite vector

$$\mathbf{A} = \begin{pmatrix} A_0 \\ A_1 \\ \dots \\ A_n \\ \dots \end{pmatrix}.$$

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

$$\Phi(\mathbf{y}) \rightleftarrows \mathbf{A}, \quad \Phi(\mathbf{y}) \in \mathbb{F}(\boldsymbol{\Omega}), \quad \mathbf{A} \in \mathbb{A}(\boldsymbol{\Omega}) \subset \mathbb{R}^\infty.$$

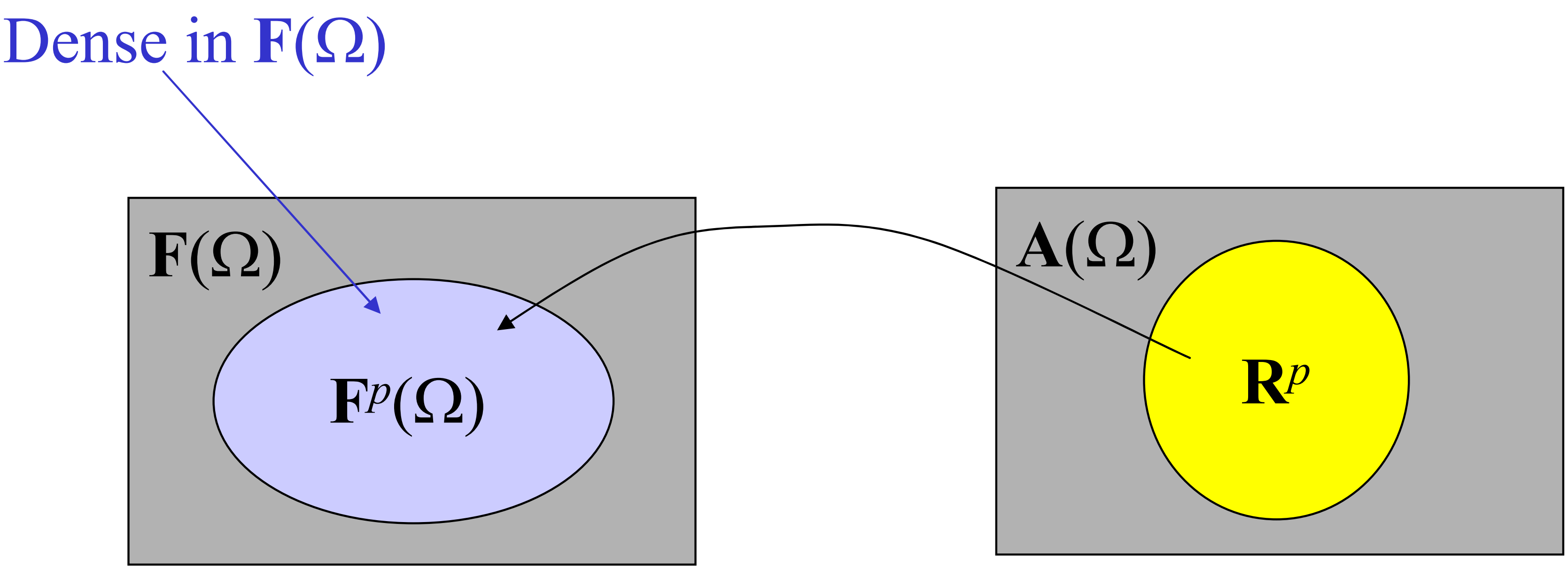


p-Truncated Vectors

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

$\mathbb{F}^p(\boldsymbol{\Omega})$ is dense in $\mathbb{F}(\boldsymbol{\Omega})$:

$$\forall \Phi(\mathbf{y}) \in \mathbb{F}(\boldsymbol{\Omega}), \quad \exists p, \Phi^p(\mathbf{y}) \in \mathbb{F}^p(\boldsymbol{\Omega}), \quad \|\Phi(\mathbf{y}) - \Phi^p(\mathbf{y})\| = \sup_{\mathbf{r} \in \Omega} |\Phi(\mathbf{y}) - \Phi^p(\mathbf{y})| < \epsilon.$$



Matrix Representation of Linear Operators

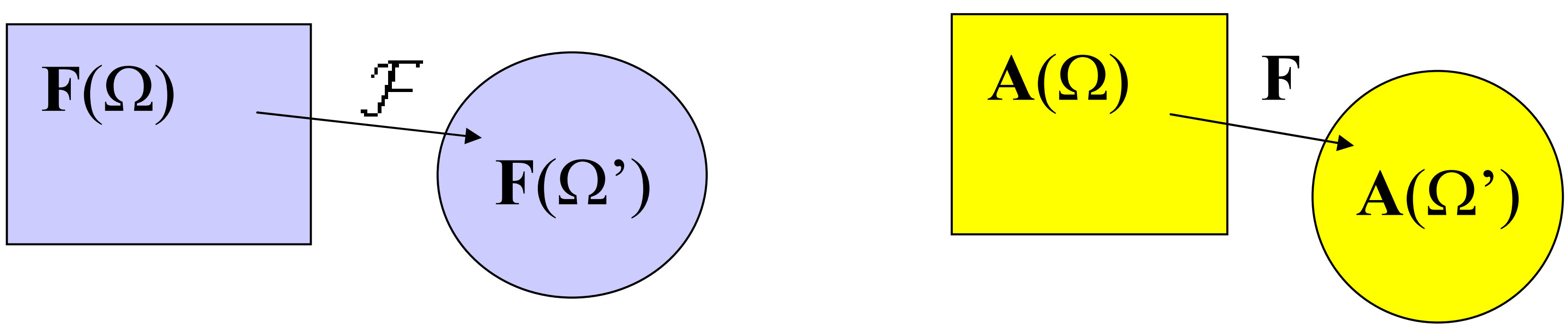
Let $\Omega' \subset \Omega$ and $\mathcal{F}$ is a mapping of $\mathbb{F}(\Omega)$ to $\mathbb{F}(\Omega')$. Such mapping can be considered as action of operator $\mathcal{F}$ on Φ :

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

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

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

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



Representation of a Linear Operator

p-Truncation (Projection) Operator

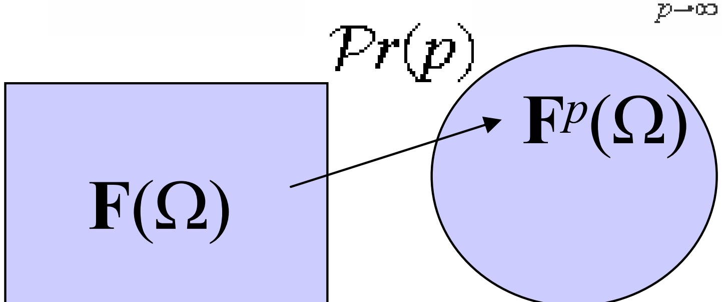
$$\mathbf{Pr}(p)\mathbf{A} = \widetilde{\mathbf{A}}, \quad \mathbf{A} \in \mathbb{A}(\boldsymbol{\Omega}), \quad \widetilde{\mathbf{A}} \in \mathbb{A}^p(\boldsymbol{\Omega}).$$

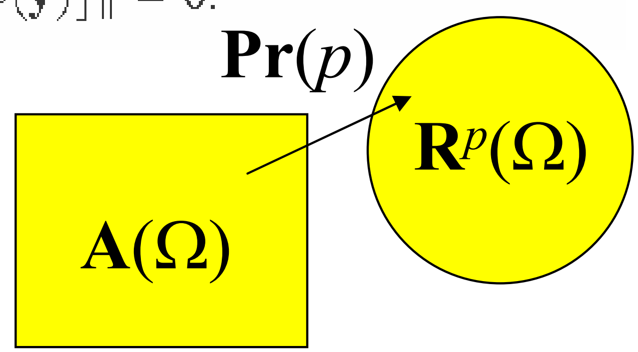
$$\mathbf{A} = \begin{pmatrix} A_0 \\ A_1 \\ \dots \\ A_{p-1} \\ A_p \\ A_{p+1} \\ \dots \end{pmatrix} \rightarrow \widetilde{\mathbf{A}} = \begin{pmatrix} A_0 \\ A_1 \\ \dots \\ A_{p-1} \\ 0 \\ 0 \\ \dots \end{pmatrix}, \qquad \widetilde{\mathbf{A}} = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 & 0 & \dots \\ 0 & 1 & \dots & 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 & 0 & 0 & \dots \\ 0 & 0 & \dots & 0 & 0 & 0 & \dots \\ 0 & 0 & \dots & 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \mathbf{A}$$

In space $\mathbb{F}(\boldsymbol{\Omega})$:

$$\mathcal{P}r(p)[\Phi(\mathbf{y})] = \Phi^p(\mathbf{y}), \quad \Phi(\mathbf{y}) \in \mathbb{F}(\boldsymbol{\Omega}), \quad \Phi^p(\mathbf{y}) \in \mathbb{F}^p(\boldsymbol{\Omega}),$$

$$\lim_{p \to \infty} \| \Phi(\mathbf{y}) - \mathcal{P}r(p)[\Phi(\mathbf{y})] \| = 0.$$





Norm of p-Truncation Operator (important for error bounds)

Norm:

$$\|\mathsf{P}r(p)\| = \frac{\sup_{\mathbf{y}\in\Omega}\|\mathsf{P}r(p)[\Phi(\mathbf{y})]\|}{\sup_{\mathbf{y}\in\Omega}\|\Phi(\mathbf{y})\|}.$$

Triangle unequality:

$$\|\mathbf{I}\| - \|\mathbf{I} - \mathsf{P}r(p)\| \leqslant \|\mathsf{P}r(p)\| \leqslant \|\mathbf{I}\| + \|\mathbf{I} - \mathsf{P}r(p)\| = 1 + \|\mathbf{I} - \mathsf{P}r(p)\|$$

$$\forall\epsilon > 0, \quad \exists p, \quad \|\mathbf{I} - \mathsf{P}r(p)\| < \epsilon,$$

so

$$\forall\epsilon > 0, \quad \exists p, \quad 1 - \epsilon < \|\mathsf{P}r(p)\| < 1 + \epsilon,$$

p-Truncated Operator

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

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

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

$$\mathrm{H}^{(p)} = \begin{pmatrix} h_{00} & h_{01} & \ldots & h_{0,p-1} & 0 & \ldots \\ h_{10} & h_{11} & \ldots & h_{1,p-1} & 0 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ h_{p-1,0} & h_{p-1,1} & \ldots & h_{p-1,p-1} & 0 & \ldots \\ 0 & 0 & \ldots & 0 & 0 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix}$$

Norm of p-Truncated Operator (important for error bounds)

