MAIT 627 Fast Multipole Methods

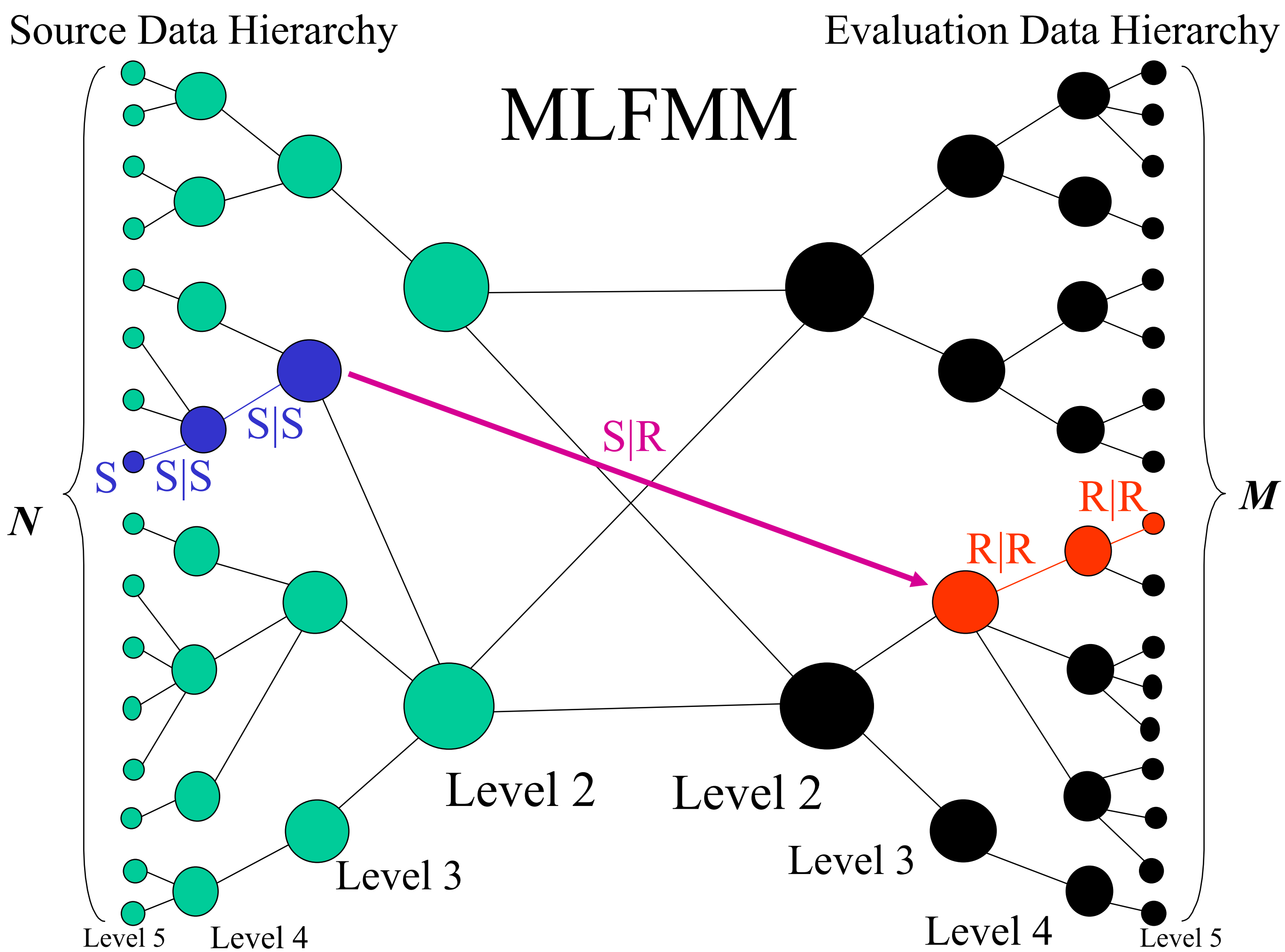
Lecture 8

Outline

- Error Bounds of MLFMM
  - A scheme for error evaluation;
- Example problem
  - S-expansion error;
  - S|S-translation error;
  - S|R-translation error;
  - R|R-translation error.
- Error and Neighborhoods

A scheme for error evaluation (1)

(How one source contributes to one evaluation points)



A scheme for error evaluation (2)

$$\Phi(\mathbf{y},\mathbf{x}_k) = \sum_{m=0}^{\infty} C_m^{(L)}(\mathbf{x}_k,\mathbf{x}_*^{(L)}) S_m(\mathbf{y}-\mathbf{x}_*^{(L)}) = \mathbf{C}^{(L)}(\mathbf{x}_k,\mathbf{x}_*^{(L)}) \cdot \mathbf{S}(\mathbf{y}-\mathbf{x}_*^{(L)})$$

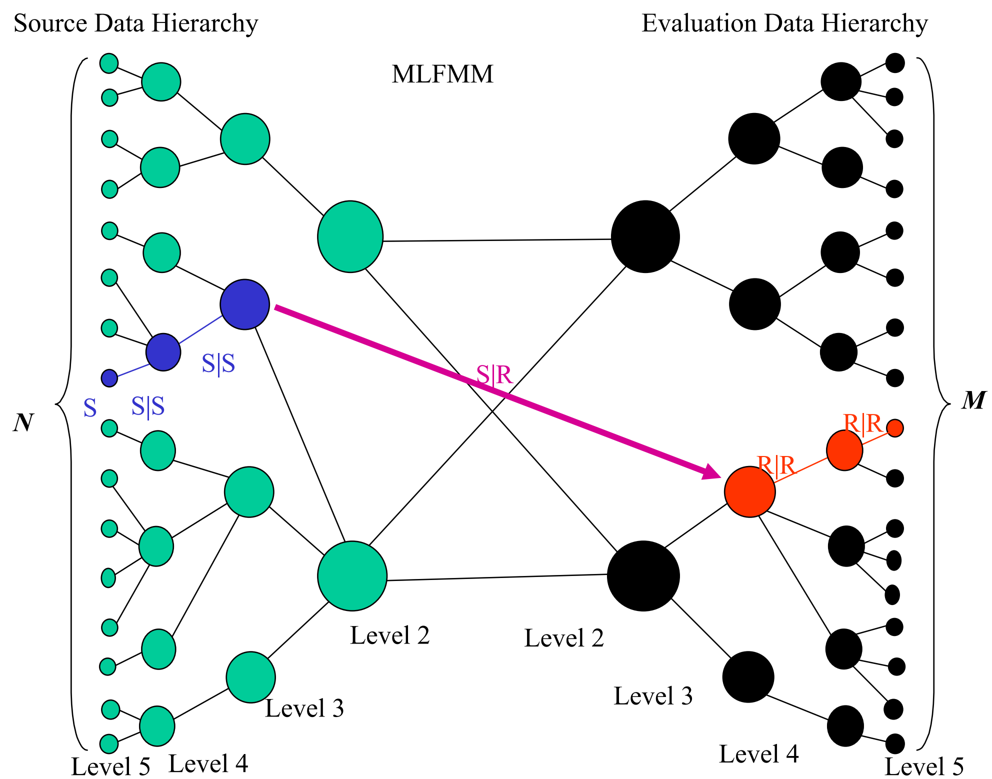
$$= \mathbf{C}^{(L-1)}(\mathbf{x}_k,\mathbf{x}_*^{(L-1)}) \cdot \mathbf{S}(\mathbf{y}-\mathbf{x}_*^{(L-1)})$$

$$= \ldots = \mathbf{C}^{(l)}(\mathbf{x}_k,\mathbf{x}_*^{(l)}) \cdot \mathbf{S}\left(\mathbf{y}-\mathbf{x}_*^{(l)}\right)$$

$$= \mathbf{D}^{(l)}(\mathbf{x}_k,\mathbf{y}_*^{(l)}) \cdot \mathbf{R}\left(\mathbf{y}-\mathbf{y}_*^{(l)}\right)$$

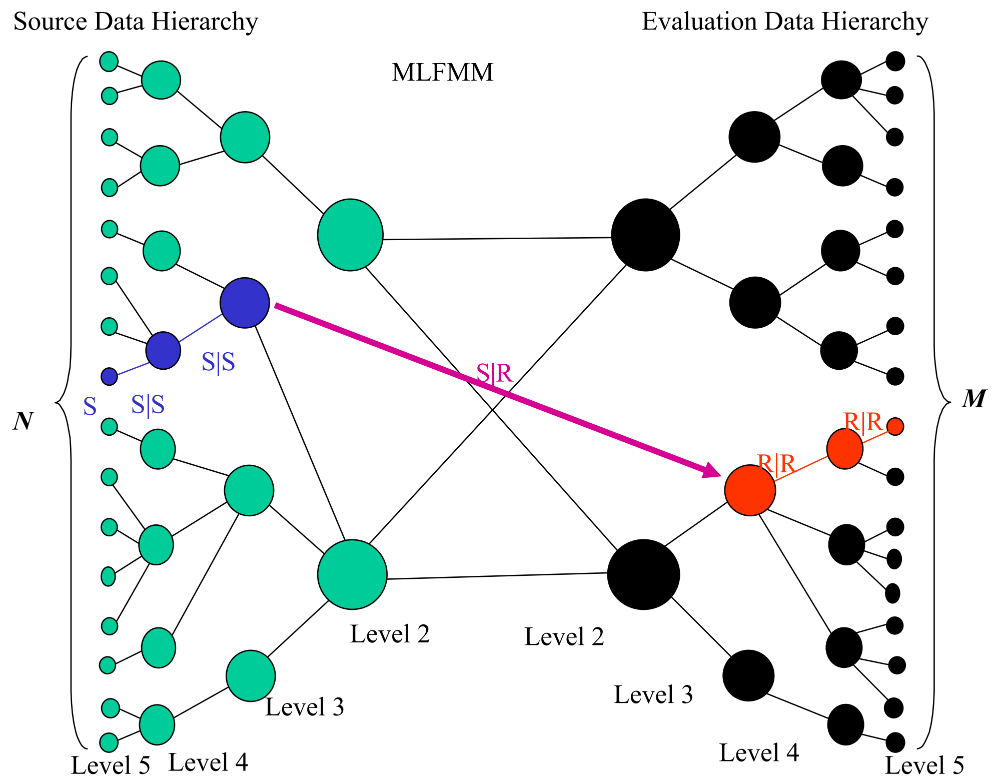
$$= \mathbf{D}^{(l+1)}(\mathbf{x}_k,\mathbf{y}_*^{(l+1)}) \cdot \mathbf{R}\left(\mathbf{y}-\mathbf{y}_*^{(l+1)}\right)$$

$$= \ldots = \mathbf{D}^{(L)}(\mathbf{x}_k,\mathbf{y}_*^{(L)}) \cdot \mathbf{R}(\mathbf{y}-\mathbf{y}_*^{(L)}).$$



A scheme for error evaluation (3)