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

$$(1-\epsilon)^2 < \|\mathsf{P}r(p)\|^2 = \frac{\|\mathsf{H}^{(p)}\|}{\|\mathsf{H}\|} = \|\mathsf{P}r(p)\|^2 < (1+\epsilon)^2,$$

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

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

$$\mathsf{H}^{(p)} = \mathsf{P}r(p)\mathsf{H}\mathsf{P}r(p)$$

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

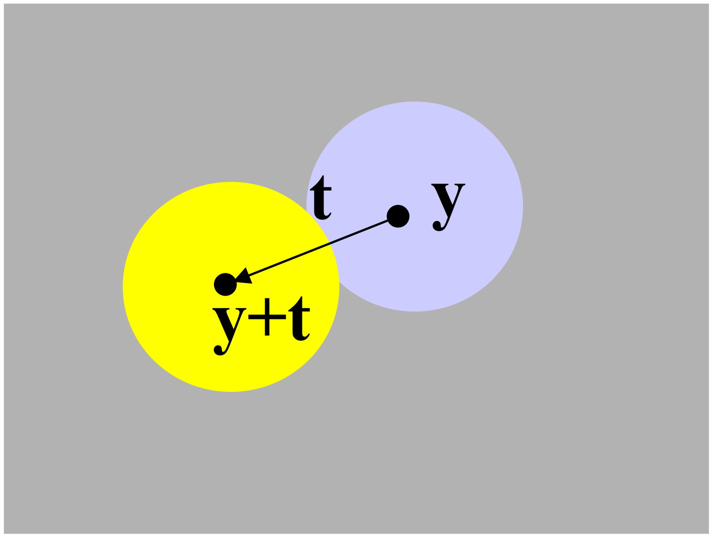
$$\|\mathsf{H}^{(p)}\| = \|\mathsf{P}r(p)\|\,\|\mathsf{H}\|\,\|\mathsf{P}r(p)\| = \|\mathsf{H}\|\,\|\mathsf{P}r(p)\|^2.$$

End of Proof.

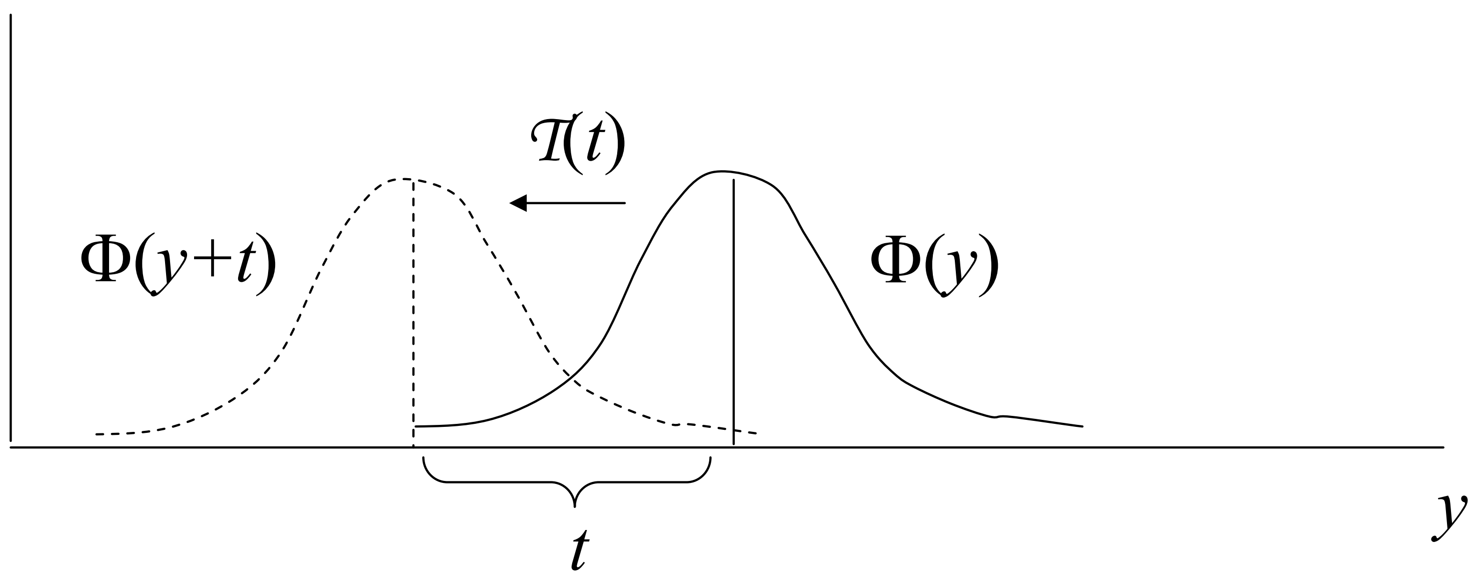
Translation Operator

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

$$\mathcal{T}(\mathbf{t})[\Phi(\mathbf{y})] = \Phi(\mathbf{y}+\mathbf{t}), \quad (\mathbf{y} \in \Omega, \quad \mathbf{y}+\mathbf{t} \in \Omega').$$



Example of Translation Operator



R|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 $C(\Omega)$. Let $\mathbf{y}-\mathbf{x}_*+\mathbf{t} \in \Omega_r(\mathbf{x}_*)$ and

$$R_n(\mathbf{y}-\mathbf{x}_*+\mathbf{t}) = \sum_{l=0}^{\infty}(R|R)_{ln}(\mathbf{t})R_l(\mathbf{y}-\mathbf{x}_*).$$

Coefficients $(R|R)_{ln}(\mathbf{t})$ are called $R|R-$ *reexpansion coefficients* (regular-to-regular) , and infinite matrix

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

is called $R|R-$ *reexpansion matrix*.

Example of R|R-reexpansion

$$R_m(x) = x^m,$$

$$R_m(x+t) = (x+t)^m = x^m + \begin{pmatrix} m \\ 1 \end{pmatrix} x^{m-1} t + \ldots + \begin{pmatrix} m \\ m-1 \end{pmatrix} x t^{m-1} + t^m$$

$$= \sum_{l=0}^{m} \begin{pmatrix} m \\ l \end{pmatrix} t^l x^{m-l} = \sum_{l=0}^{m} \begin{pmatrix} m \\ l \end{pmatrix} t^{m-l} x^l = \sum_{l=0}^{m} \begin{pmatrix} m \\ l \end{pmatrix} t^{m-l} R_l(x),$$

$$(R|R)_{lm}(t) = \begin{cases} \begin{pmatrix} m \\ l \end{pmatrix} t^{m-l}, & l \leqslant m, \\ 0, & l > m. \end{cases}$$

R|R-translation operator

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

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

$$(\mathcal{R}|\mathcal{R})(\mathbf{t}) = \mathcal{T}(\mathbf{t}).$$

Why the same operator named differently?

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

The first letter shows the basis for $\Phi(\mathbf{y})$

The second letter shows the basis for $\Phi(\mathbf{y}+\mathbf{t})$

$$\mathcal{T}(\mathbf{t}) = \begin{cases} (\mathcal{R}|\mathcal{R})(\mathbf{t}) \\ (\mathcal{S}|\mathcal{S})(\mathbf{t}) \\ (\mathcal{S}|\mathcal{R})(\mathbf{t}) \\ (\mathcal{R}|\mathcal{S})(\mathbf{t}) \end{cases}$$

Needed only to show the expansion basis (for operator representation)

Matrix representation of R|R-translation operator

Consider $\Phi(\mathbf{y}) = \sum_{n=0}^{\infty} A_n(\mathbf{x}_*) R_n(\mathbf{y} - \mathbf{x}_*)$.

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

$$= \sum_{n=0}^{\infty} A_n(\mathbf{x}_*) R_n(\mathbf{y} - \mathbf{x}_* + \mathbf{t})$$

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

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

$$= \sum_{l=0}^{\infty} \widetilde{A}_l(\mathbf{x}_*, \mathbf{t}) R_l(\mathbf{y} - \mathbf{x}_*),$$

Coefficients of shifted function

Coefficients of original function

$$\widetilde{A}_l(\mathbf{x}_*, \mathbf{t}) = \sum_{n=0}^{\infty} (R|R)_{ln}(\mathbf{t}) A_n(\mathbf{x}_*), \quad \widetilde{\mathbf{A}}(\mathbf{x}_*, \mathbf{t}) = (\mathbf{R}|\mathbf{R})(\mathbf{t}) \mathbf{A}(\mathbf{x}_*).$$

Reexpansion of the same function over shifted basis

Compact notation:

$$\Phi(\mathbf{y}) = \sum_{n=0}^{\infty} A_n(\mathbf{x}_*)R_n(\mathbf{y}-\mathbf{x}_*) = \mathbf{A}(\mathbf{x}_*) \circ \mathbf{R}(\mathbf{y}-\mathbf{x}_*),$$

$$\Phi(\mathbf{y}+\mathbf{t}) = \sum_{l=0}^{\infty} \widetilde{A}_l(\mathbf{x}_*,\mathbf{t})R_l(\mathbf{y}-\mathbf{x}_*) = \widetilde{\mathbf{A}}(\mathbf{x}_*,\mathbf{t}) \circ \mathbf{R}(\mathbf{y}-\mathbf{x}_*)$$

We have:

$$\Phi(\mathbf{y}) = \Phi((\mathbf{y}-\mathbf{t})+\mathbf{t}) = \widetilde{\mathbf{A}}(\mathbf{x}_*,\mathbf{t}) \circ \mathbf{R}((\mathbf{y}-\mathbf{t})-\mathbf{x}_*)$$
$$= \widetilde{\mathbf{A}}(\mathbf{x}_*,\mathbf{t}) \circ \mathbf{R}(\mathbf{y}-\mathbf{x}_*-\mathbf{t}).$$