$$
\begin{aligned}
\mathbf{D}^{(L)}(\mathbf{x}_k,\mathbf{y}_*^{(L)}) &= (\mathrm{R|R})(\mathbf{y}_*^{(L)}-\mathbf{y}_*^{(L-1)})\mathbf{D}^{(L-1)}(\mathbf{x}_k,\mathbf{y}_*^{(L-1)}) \\
&= [(\mathrm{R|R})(\mathbf{y}_*^{(L)}-\mathbf{y}_*^{(L-1)})\circ(\mathrm{R|R})(\mathbf{y}_*^{(L-1)}-\mathbf{y}_*^{(L-2)})]\mathbf{D}^{(L-2)}(\mathbf{x}_k,\mathbf{y}_*^{(L-2)}) \\
&= \ldots = \left[(\mathrm{R|R})(\mathbf{y}_*^{(L)}-\mathbf{y}_*^{(L-1)})\circ(\mathrm{R|R})(\mathbf{y}_*^{(L-1)}-\mathbf{y}_*^{(L-2)})\circ\ldots\circ(\mathrm{R|R})\left\{\mathbf{y}_*^{(l+1)}-\mathbf{y}_*^{(l)}\right\}\right]\mathbf{D}^{(l)}(\mathbf{x}_k,\mathbf{y}_*^{(l)}) \\
&= \left[(\mathrm{R|R})(\mathbf{y}_*^{(L)}-\mathbf{y}_*^{(L-1)})\circ\ldots\circ(\mathrm{R|R})\left\{\mathbf{y}_*^{(l+1)}-\mathbf{y}_*^{(l)}\right\}\circ(\mathrm{S|R})\left\{\mathbf{y}_*^{(l)}-\mathbf{x}_*^{(l)}\right\}\right]\mathrm{C}^{(l)}(\mathbf{x}_k,\mathbf{x}_*^{(l)}) \\
&= \left[(\mathrm{R|R})(\mathbf{y}_*^{(L)}-\mathbf{y}_*^{(L-1)})\circ\ldots\circ(\mathrm{R|R})\left\{\mathbf{y}_*^{(l+1)}-\mathbf{y}_*^{(l)}\right\}\circ(\mathrm{S|R})\left\{\mathbf{y}_*^{(l)}-\mathbf{x}_*^{(l)}\right\}\circ(\mathrm{S|S})\left\{\mathbf{x}_*^{(l)}-\mathbf{x}_*^{(l+1)}\right\}\right]\mathrm{C}^{(l+1)}(\mathbf{x}_k,\mathbf{x}_*^{(l+1)}) \\
&= \ldots \\
&= \left[(\mathrm{R|R})(\mathbf{y}_*^{(L)}-\mathbf{y}_*^{(L-1)})\circ\ldots\circ(\mathrm{R|R})\left\{\mathbf{y}_*^{(l+1)}-\mathbf{y}_*^{(l)}\right\}\circ(\mathrm{S|R})\left\{\mathbf{y}_*^{(l)}-\mathbf{x}_*^{(l)}\right\}\circ(\mathrm{S|S})\left\{\mathbf{x}_*^{(l)}-\mathbf{x}_*^{(l+1)}\right\}\circ\ldots\circ(\mathrm{S|S})(\mathbf{x}_*^{(L-1)}-\mathbf{x}_*^{(L)})\right]\mathrm{C}^{(L)}(\mathbf{x}_k,\mathbf{x}_*^{(L)})
\end{aligned}
$$



A scheme for error evaluation (4)

Consider computation of the final coefficients with p-truncated matrices

$$\begin{aligned}
\mathbf{D}^{(L)}(\mathbf{x}_k,\mathbf{y}_*^{(L)}) = & [\Pr(p)\circ(\mathbf{R}|\mathbf{R})(\mathbf{y}_*^{(L)}-\mathbf{y}_*^{(L-1)})\circ\Pr(p)]\circ\ldots\circ \\
& \left[\Pr(p)\circ(\mathbf{R}|\mathbf{R})\left(\mathbf{y}_*^{(l+1)}-\mathbf{y}_*^{(l)}\right)\circ\Pr(p)\right]\circ \\
& \left[\Pr(p)\circ(\mathbf{S}|\mathbf{R})\left(\mathbf{y}_*^{(l)}-\mathbf{x}_*^{(l)}\right)\circ\Pr(p)\right]\circ \\
& \left[\Pr(p)\circ(\mathbf{S}|\mathbf{S})\left(\mathbf{x}_*^{(l)}-\mathbf{x}_*^{(l+1)}\right)\circ\Pr(p)\right]\circ\ldots\circ \\
& [\Pr(p)\circ(\mathbf{S}|\mathbf{S})(\mathbf{x}_*^{(L-2)}-\mathbf{x}_*^{(L-1)})\circ\Pr(p)]\circ \\
& [\Pr(p)\circ(\mathbf{S}|\mathbf{S})(\mathbf{x}_*^{(L-1)}-\mathbf{x}_*^{(L)})\circ\Pr(p)]\mathbf{C}^{(L)}(\mathbf{x}_k,\mathbf{x}_*^{(L)})
\end{aligned}$$

These truncation operators can be skipped! ($\Pr^2=\Pr$)

So:

$$\begin{aligned}
\mathbf{D}^{(L)}(\mathbf{x}_k,\mathbf{y}_*^{(L)}) = & [\Pr(p)\circ(\mathbf{R}|\mathbf{R})(\mathbf{y}_*^{(L)}-\mathbf{y}_*^{(L-1)})]\circ\ldots\circ \\
& \left[\Pr(p)\circ(\mathbf{R}|\mathbf{R})\left(\mathbf{y}_*^{(l+1)}-\mathbf{y}_*^{(l)}\right)\right]\circ \\
& \left[\Pr(p)\circ(\mathbf{S}|\mathbf{R})\left(\mathbf{y}_*^{(l)}-\mathbf{x}_*^{(l)}\right)\right]\circ \\
& \left[\Pr(p)\circ(\mathbf{S}|\mathbf{S})\left(\mathbf{x}_*^{(l)}-\mathbf{x}_*^{(l+1)}\right)\right]\circ\ldots\circ \\
& [\Pr(p)\circ(\mathbf{S}|\mathbf{S})(\mathbf{x}_*^{(L-2)}-\mathbf{x}_*^{(L-1)})]\circ \\
& [\Pr(p)\circ(\mathbf{S}|\mathbf{S})(\mathbf{x}_*^{(L-1)}-\mathbf{x}_*^{(L)})]\circ\Pr(p)\mathbf{C}^{(L)}(\mathbf{x}_k,\mathbf{x}_*^{(L)})
\end{aligned}$$