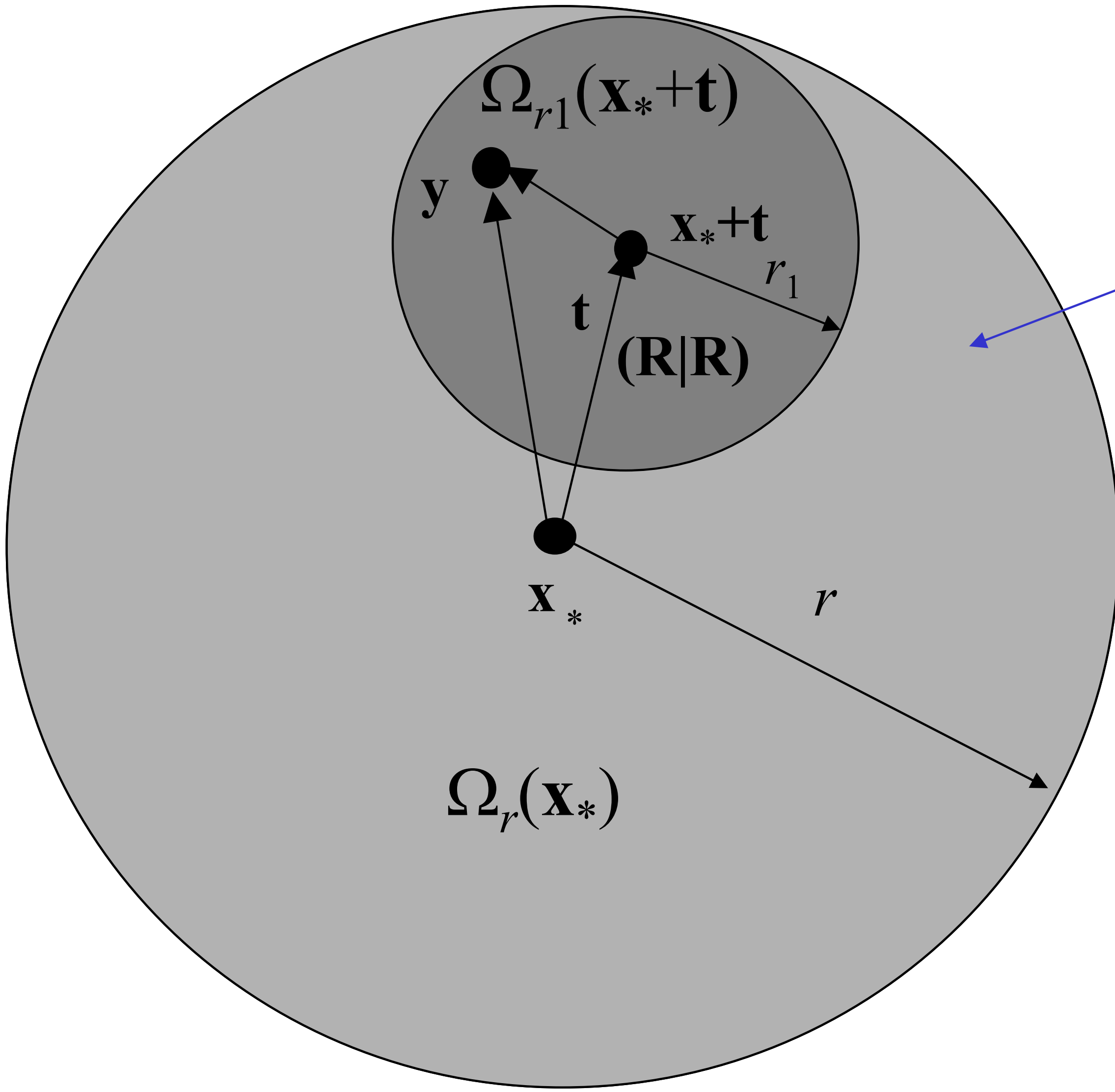
Also

$$\Phi(\mathbf{y}) = \mathbf{A}(\mathbf{x}_*) \circ \mathbf{R}(\mathbf{y}-\mathbf{x}_*) = \mathbf{A}(\mathbf{x}_*+\mathbf{t}) \circ \mathbf{R}(\mathbf{y}-\mathbf{x}_*-\mathbf{t}),$$

so

$$\mathbf{A}(\mathbf{x}_*+\mathbf{t}) = \widetilde{\mathbf{A}}(\mathbf{x}_*,\mathbf{t}) = (\mathbf{R}|\mathbf{R})(\mathbf{t})\mathbf{A}(\mathbf{x}_*).$$

R|R-reexpansion of the same function over shifted basis (2)



Original expansion Is valid only here!

$|\mathbf{y} - \mathbf{x}_* - \mathbf{t}| < r_1 = r - |\mathbf{t}|$

Since $\Omega_{r1}(\mathbf{x}_*+\mathbf{t}) \subset \Omega_r(\mathbf{t})$!

Example of power series reexpansion

$$R_m(x) = x^m$$

$$\Phi(y, x_i) = \sum_{m=0}^{\infty} A_m(x_{*1}, x_i) R_m(y - x_{*1}) = \sum_{m=0}^{\infty} A_m(x_{*2}, x_i) R_m(y - x_{*2}),$$

$$\mathbf{A}(x_{*2}, x_i) = (\mathbf{R}|\mathbf{R})(x_{*2} - x_{*1}) \bullet \mathbf{A}(x_{*1}, x_i).$$

$$\begin{pmatrix} A_0(x_{*2}, x_i) \\ A_1(x_{*2}, x_i) \\ A_2(x_{*2}, x_i) \\ \ldots \end{pmatrix} = \begin{pmatrix} 1 & \binom{1}{0}(x_{*2} - x_{*1}) & \binom{2}{0}(x_{*2} - x_{*1})^2 & \ldots \\ 0 & 1 & \binom{2}{1}(x_{*2} - x_{*1}) & \ldots \\ 0 & 0 & 1 & \ldots \\ \ldots & \ldots & \ldots & \ldots \end{pmatrix} \begin{pmatrix} A_0(x_{*1}, x_i) \\ A_1(x_{*1}, x_i) \\ A_2(x_{*1}, x_i) \\ \ldots \end{pmatrix}$$

S|S-reexpansion

Let $\mathbf{y}-\mathbf{x}_* \in \Omega_r(\mathbf{x}_*) \subset \mathbb{R}^d, \quad \Omega_r(\mathbf{x}_*) : |\mathbf{y}-\mathbf{x}_*| > r,$ and $\{S_n(\mathbf{y}-\mathbf{x}_*)\}$ be a singular basis in $C(\Omega)$. Let $\mathbf{y}-\mathbf{x}_*+\mathbf{t} \in \Omega_r(\mathbf{x}_*)$ and

$$S_n(\mathbf{y}-\mathbf{x}_*+\mathbf{t}) = \sum_{l=0}^{\infty}(S|S)_{ln}(\mathbf{t})S_l(\mathbf{y}-\mathbf{x}_*).$$

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

$$(\mathbf{S}|\mathbf{S})(\mathbf{t}) = \begin{pmatrix} (S|S)_{00} & (S|S)_{01} & \cdots \\ (S|S)_{10} & (S|S)_{11} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix}$$

is called $S|S-$ *reexpansion matrix*.

S|S-translation operator

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

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

$$(\mathcal{S}|\mathcal{S})(\mathbf{t}) = \mathcal{T}(\mathbf{t}).$$

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)

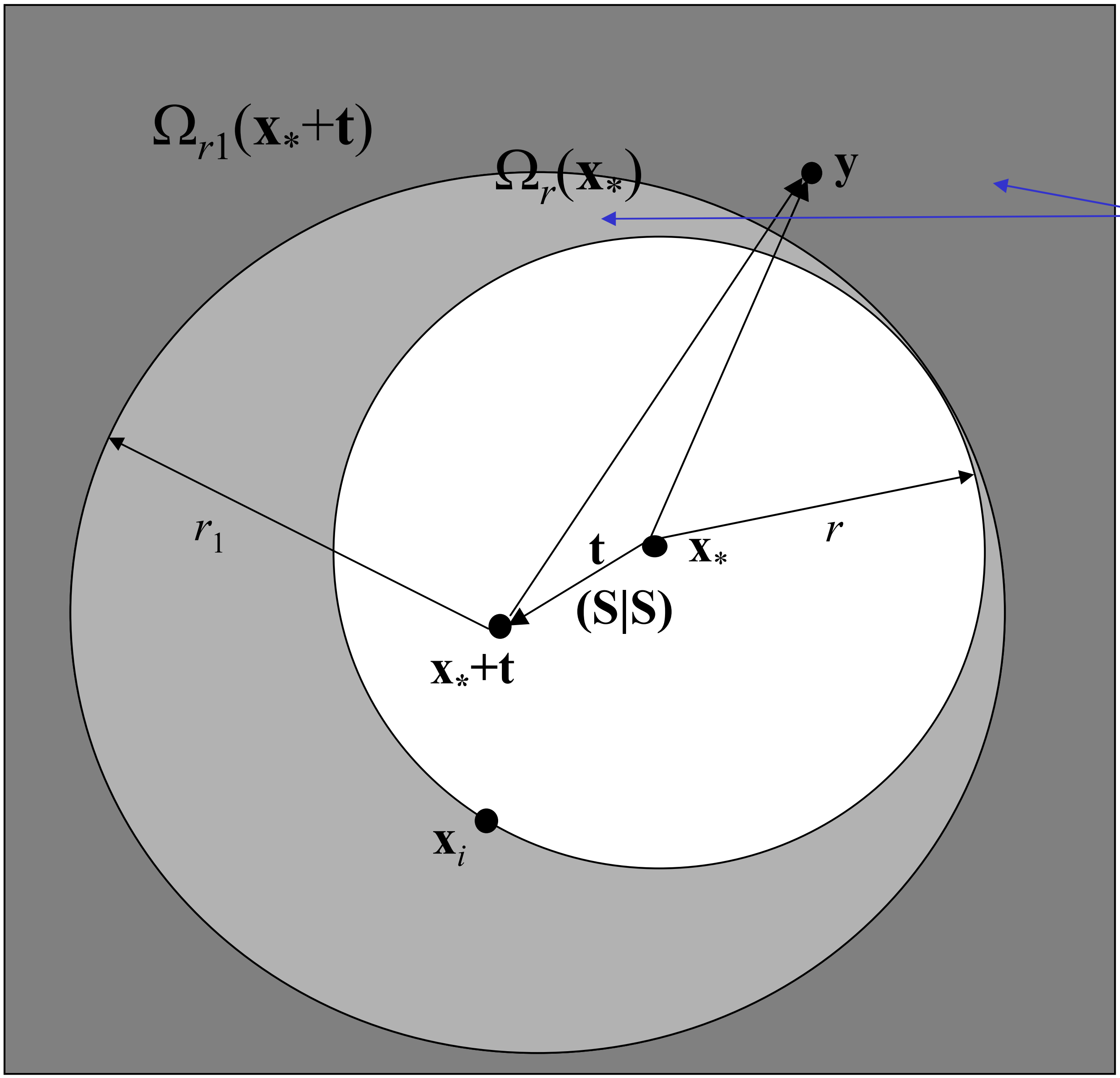
$$\Phi(\mathbf{y}) = \mathbf{B}(\mathbf{x}_*) \circ \mathbf{S}(\mathbf{y} - \mathbf{x}_*),$$

$$\Phi(\mathbf{y} + \mathbf{t}) = \widetilde{\mathbf{B}}(\mathbf{x}_*, \mathbf{t}) \circ \mathbf{S}(\mathbf{y} - \mathbf{x}_*)$$

$$\Phi(\mathbf{y}) = \widetilde{\mathbf{B}}(\mathbf{x}_*, \mathbf{t}) \circ \mathbf{S}(\mathbf{y} - \mathbf{x}_* - \mathbf{t}).$$

$$\widetilde{\mathbf{B}}(\mathbf{x}_*, \mathbf{t}) = (\mathbf{S}|\mathbf{S})(\mathbf{t})\mathbf{B}(\mathbf{x}_*) = \mathbf{B}(\mathbf{x}_* + \mathbf{t}).$$

But picture is different…



Original expansion
Is valid only here!

$|\mathbf{y} - \mathbf{x}_* - \mathbf{t}| > r_1 = r + |\mathbf{t}|$

Since
$\Omega_{r1}(\mathbf{x}_*+\mathbf{t}) \subset \Omega_r(\mathbf{t})$!

Also

$|\mathbf{x}_i - \mathbf{x}_*| < r$

singular point !

S|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 $C(\Omega_r(\mathbf{x}_*))$, then

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

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

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

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
then 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.

S|R-translation operator

Translation operator $\mathcal{T}(\mathbf{t})$ which is represented in singular basis by the $S|R-$ *reexpansion matrix* is called $\mathcal{S}|\mathcal{R}$-translation operator if the basis of expansion is changed with the translation operation from singular $\{S_n(\mathbf{y}-\mathbf{x}_*)\}$ to regular $\{R_n(\mathbf{y}-\mathbf{x}_*+\mathbf{t})\}$

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

$$(\mathcal{S}|\mathcal{R})(\mathbf{t}) = \mathcal{T}(\mathbf{t}).$$

S|R-operator has almost the same properties as S|S and R|R

(**t** cannot be zero)

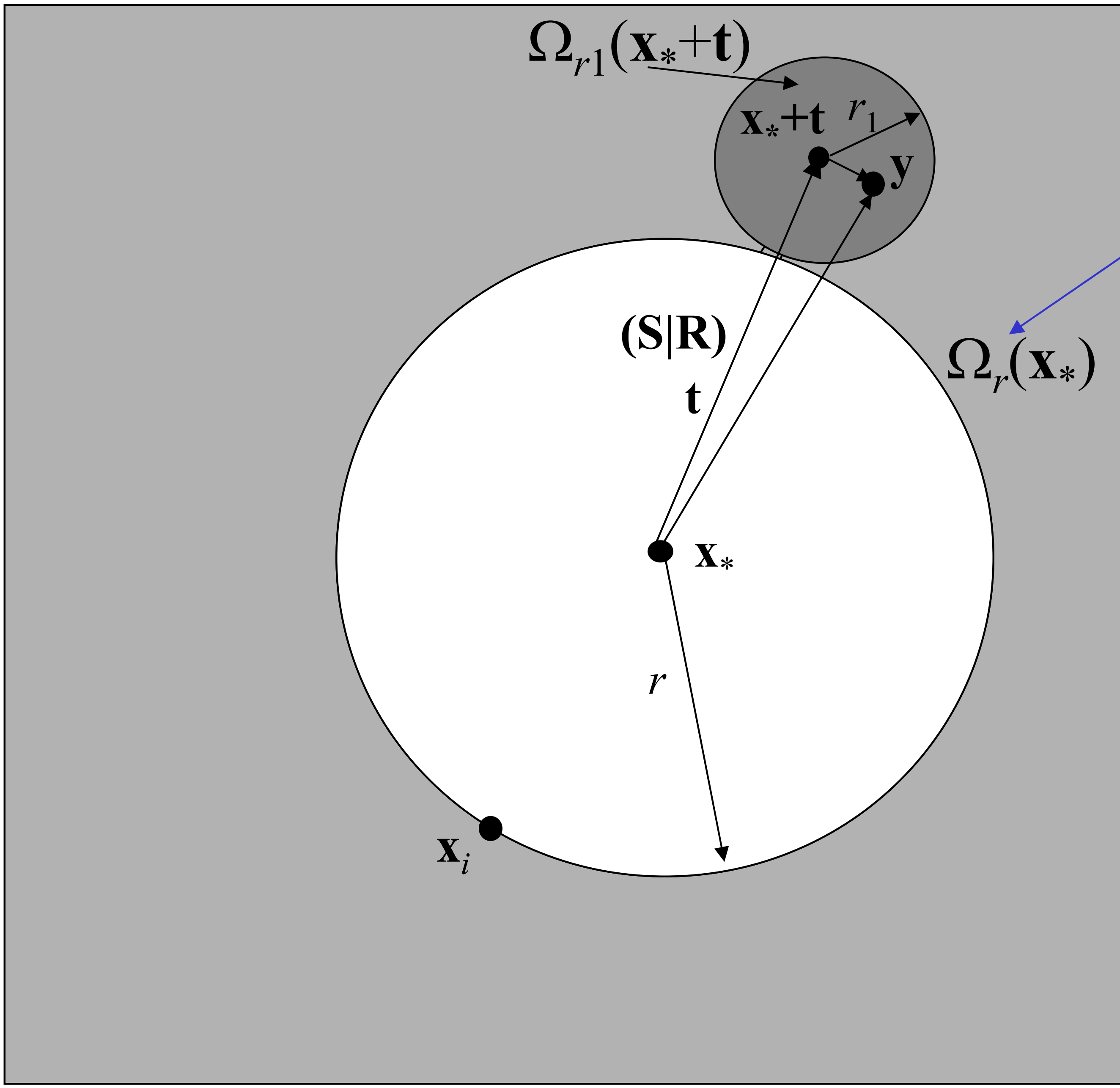
$$\Phi(\mathbf{y}) = \mathrm{B}(\mathbf{x}_*) \circ \mathbf{S}(\mathbf{y} - \mathbf{x}_*),$$

$$\Phi(\mathbf{y} + \mathbf{t}) = \widetilde{\mathrm{A}}(\mathbf{x}_*, \mathbf{t}) \circ \mathrm{R}(\mathbf{y} - \mathbf{x}_*)$$

$$\Phi(\mathbf{y}) = \widetilde{\mathrm{A}}(\mathbf{x}_*, \mathbf{t}) \circ \mathrm{R}(\mathbf{y} - \mathbf{x}_* - \mathbf{t}).$$

$$\widetilde{\mathrm{A}}(\mathbf{x}_*, \mathbf{t}) = (\mathbf{S}|\mathbf{R})(\mathbf{t})\mathrm{B}(\mathbf{x}_*).$$

Picture is different…



Original expansion
Is valid only here!

$|\mathbf{y} - \mathbf{x}_* - \mathbf{t}| < r_1 = |\mathbf{t}| - r$

Since
$\Omega_{r1}(\mathbf{x}_*+\mathbf{t}) \subset \Omega_r(\mathbf{t})$!

Also

$|\mathbf{x}_i - \mathbf{x}_*| < r$

singular point !

Properties of the translation operator

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

- $\mathcal{T}(\mathbf{0}) = \mathcal{I}$ (identity operator). Proof:

$$\mathcal{T}(\mathbf{0})[\Phi(\mathbf{y})] = \Phi(\mathbf{y}).$$

- $\mathcal{T}(\mathbf{t}_1+\mathbf{t}_2) = \mathcal{T}(\mathbf{t}_1)\circ\mathcal{T}(\mathbf{t}_2) = \mathcal{T}(\mathbf{t}_2)\circ\mathcal{T}(\mathbf{t}_1)$. Proof:

$$\mathcal{T}(\mathbf{t}_1)\circ\mathcal{T}(\mathbf{t}_2)[\Phi(\mathbf{y})] = \Phi(\mathbf{y}+\mathbf{t}_2+\mathbf{t}_1) = \mathcal{T}(\mathbf{t}_2+\mathbf{t}_1)[\Phi(\mathbf{y})] = \mathcal{T}(\mathbf{t}_1+\mathbf{t}_2)[\Phi(\mathbf{y})].$$

- (corollary 1): $\mathcal{T}^{-1}(\mathbf{t}) = \mathcal{T}(-\mathbf{t})$. Proof:

$$\mathcal{I} = \mathcal{T}(\mathbf{0}) = \mathcal{T}(\mathbf{t}-\mathbf{t}) = \mathcal{T}(\mathbf{t})\circ\mathcal{T}(-\mathbf{t}).$$

- (corollary 2): $\mathcal{T}^n(\mathbf{t}) = \mathcal{T}(n\mathbf{t})$. Proof (use induction):

$$\mathcal{T}(n\mathbf{t}) = \mathcal{T}((n-1)\mathbf{t})\circ\mathcal{T}(\mathbf{t}) = \mathcal{T}^{n-1}(\mathbf{t})\circ\mathcal{T}(\mathbf{t}) = \mathcal{T}^n(\mathbf{t}).$$

Spectrum of the translation operator

eigen value *eigen function*

$$\mathcal{T}(\mathbf{t})[\Psi(\mathbf{y})] = \lambda\Psi(\mathbf{y}), \quad \mathbf{y} \in \mathbb{R}^d.$$

Any function of type

$$\forall \mathbf{a} \in \mathbb{R}^d, \quad \Psi(\mathbf{y}) = e^{\mathbf{a}\cdot\mathbf{y}}, \quad \lambda = e^{\mathbf{a}\cdot\mathbf{t}}.$$

Check:

$$\mathcal{T}(\mathbf{t})[\Psi(\mathbf{y})] = \Psi(\mathbf{y}+\mathbf{t}) = e^{\mathbf{a}\cdot(\mathbf{y}+\mathbf{t})} = e^{\mathbf{a}\cdot\mathbf{t}}e^{\mathbf{a}\cdot\mathbf{y}} = \lambda\Psi(\mathbf{y}).$$

Relation to differential operator:

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

*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

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

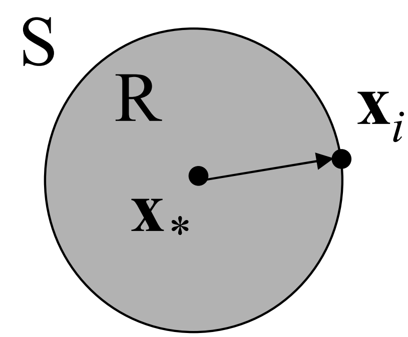
$|y - x_*| < |x_i - x_*|$:

R-expansion

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

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

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



$|y - x_*| > |x_i - x_*|$:

S-expansion

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

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

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

In this case we have

$(|y - x_*| < |t|)$

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

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

So

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

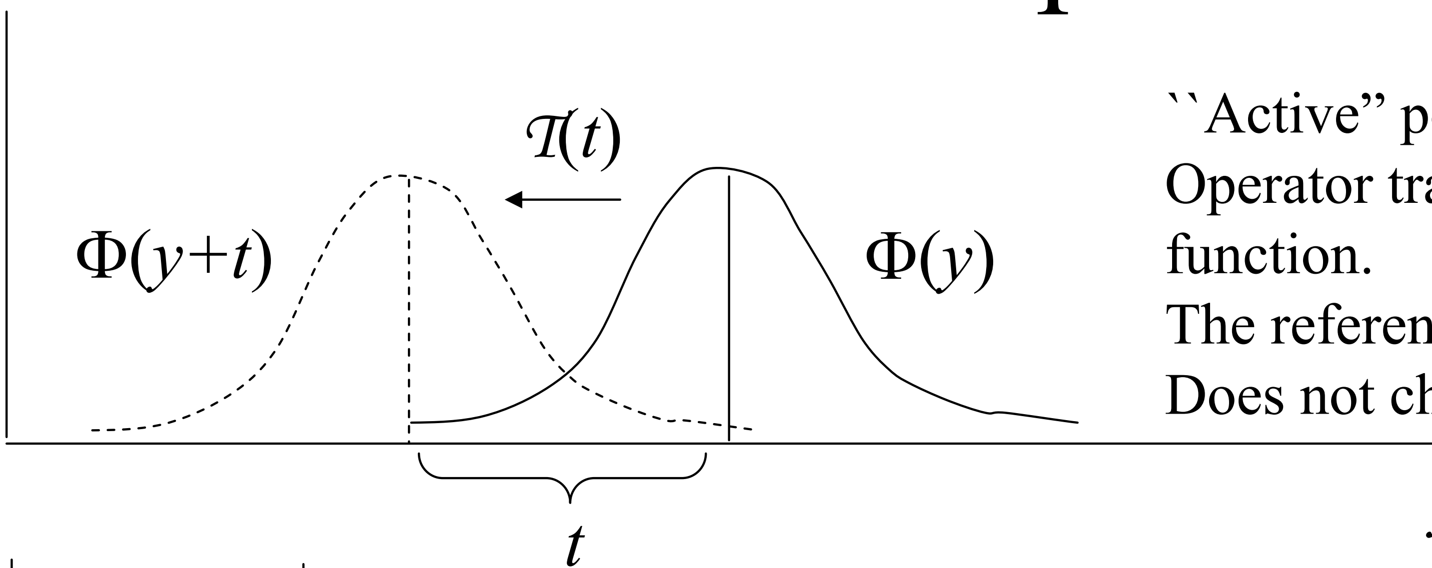
$$(\mathbf{S}|\mathbf{R})(t) = \begin{pmatrix} t^{-1} & t^{-2} & t^{-3} & \ldots \\ -t^{-2} & -2t^{-3} & -3t^{-4} & \ldots \\ t^{-3} & 3t^{-4} & 6t^{-5} & \ldots \\ \ldots & \ldots & \ldots & \ldots \end{pmatrix}$$

Norm of the Translation Operator

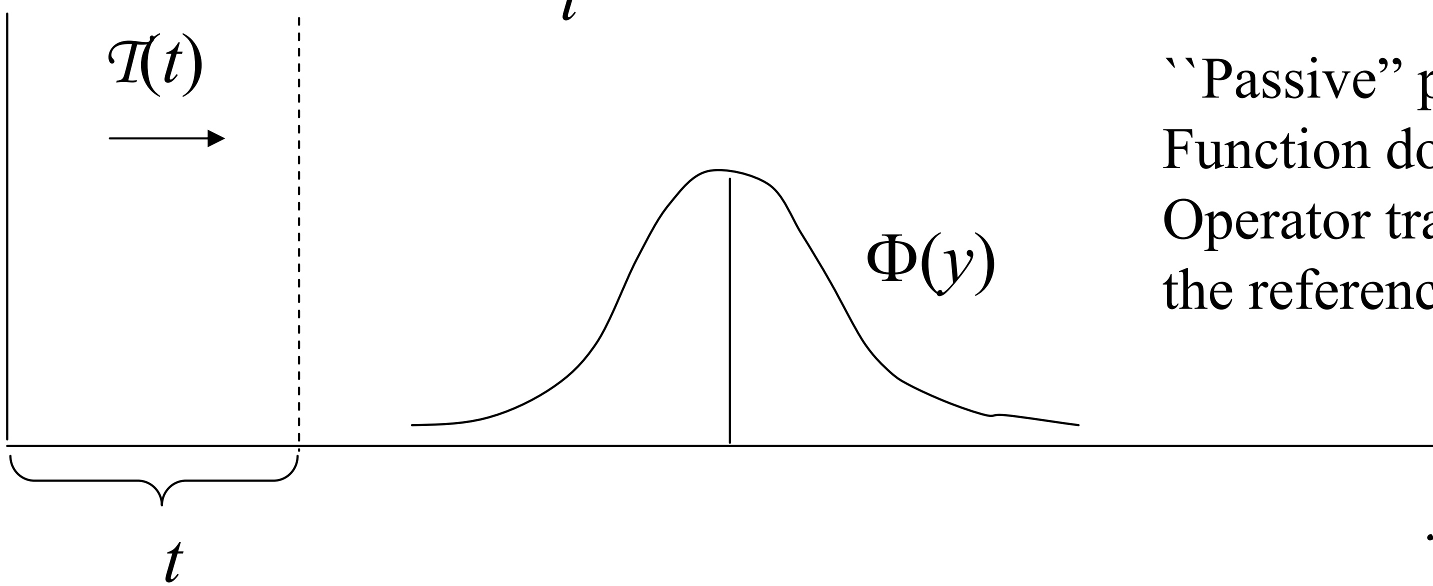
Theorem. Let $\mathbb{F}(\Omega)$ be a set of functions bounded in $\mathbb{R}^d$. Then $\| \mathcal{T}(\mathbf{t}) \| = 1$.
Proof.

$$\| \mathcal{T}(\mathbf{t}) \| = \frac{\| \mathcal{T}(\mathbf{t})\Phi(\mathbf{y}) \|}{\| \Phi(\mathbf{y}) \|} = \frac{\| \Phi(\mathbf{y}+\mathbf{t}) \|}{\| \Phi(\mathbf{y}) \|} = \frac{\sup_{\mathbf{y}\in\mathbb{R}^d} |\Phi(\mathbf{y}+\mathbf{t})|}{\sup_{\mathbf{y}\in\mathbb{R}^d} |\Phi(\mathbf{y})|} = 1.$$

Active and Passive points of view on translation operator

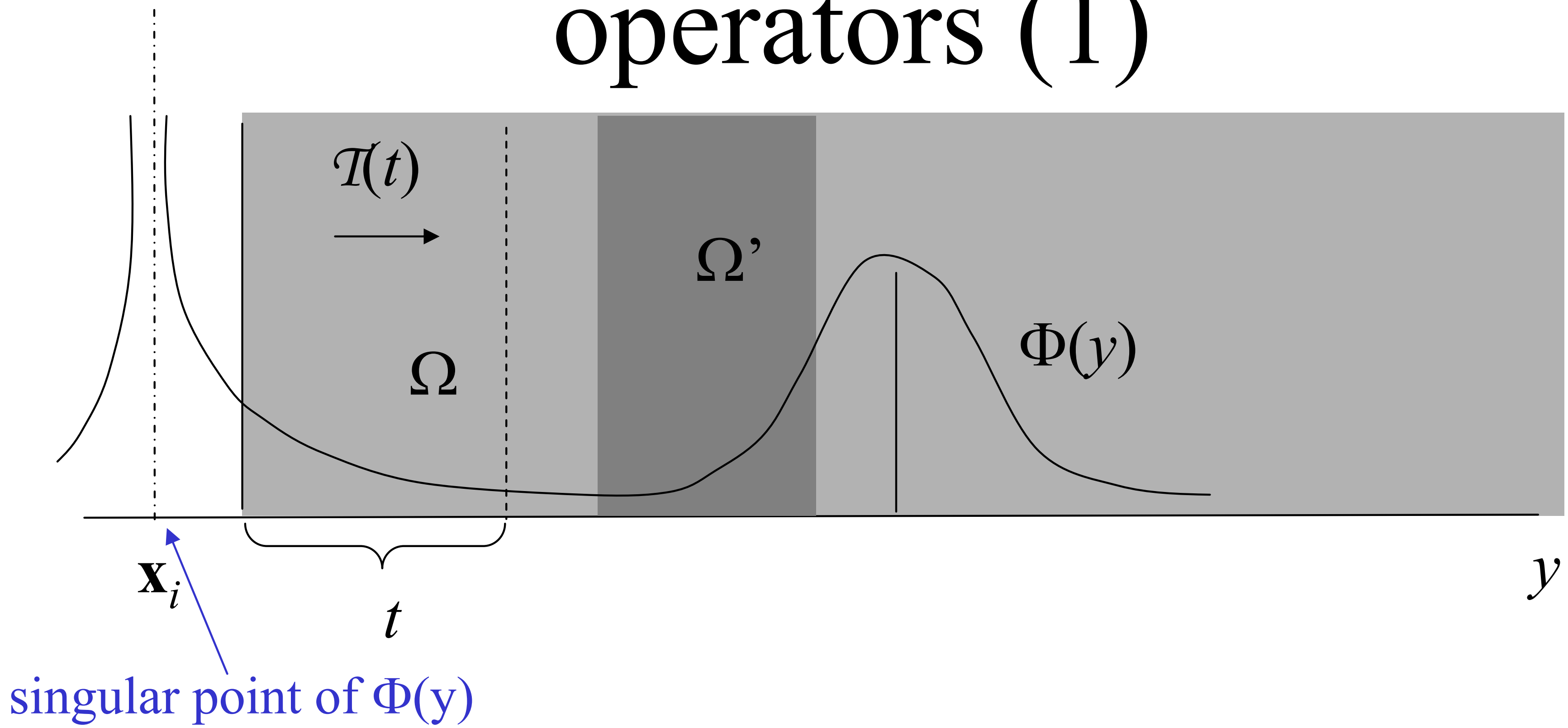


``Active" point of view:
Operator transforms
function.
The reference frame
Does not change.



``Passive" point of view:
Function does not change.
Operator transforms
the reference frame.