A scheme for error evaluation (5)

p-truncated functions:

$$\hat{\Phi}_L(\mathbf{y},\mathbf{x}_k) = \widehat{\mathbf{C}}^{(L)}(\mathbf{x}_k,\mathbf{x}_*^{(L)}) \cdot \mathbf{S}(\mathbf{y}-\mathbf{x}_*^{(L)})$$

$$\hat{\Phi}_{L-1}(\mathbf{y},\mathbf{x}_k) = \widehat{\mathbf{C}}^{(L-1)}(\mathbf{x}_k,\mathbf{x}_*^{(L-1)}) \cdot \mathbf{S}(\mathbf{y}-\mathbf{x}_*^{(L-1)})$$

$$\ldots$$

$$\hat{\Phi}_l(\mathbf{y},\mathbf{x}_k) = \widehat{\mathbf{C}}^{(l)}(\mathbf{x}_k,\mathbf{x}_*^{(l)}) \cdot \mathbf{S}\left(\mathbf{y}-\mathbf{x}_*^{(l)}\right)$$

$$\hat{\Psi}_l(\mathbf{y},\mathbf{x}_k) = \widehat{\mathbf{D}}^{(l)}(\mathbf{x}_k,\mathbf{y}_*^{(l)}) \cdot \mathbf{R}\left(\mathbf{y}-\mathbf{y}_*^{(l)}\right)$$

$$\hat{\Psi}_{l+1}(\mathbf{y},\mathbf{x}_k) = \widehat{\mathbf{D}}^{(l+1)}(\mathbf{x}_k,\mathbf{y}_*^{(l+1)}) \cdot \mathbf{R}\left(\mathbf{y}-\mathbf{y}_*^{(l+1)}\right)$$

$$\ldots$$

$$\hat{\Psi}_L(\mathbf{y},\mathbf{x}_k) = \widehat{\mathbf{D}}^{(L)}(\mathbf{x}_k,\mathbf{y}_*^{(L)}) \cdot \mathbf{R}(\mathbf{y}-\mathbf{y}_*^{(L)}).$$

The error comes only from truncation operator

$$\widehat{\mathbf{C}}^{(\alpha)} = \Pr(p) \circ (\mathbf{S}|\mathbf{S})(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)})\widehat{\mathbf{C}}^{(\alpha+1)}, \quad \alpha = L-1,\ldots,l$$

$$\widehat{\mathbf{D}}^{(l)} = \Pr(p) \circ (\mathbf{S}|\mathbf{R})\left(\mathbf{y}_*^{(l)} - \mathbf{x}_*^{(l)}\right)\widehat{\mathbf{C}}^{(l)},$$

$$\widehat{\mathbf{D}}^{(\alpha)} = \Pr(p) \circ (\mathbf{R}|\mathbf{R})(\mathbf{y}_*^{(\alpha)} - \mathbf{y}_*^{(\alpha+1)})\widehat{\mathbf{C}}^{(\alpha+1)}, \quad \alpha = l,\ldots,L-1$$

Truncated Translation Theorem

Let $\{F_n(\mathbf{y})\}$ and $\{G_n(\mathbf{y})\}$ be two expansion bases in Ω, and the reexpansion series converges everywhere in Ω :

$$\forall \mathbf{y} \in \Omega, \quad F_n(\mathbf{y}) = \sum_{m=0}^{\infty} (F|G)_{mn} G_m(\mathbf{y}), \quad n = 0, 1, 2, \ldots$$

Let also $\{A_n\}$ be a set of coefficients, such that the duble sum converges absolutely and uniformly in Ω :

$$\forall \mathbf{y} \in \Omega, \quad \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} A_n (F|G)_{mn} G_m(\mathbf{y}) = \Phi(\mathbf{y}),$$

$$\forall \epsilon, \exists p(\epsilon), \quad \sum_{n=0}^{\infty} \sum_{m=p}^{\infty} |A_n (F|G)_{mn} G_m(\mathbf{y})| < \epsilon, \quad \sum_{n=p}^{\infty} \sum_{m=0}^{\infty} |A_n (F|G)_{mn} G_m(\mathbf{y})| < \epsilon.$$

Then

$$\left| \Phi(\mathbf{y}) - \sum_{n=0}^{p-1} \sum_{m=0}^{p-1} A_n (F|G)_{mn} G_m(\mathbf{y}) \right| < 2\epsilon.$$

Proof

Let us denote

$$c_{mn} = (F|G)_{mn} A_n G_m(\mathbf{y})$$

$$\left|\Phi(\mathbf{y}) - \sum_{n=0}^{p-1}\sum_{m=0}^{p-1} c_{mn}\right| = \left|\sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_{mn} - \sum_{n=0}^{p-1}\sum_{m=0}^{p-1} c_{mn}\right| =$$

$$= \left|\sum_{m=0}^{p-1}\sum_{n=0}^{\infty} c_{mn} + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} c_{mn} - \sum_{m=0}^{p-1}\sum_{n=0}^{p-1} c_{mn}\right|$$

$$= \left|\sum_{m=0}^{p-1}\sum_{n=0}^{p-1} c_{mn} + \sum_{m=0}^{p-1}\sum_{n=p}^{\infty} c_{mn} + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} c_{mn} - \sum_{m=0}^{p-1}\sum_{n=0}^{p-1} c_{mn}\right|$$

$$= \left|\sum_{m=0}^{p-1}\sum_{n=p}^{\infty} c_{mn} + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} c_{mn}\right| \leqslant \sum_{m=0}^{p-1}\sum_{n=p}^{\infty}|c_{mn}| + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty}|c_{mn}|$$

$$\leqslant \sum_{m=0}^{\infty}\sum_{n=p}^{\infty}|c_{mn}| + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty}|c_{mn}| < \epsilon + \epsilon = 2\epsilon.$$

A scheme for error evaluation (5)