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



$\Phi(\mathbf{y})$ is bounded in Ω.
$\Omega' \subset \Omega$.
Therefore $\Phi(\mathbf{y})$ is bounded in Ω', and

$$\|\Phi(\mathbf{y})\|_{\Omega'} = \sup_{\mathbf{y}\in\Omega'}|\Phi(\mathbf{y})| \leqslant \sup_{\mathbf{y}\in\Omega}|\Phi(\mathbf{y})| = \|\Phi(\mathbf{y})\|_{\Omega}.$$

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.

$$\Omega' \subset \Omega$$

$$\|(\mathcal{R}|\mathcal{R})(\mathbf{t})\| = \frac{\sup_{\mathbf{y}\in\Omega'}|\Phi(\mathbf{y})|}{\sup_{\mathbf{y}\in\Omega}|\Phi(\mathbf{y})|} \leqslant 1,$$

$$\|(\mathcal{S}|\mathcal{S})(\mathbf{t})\| = \frac{\sup_{\mathbf{y}\in\Omega'}|\Phi(\mathbf{y})|}{\sup_{\mathbf{y}\in\Omega}|\Phi(\mathbf{y})|} \leqslant 1,$$

$$\|(\mathcal{S}|\mathcal{R})(\mathbf{t})\| = \frac{\sup_{\mathbf{y}\in\Omega'}|\Phi(\mathbf{y})|}{\sup_{\mathbf{y}\in\Omega}|\Phi(\mathbf{y})|} \leqslant 1.$$

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

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

then

$$\|(\mathcal{R}|\mathcal{R})(\mathbf{t})(\Phi(\mathbf{y}) - \Phi^p(\mathbf{y}))\| = \|(\mathcal{R}|\mathcal{R})(\mathbf{t})\|\,\|\Phi(\mathbf{y}) - \Phi^p(\mathbf{y})\| < \epsilon,$$
$$\|(\mathcal{S}|\mathcal{S})(\mathbf{t})(\Phi(\mathbf{y}) - \Phi^p(\mathbf{y}))\| = \|(\mathcal{S}|\mathcal{S})(\mathbf{t})\|\,\|\Phi(\mathbf{y}) - \Phi^p(\mathbf{y})\| < \epsilon,$$
$$\|(\mathcal{S}|\mathcal{R})(\mathbf{t})(\Phi(\mathbf{y}) - \Phi^p(\mathbf{y}))\| = \|(\mathcal{S}|\mathcal{R})(\mathbf{t})\|\,\|\Phi(\mathbf{y}) - \Phi^p(\mathbf{y})\| < \epsilon.$$

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:

$$X = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\}, \quad \mathbf{x}_i \in R^d, \quad i = 1, ..., N,$$

$$Y = \{\mathbf{y}_1, \mathbf{y}_2, ..., \mathbf{y}_M\}, \quad \mathbf{y}_j \in R^d, \quad j = 1, ..., M.$$

- We have functions (potentials):

$$\Phi(\mathbf{x}_i, \mathbf{y}) : R^d \to R, \quad \mathbf{y} \in R^d, \quad i = 1, ..., N.$$

- These functions can be factorized as (local expansion):

$$\Phi(\mathbf{x}_i, \mathbf{y}) = \mathbf{A}(\mathbf{x}_i, \mathbf{x}_*) \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_*), \quad |\mathbf{y} - \mathbf{x}_*| < r < |\mathbf{x}_i - \mathbf{x}_*|, \quad i = 1, ..., N$$

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

$$\Phi(\mathbf{x}_i, \mathbf{y}) = \mathbf{B}(\mathbf{x}_i, \mathbf{x}_*) \circ \mathbf{S}(\mathbf{x} - \mathbf{x}_*), \quad |\mathbf{y} - \mathbf{x}_*| > R > |\mathbf{x}_i - \mathbf{x}_*|, \quad i = 1, ..., N$$

- The product is distributive operation with respect to addition

$$(u_1\mathbf{A}_1 + u_2\mathbf{A}_2) \circ \mathbf{F} = u_1\mathbf{A}_1 \circ \mathbf{F} + u_2\mathbf{A}_2 \circ \mathbf{F}, \quad \mathbf{F} = \mathbf{S}, \mathbf{R}$$

Summary of formal requirements for functions that can be used in FMM (2)

- R-expansion coefficients can be $R|R$-translated:

$$|\mathbf{x} - \mathbf{x}_{*2}| < |\mathbf{x}_i - \mathbf{x}_{*1}| - |\mathbf{x}_{*1} - \mathbf{x}_{*2}| :$$

$$\mathbf{A}(\mathbf{x}_i, \mathbf{x}_{*2}) = (\mathbf{R}|\mathbf{R})(\mathbf{x}_{*2} - \mathbf{x}_{*1})\mathbf{A}(\mathbf{x}_i, \mathbf{x}_{*1})$$

- S-expansion coefficients can be $S|S$-translated:

$$|\mathbf{x} - \mathbf{x}_{*2}| > |\mathbf{x}_{*1} - \mathbf{x}_{*2}| + |\mathbf{x}_i - \mathbf{x}_{*1}|,$$

$$\mathbf{B}(\mathbf{x}_i, \mathbf{x}_{*2}) = (\mathbf{S}|\mathbf{S})(\mathbf{x}_{*2} - \mathbf{x}_{*1})\mathbf{B}(\mathbf{x}_i, \mathbf{x}_{*1})$$

- S-expansion coefficients can be $S|R$-translated (converted to R-expansion coefficients)

$$|\mathbf{x} - \mathbf{x}_{*2}| < |\mathbf{x}_{*1} - \mathbf{x}_{*2}| + |\mathbf{x}_i - \mathbf{x}_{*1}|,$$

$$\mathbf{A}(\mathbf{x}_i, \mathbf{x}_{*2}) = (\mathbf{S}|\mathbf{R})(\mathbf{x}_{*2} - \mathbf{x}_{*1})\mathbf{B}(\mathbf{x}_i, \mathbf{x}_{*1})$$

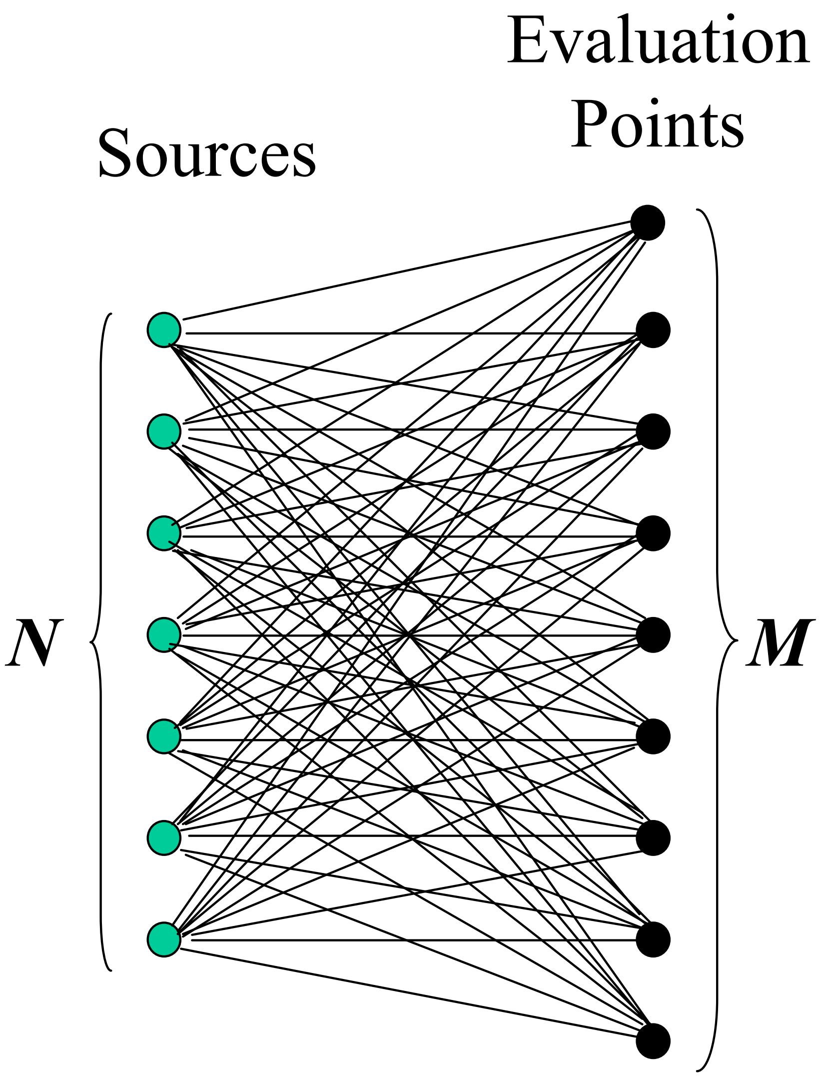
- And we are looking for sums:

$$v_j = \sum_{i=1}^{N} u_i \Phi(\mathbf{y}_j, \mathbf{x}_i), \quad j = 1, \ldots, M.$$

- Some generalization are possible, say instead of $\Phi(\mathbf{y}_j, \mathbf{x}_i)$ we can consider $\Phi_i(\mathbf{y}_j)$, etc.

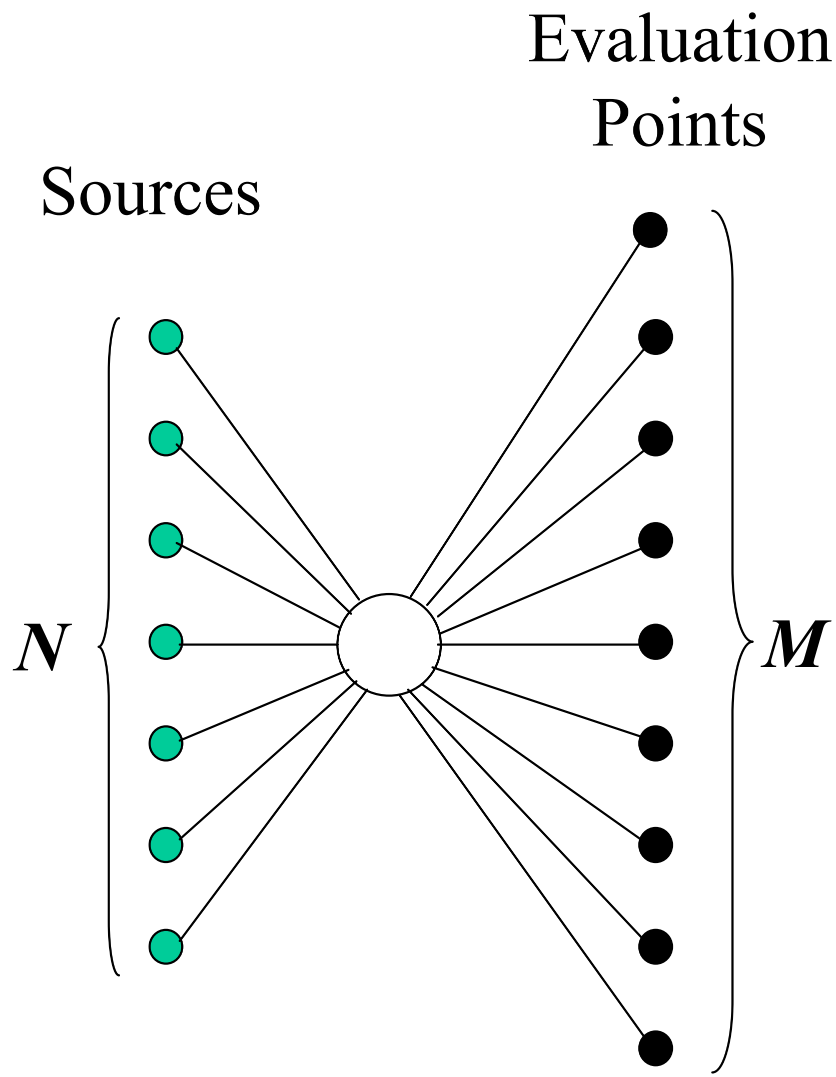
Middleman Algorithm

Standard algorithm



Total number of operations: ***O(NM)***

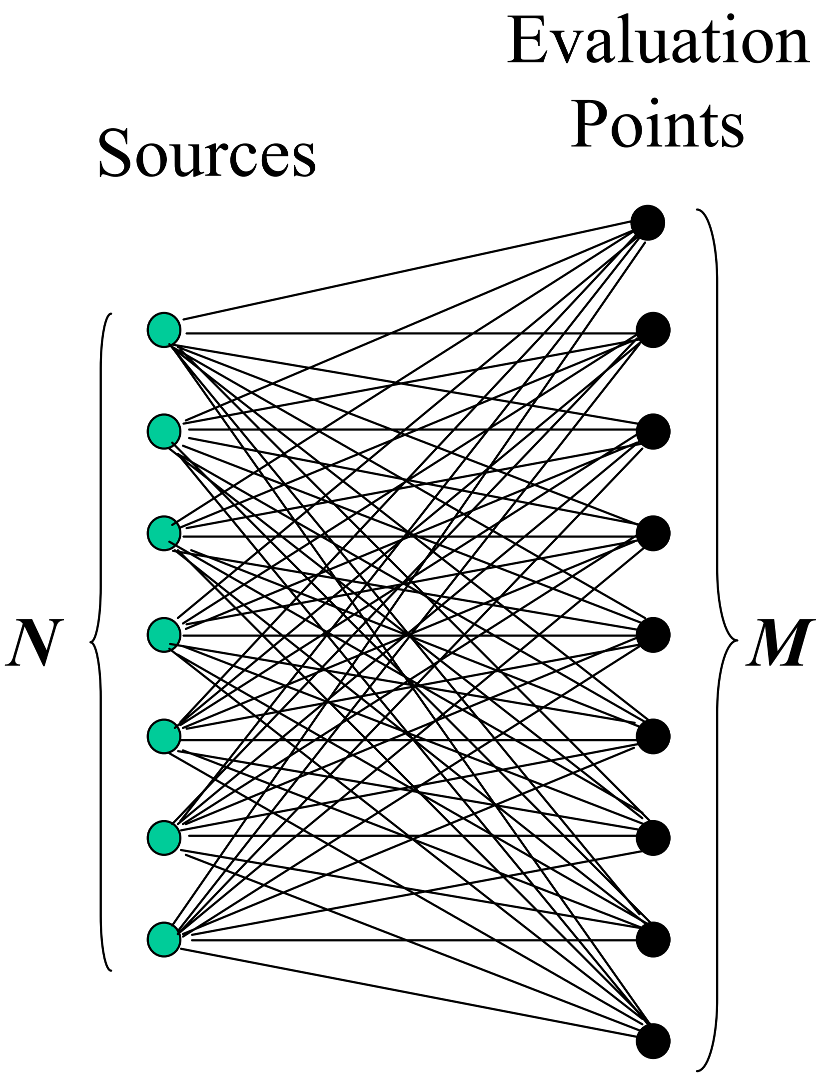
Middleman algorithm



Total number of operations: ***O(N+M)***

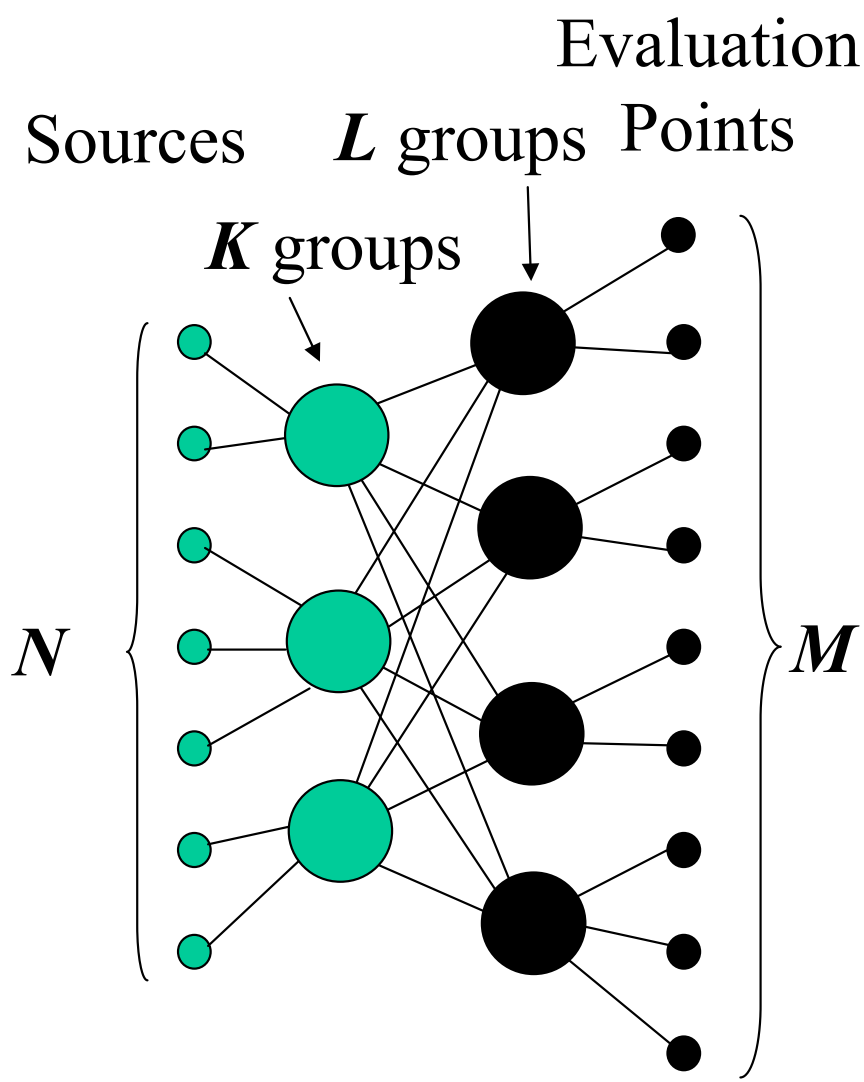
Idea of a Single Level FMM

Standard algorithm



Total number of operations: ***O(NM)***

SLFMM

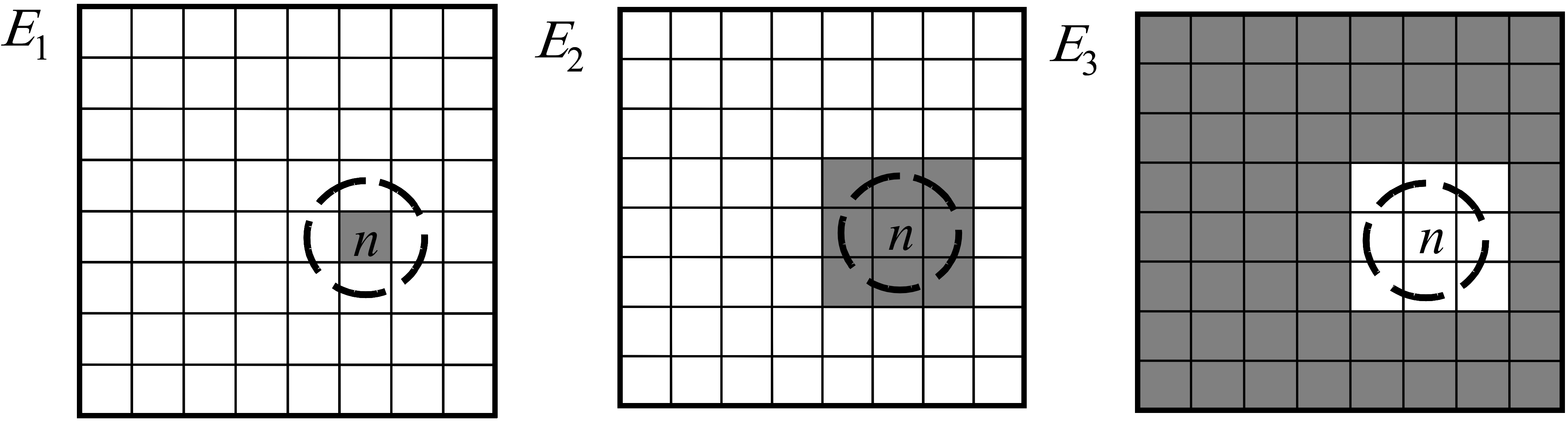


Total number of operations: ***O(N+M+KL)***

Spatial Domains

Potentials due to sources in these spatial domains

$\Phi_1^{(n)}(\mathbf{y})$ $\Phi_2^{(n)}(\mathbf{y})$ $\Phi_3^{(n)}(\mathbf{y})$



$I_1(n) = n$ $\quad I_2(n) = \{Neighbors(n)\} \cup n$

$I_3(n) = \{All\ boxes\} \setminus I_2(n)$

Boxes with these numbers belong to these spatial domains

Definition of potentials

$$\Phi_1^{(n)}(\mathbf{y}) = \sum_{\mathbf{x}_i \in E_1(n)} u_i \Phi(\mathbf{y}, \mathbf{x}_i),$$

$$\Phi_2^{(n)}(\mathbf{y}) = \sum_{\mathbf{x}_i \in E_2(n)} u_i \Phi(\mathbf{y}, \mathbf{x}_i),$$

$$\Phi_3^{(n)}(\mathbf{y}) = \sum_{\mathbf{x}_i \in E_3(n)} u_i \Phi(\mathbf{y}, \mathbf{x}_i),$$

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

$$\Phi(\mathbf{y}) = \sum_{i=1}^{N} u_i \Phi(\mathbf{y}, \mathbf{x}_i) = \sum_{\mathbf{x}_i \in E_2(n) \cup E_3(n)} u_i \Phi(\mathbf{y}, \mathbf{x}_i) = \Phi_2^{(n)}(\mathbf{y}) + \Phi_3^{(n)}(\mathbf{y}$$

for arbitrary n.