For uniformly and absolutely convergent series:

$$\begin{aligned}
&\left|\widehat{\Phi}_\alpha(\mathbf{y},\mathbf{x}_k) - \widehat{\Phi}_{\alpha+1}(\mathbf{y},\mathbf{x}_k)\right| \\
&= \left| \sum_{m=0}^{p-1} \widehat{C_m}^{(\alpha)} S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)}) - \sum_{n=0}^{p-1} \widehat{C_n}^{(\alpha+1)} S_n(\mathbf{y}-\mathbf{x}_*^{(\alpha+1)}) \right| \\
&= \left| \sum_{m=0}^{p-1} \sum_{n=0}^{p-1} (S|S)_{mn}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)}) \widehat{C_n}^{(\alpha+1)} S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)}) \right. \\
&\quad \left. - \sum_{n=0}^{p-1} \widehat{C_n}^{(\alpha+1)} \sum_{m=0}^{\infty} (S|S)_{nm}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)}) S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)}) \right| \\
&= \left| \sum_{n=0}^{p-1} \widehat{C_n}^{(\alpha+1)} \sum_{m=p}^{\infty} (S|S)_{nm}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)}) S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)}) \right| \\
&\leqslant \sum_{n=0}^{p-1} \sum_{m=p}^{\infty} \left| \widehat{C_n}^{(\alpha+1)} (S|S)_{nm}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)}) S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)}) \right| \\
&< \sum_{n=0}^{\infty} \sum_{m=p}^{\infty} \left| \widehat{C_n}^{(\alpha+1)} (S|S)_{nm}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)}) S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)}) \right| < \epsilon_{\max}(p).
\end{aligned}$$

A scheme for error evaluation (6)

For uniformly and absolutely convergent series it is possible to find such $\varepsilon_{max}(p)$ that for given minimum(maximum) translation distance the max abs difference between two subsequent functions is smaller than $\varepsilon_{max}(p)$.

In this case the total error of FMM does not exceed:

$$FMMError \leqslant N\left[\epsilon_{\max}^{(\exp)}(p) + (L-2)\epsilon_{\max}^{(S|S)}(p) + \epsilon_{\max}^{(S|R)}(p) + (L-2)\epsilon_{\max}^{(R|R)}(p)\right].$$

$$\lim_{p\to\infty}\epsilon_{\max}^{(\exp)}(p) = 0, \quad \lim_{p\to\infty}\epsilon_{\max}^{(S|S)}(p) = 0, \quad \lim_{p\to\infty}\epsilon_{\max}^{(S|R)}(p) = 0, \quad \lim_{p\to\infty}\epsilon_{\max}^{(R|R)}(p) = 0.$$

If

$$\epsilon(p) = \max\left(\epsilon_{\max}^{(\exp)}(p), \epsilon_{\max}^{(S|S)}(p), \epsilon_{\max}^{(S|R)}(p), \epsilon_{\max}^{(R|R)}(p)\right),$$

$$FMMError \leqslant 2N(L-1)\epsilon(p).$$

Example Problem

Problem:
Evaluate the MLFMM error for computation of function

$$v(y) = \sum_{k=0}^{N} u_k \Phi(y, x_k),$$

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

where y and x_k are points in a box of size D and space is subdivided by the binary tree to the maximum level L.

This example is also good to evaluate 2D problem, by treating x and y as complex numbers!

We have…

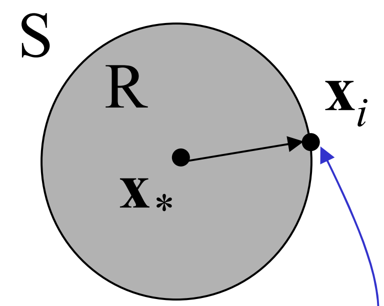
$|y - x_*| < |x_i - x_*|$:

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

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

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

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

Singular Point is located at the Boundary of regions for the R- and S-expansions!

S|R-operator

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

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

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

So

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

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

S|S-operator

$$S_n(y-x_{*1}) = \sum_{m=0}^{\infty}(S|S)_{mn}(t)S_m(y-x_{*2}), \quad t = x_{*2} - x_{*1}$$

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

$$\begin{aligned}
S_n(y-x_{*1}) &= (y-x_{*1})^{-n-1} = (y - x_{*2} - (x_{*1} - x_{*2}))^{-n-1} \\
&= (y-x_{*2})^{-n-1}\left[1 - \frac{x_{*1}-x_{*2}}{y-x_{*2}}\right]^{-n-1} \\
&= \sum_{m=0}^{\infty}\frac{(-1)^m(m+n)!}{m!n!}(x_{*2}-x_{*1})^m(y-x_{*2})^{-n-m-1} \\
&= \sum_{m=0}^{\infty}\frac{(-1)^m(m+n)!}{m!n!}t^m S_{n+m}(y-x_{*2}) = \sum_{m=n}^{\infty}\frac{(-1)^{m-n}m!}{n!(m-n)!}t^{m-n}S_m(y-x_{*2})
\end{aligned}$$

$$(S|S)_{mn}(t) = \begin{cases} 0, & m < n \\ \frac{(-1)^{m-n}m!}{n!(m-n)!}t^{m-n}, & m \geqslant n. \end{cases}$$

S|S-operator (2)

$$S_n(y-x_{*1}) = \sum_{m=0}^{\infty}(S|S)_{mn}(t)S_m(y-x_{*2}), \quad t = x_{*2} - x_{*1}$$

$$(S|S)_{mn}(t) = \begin{cases} 0, & m < n \\ \frac{(-1)^{m-n}m!}{n!(m-n)!}t^{m-n}, & m \geqslant n. \end{cases}$$

$$(\mathbf{S}|\mathbf{S})(t) = (S|S)_{mn}(t) = \begin{pmatrix} 1 & 0 & 0 & 0 & \ldots \\ -t & 1 & 0 & 0 & \ldots \\ t^2 & -2t & 1 & 0 & \ldots \\ -t^3 & 3t^2 & -3t & 1 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix}$$

R|R-operator

$$R_n(y - x_{*1}) = \sum_{m=0}^{\infty} (R|R)_{mn}(t) R_m(y - x_{*2}), \quad t = x_{*2} - x_{*1}$$

$$R_n(y - x_{*1}) = (y - x_{*1})^n = (y - x_{*2} - (x_{*1} - x_{*2}))^n$$

$$= \sum_{m=0}^{n} \frac{(-1)^m n!}{m!(n-m)!} (x_{*2} - x_{*1})^{n-m} (y - x_{*2})^m$$

$$= \sum_{m=0}^{n} \frac{(-1)^m n!}{m!(n-m)!} t^{n-m} R_m(y - x_{*2}).$$

$$(R|R)_{mn}(t) = \begin{cases} 0, & m > n \\ \frac{(-1)^m n!}{m!(n-m)!} t^{n-m}, & m \leqslant n. \end{cases}$$

R|R-operator(2)

$$R_n(y-x_{*1}) = \sum_{m=0}^{n} (R|R)_{mn}(t) R_m(y-x_{*2}), \quad t = x_{*2} - x_{*1}$$

$$(R|R)_{mn}(t) = \begin{cases} 0, & m > n \\ \frac{(-1)^m n!}{m!(n-m)!} t^{n-m}, & m \leqslant n. \end{cases}$$

$$(\mathbf{R}|\mathbf{R})(t) = (R|R)_{mn}(t) = \begin{pmatrix} 1 & t & t^2 & t^3 & \ldots \\ 0 & -1 & -2t & -3t^2 & \ldots \\ 0 & 0 & 1 & 3t & \ldots \\ 0 & 0 & 0 & -1 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix}$$

S-Expansion Error

$$\Phi(y,x_k) = \frac{1}{y-x_k} = \sum_{m=0}^{\infty} b_m(x_k,x_{*1})S_m(y-x_{*1}),$$

$$b_m(x_k,x_{*1}) = (x_k - x_{*1})^m, \quad m = 0,1,...,$$

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

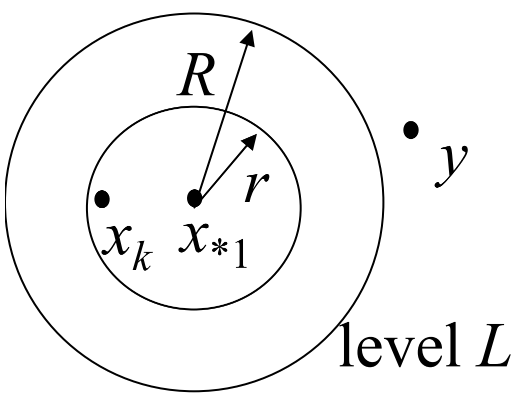
Assume

$$|x_k - x_{*1}| \leqslant r, \quad |y - x_{*1}| \geqslant R.$$

$$ExpansionError(p,R,r) \leqslant \left| \sum_{m=0}^{\infty} b_m(x_k,x_{*1})S_m(y-x_{*1}) - \sum_{m=0}^{p-1} b_m(x_k,x_{*1})S_m(y-x_{*1}) \right|$$

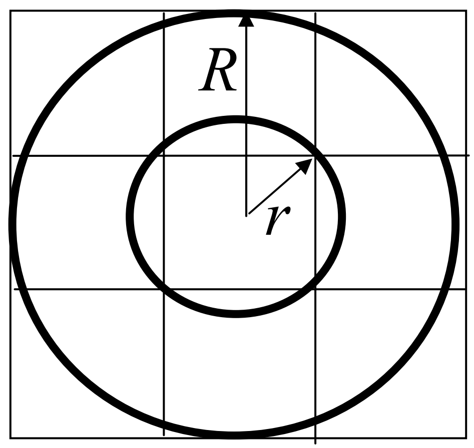
$$= \left| \sum_{m=p}^{\infty} b_m(x_k,x_{*1})S_m(y-x_{*1}) \right| \leqslant \sum_{m=p}^{\infty} |b_m(x_k,x_{*1})S_m(y-x_{*1})|$$

$$= \frac{1}{|y-x_{*1}|} \sum_{m=p}^{\infty} \left(\frac{r}{R}\right)^m \leqslant \frac{1}{R}\left(\frac{r}{R}\right)^p \frac{1}{1-r/R} = \left(\frac{r}{R}\right)^p \frac{1}{R-r}.$$



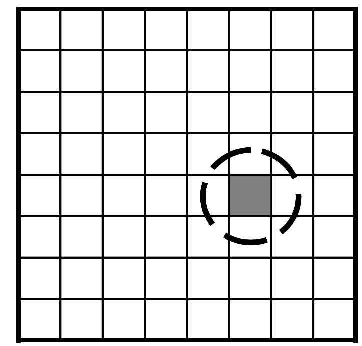
S-Expansion Error

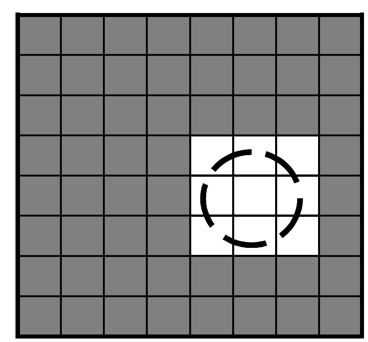
$$ExpansionError(p, R, r) \leqslant \left(\frac{r}{R}\right)^p \frac{1}{R - r}.$$



$d = 1$: $r/R = 1/3$,

$d = 2$: $r/R = \sqrt{2}/3 < 1/2$.





S|S-Translation Error

Translation from level α+1 to α:

$$\widehat{\mathbf{C}}^{(\alpha)} = (\mathbf{S}|\mathbf{S})(t)\widehat{\mathbf{C}}^{(\alpha+1)}$$

$$\begin{pmatrix} \widehat{C}_0^{(\alpha)} \\ \widehat{C}_1^{(\alpha)} \\ \widehat{C}_2^{(\alpha)} \\ \widehat{C}_3^{(\alpha)} \\ \ldots \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & \ldots \\ -t & 1 & 0 & 0 & \ldots \\ t^2 & -2t & 1 & 0 & \ldots \\ -t^3 & 3t^2 & -3t & 1 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix} \begin{pmatrix} \widehat{C}_0^{(\alpha+1)} \\ \widehat{C}_1^{(\alpha+1)} \\ \widehat{C}_2^{(\alpha+1)} \\ \widehat{C}_3^{(\alpha+1)} \\ \ldots \end{pmatrix}$$

$$\widehat{C}_0^{(\alpha)} = \widehat{C}_0^{(\alpha+1)},$$

$$\widehat{C}_1^{(\alpha)} = -t\widehat{C}_0^{(\alpha+1)} + \widehat{C}_1^{(\alpha+1)},$$

$$\widehat{C}_2^{(\alpha)} = t^2\widehat{C}_0^{(\alpha+1)} - 2t\widehat{C}_1^{(\alpha+1)} + \widehat{C}_2^{(\alpha+1)},$$

$$\ldots$$

p first coefficients at level α can be exactly computed from *p* first coefficients at level α+1.