SLFMM Algorithm

Step 1. Generate S-expansion coefficients for each box

$$\Phi_1^{(n)}(\mathbf{x}) = \mathbf{C}^{(n)} \circ \mathbf{S}(\mathbf{x} - \mathbf{x}_c^{(n)}),$$

$$\mathbf{C}^{(n)} = \sum_{\mathbf{x}_i \in E_1(n,L)} u_i \mathbf{B}\left(\mathbf{x}_i, \mathbf{x}_c^{(n)}\right).$$

loop over all non-empty source boxes

For $n \in NonEmptySource$

Get $\mathbf{x}_c^{(n)}$, the center of the box;

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

loop over all sources in the box

For $\mathbf{x}_i \in E_1(n)$

Get $\mathbf{B}\ (\mathbf{x}_i, \mathbf{x}_c^{(n)})$, the S-expansion coefficients near the center of the box;

$\mathbf{C}^{(n)} = \mathbf{C}^{(n)} + u_i\mathbf{B}\ (\mathbf{x}_i, \mathbf{x}_c^{(n)})$;

End;

End;

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

SLFMM Algorithm

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

$$\Phi_3^{(n)}(\mathbf{y}) = \mathbf{D}^{(n)} \circ \mathbf{R}(\mathbf{y} - \mathbf{x}_c^{(n)}),$$

$$\mathbf{D}^{(n)} = \sum_{m \in I_3(n)} (\mathbf{S}|\mathbf{R})\left(\mathbf{x}_c^{(n)} - \mathbf{x}_c^{(m)}\right)\mathbf{C}^{(m)}.$$

loop over all non-empty evaluation boxes

For $n \in$ *NonEmptyEvaluation*

Get $\mathbf{x}_c^{(n)}$, the center of the box;

$\mathbf{D}^{(n)} = \mathbf{0}$;

loop over all non-empty source boxes outside the neighborhood of the *n*-th box

For $m \in I_3(n)$

Get $\mathbf{x}_c^{(m)}$, the center of the box;

$\mathbf{D}^{(n)} = \mathbf{D}^{(n)} + (\mathbf{S}|\mathbf{R})(\mathbf{x}_c^{(n)} - \mathbf{x}_c^{(m)})\, \mathbf{C}^{(m)}$;

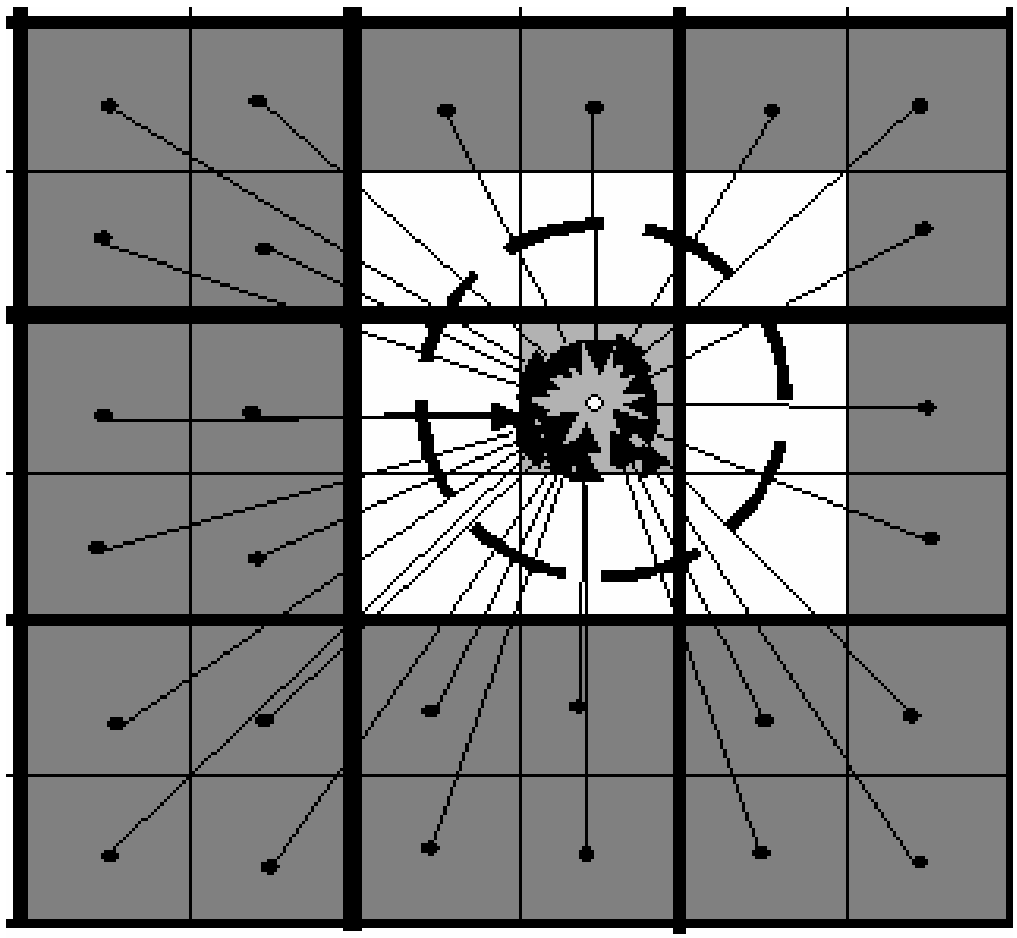
End;

End;

Implementation can be different!

All we need is to get $\mathbf{D}^{(n)}$.

S|R-translation



SLFMM Algorithm

Step 3. Final Summation

$$v_j = \Phi(\mathbf{y}_j) = \sum_{\mathbf{x}_i \in E_2(n)} \Phi(\mathbf{y}_j, \mathbf{x}_i) + \mathbf{D}^{(n)} \circ \mathbf{R}(\mathbf{y}_j - \mathbf{x}_c^{(n)}), \quad \mathbf{y}_j \in E_1(n).$$

For $n \in NonEmptyEvaluation$ ← loop over all boxes containing evaluation points

Get $\mathbf{x}_c^{(n)}$, the center of the box;

For $\mathbf{y}_j \in E_1(n)$ ← loop over all evaluation points in the box

$v_j = \mathbf{D}^{(n)} \circ \mathbf{R}(\mathbf{y}_j - \mathbf{x}_c^{(n)})$;

For $\mathbf{x}_i \in E_2(n)$ ← loop over all sources in the neighborhood of the *n*-th box

$v_j = v_j + \Phi(\mathbf{y}_j , \mathbf{x}_i)$;

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 PxP 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: $O(PN+ P^2K^2 +PM+Ms) =$
  $O(PN+ P^2K^2 +PM+MN/K)$

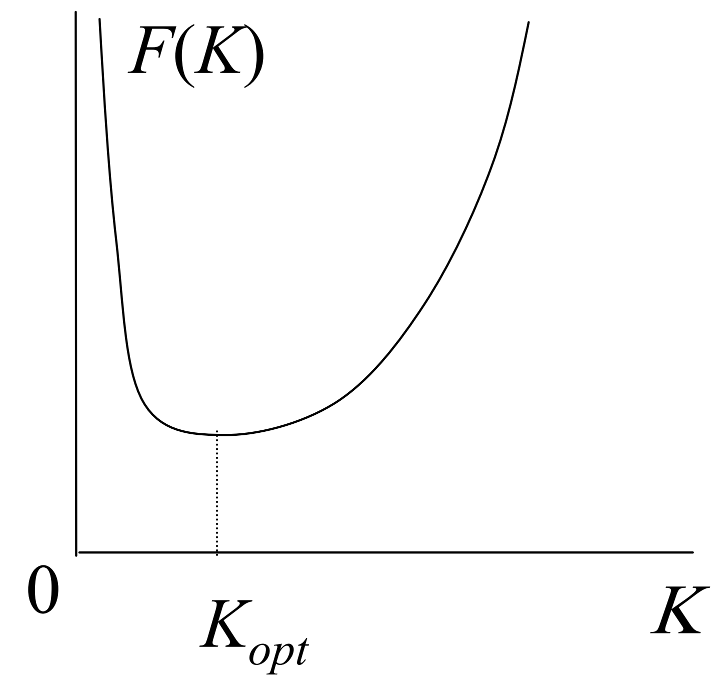
Selection of Optimal *K* (or *s*)

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

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

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

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



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:

$$O(PN + P^{4/3}N^{4/3}) = O(P^{4/3}N^{4/3}).$$

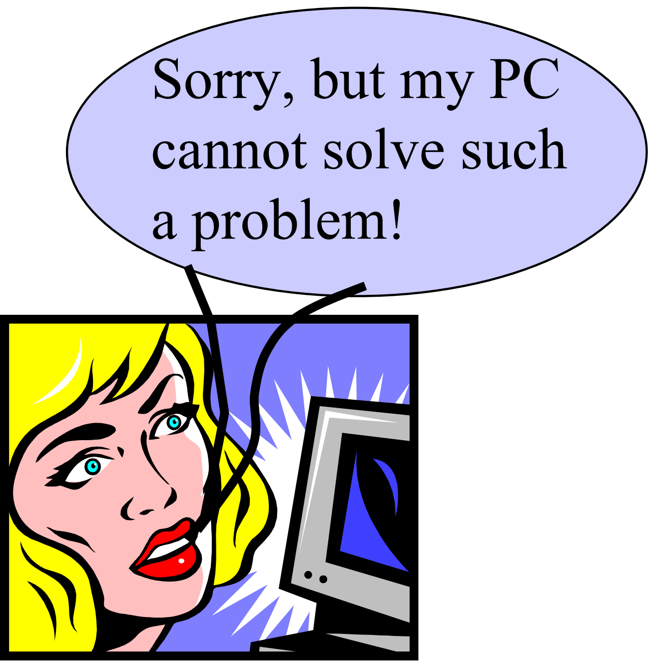
Example of Complexity:

$$P = 10, \;\; N = 10^5$$

Straightforward $O(N^2)$: Complexity ~ 10^{10}

SLFMM $O((PN)^{4/3})$: Complexity ~ 10^8

100 Times CPU savings !



$$P = 10, \;\; N = 10^8$$

Straightforward $O(N^2)$: Complexity ~ 10^{16}

SLFMM $O((PN)^{4/3})$: Complexity ~ 10^{12}

10000 Times CPU savings !