This is exact translation of first *p* coefficients!

S|S-Translation Error(2)

Translation from level α+1 to α:

$$\widehat{C_m}^{(\alpha)} = \sum_{n=0}^{p-1} (S|S)_{mn}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)})\widehat{C_n}^{(\alpha+1)} = \sum_{n=0}^{\infty} (S|S)_{mn}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)})\widehat{C_n}^{(\alpha+1)}$$

$$\text{since } (S|S)_{mn}(t) = 0, \quad m < n \leqslant p.$$

So:

$$\left|\Phi(\mathbf{y},\mathbf{x}_k) - \widehat{\Phi}_\alpha(\mathbf{y},\mathbf{x}_k)\right| \leqslant \left(\frac{2^{L-\alpha} r}{2^{L-\alpha} R}\right)^p \frac{1}{2^{L-\alpha}(R-r)}$$

$$\leqslant \left(\frac{r}{R}\right)^p \frac{1}{(R-r)} = ExpansionError(p,R,r)$$

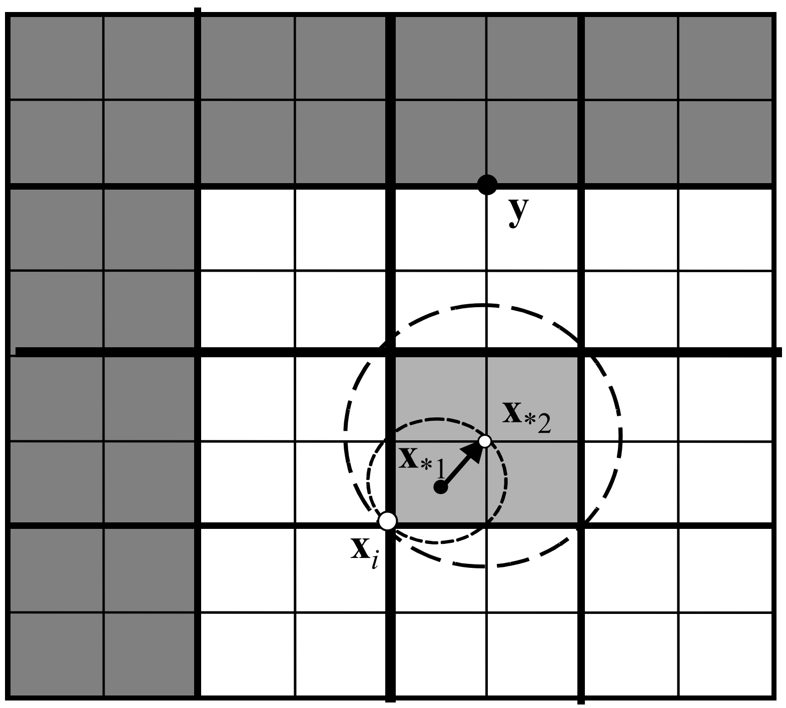
This factor shows that we are on level α

For any level α!

S|S-Translation Error(3)

$$\left|\Phi(\mathbf{y},\mathbf{x}_k) - \widehat{\Phi}_\alpha(\mathbf{y},\mathbf{x}_k)\right| \leqslant \left(\frac{2^{L-\alpha} r}{2^{L-\alpha} R}\right)^p \frac{1}{2^{L-\alpha}(R-r)}$$

$$\leqslant \left(\frac{r}{R}\right)^p \frac{1}{(R-r)} = ExpansionError(p,R,r)$$



In this example S|S-translations do not cause any additional error!

S|R-Translation Error

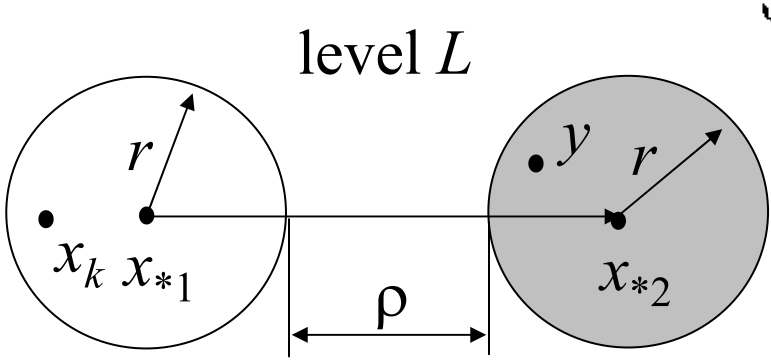
Note that in result of S|S-translations, first p coefficients are exact!

$$c_{mn} = (S|R)_{mn}(t) b_n(x_k, x_{*1}) R_m(y - x_{*2}) = \frac{(-1)^m (m+n)!}{m!n!t^{m+n+1}} (x_k - x_{*1})^n (y - x_{*2})^m$$

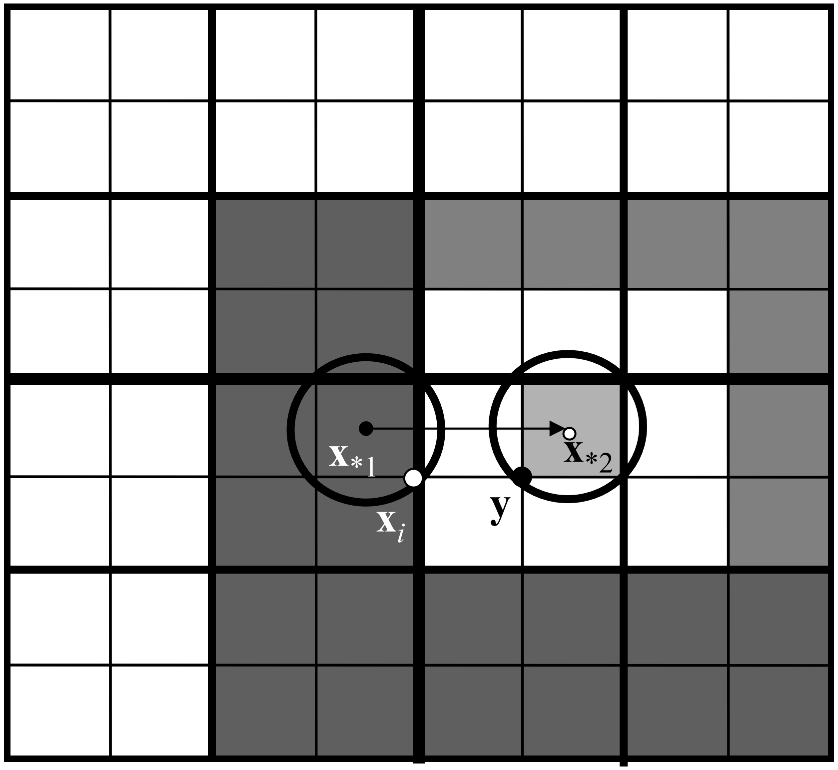
$$|x_k - x_{*1}| \leqslant 2^{L-l} r, \quad |y - x_{*2}| \leqslant 2^{L-l} r, \quad |x_{*2} - x_{*1}| \geqslant 2^{L-l} r + 2^{L-l} r + 2^{L-l} \rho$$

Translation with p –truncated operator $(S|R)^{(p)}_{mn}(t)$ yields

$$\Psi^{(l)}(y, x_k) = \sum_{m=0}^{p-1} \sum_{n=0}^{p-1} c_{mn}.$$



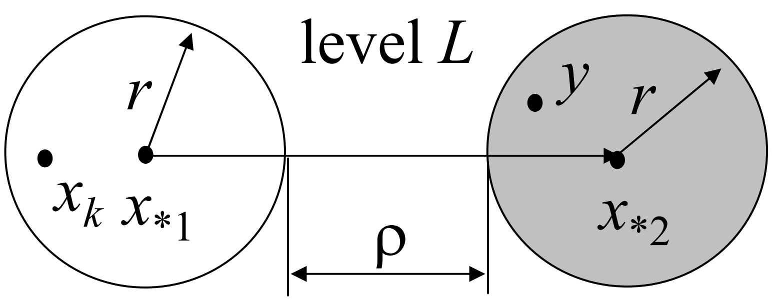
S|R-Translation Error (2)



$d = 1$: $\rho / r = 2$,

$d = 2$: $\rho / r = 2(2 - \sqrt{2})/\sqrt{2}$

$= 2(\sqrt{2} - 1) > 0.8$



S|R-Translation Error (3)

$$\left|\Phi(y,x_k) - \Psi^{(l)}(y,x_k)\right| = \left|\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} c_{mn} - \sum_{m=0}^{p-1}\sum_{n=0}^{p-1} c_{mn}\right|$$

$$= \left|\sum_{m=0}^{p-1}\sum_{n=0}^{\infty} c_{mn} + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} c_{mn} - \sum_{m=0}^{p-1}\sum_{n=0}^{p-1} c_{mn}\right|$$

$$= \left|\sum_{m=0}^{p-1}\sum_{n=0}^{p-1} c_{mn} + \sum_{m=0}^{p-1}\sum_{n=p}^{\infty} c_{mn} + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} c_{mn} - \sum_{m=0}^{p-1}\sum_{n=0}^{p-1} c_{mn}\right|$$

Long one!

$$= \left|\sum_{m=0}^{p-1}\sum_{n=p}^{\infty} c_{mn} + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} c_{mn}\right| \leqslant \sum_{m=0}^{p-1}\sum_{n=p}^{\infty} |c_{mn}| + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} |c_{mn}|$$

$$\leqslant \sum_{m=0}^{\infty}\sum_{n=p}^{\infty} |c_{mn}| + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} |c_{mn}| = \sum_{n=p}^{\infty}\sum_{m=0}^{\infty} |c_{mn}| + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} |c_{mn}|$$

$$= \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} |c_{nm}| + \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} |c_{mn}| = \sum_{m=p}^{\infty}\sum_{n=0}^{\infty} \left(|c_{nm}| + |c_{mn}|\right)$$

continued →

S|R-Translation Error (4)

$$= \frac{1}{|t|}\sum_{m=p}^{\infty}\sum_{n=0}^{\infty}\frac{(m+n)!}{m!n!}\left[\frac{|x_k - x_{*1}|^n |y - x_{*2}|^m + |x_k - x_{*1}|^m |y - x_{*2}|^n}{|t|^{m+n}}\right]$$

$$\leqslant \frac{1}{\left(2^{L-l}r + 2^{L-l}r + 2^{L-l}\rho\right)}\sum_{m=p}^{\infty}\sum_{n=0}^{\infty}\frac{(m+n)!}{m!n!}\frac{\left(2^{L-l}r\right)^n\left(2^{L-l}r\right)^m + \left(2^{L-l}r\right)^m\left(2^{L-l}r\right)^n}{\left(2^{L-l}r + 2^{L-l}r + 2^{L-l}\rho\right)^{n+m}}$$

$$= \frac{1}{2^{L-l}r(2+\frac{\rho}{r})}\sum_{m=p}^{\infty}\sum_{n=0}^{\infty}\frac{(m+n)!}{m!n!}\frac{2r^{n+m}}{r^{n+m}(2+\frac{\rho}{r})^{n+m}}$$

$$= \frac{2}{2^{L-l}r(2+\frac{\rho}{r})}\sum_{m=p}^{\infty}\sum_{n=0}^{\infty}\frac{(m+n)!}{m!n!}\frac{1}{(2+\frac{\rho}{r})^{n+m}}$$

It is really long!

$$= \frac{2}{2^{L-l}r(2+\frac{\rho}{r})}\sum_{m=p}^{\infty}\frac{1}{(2+\frac{\rho}{r})^{m}}\sum_{n=0}^{\infty}\frac{(m+n)!}{m!n!}\frac{1}{(2+\frac{\rho}{r})^{n}}$$

we used this

$$= \frac{2}{2^{L-l}r(2+\frac{\rho}{r})}\sum_{m=p}^{\infty}\frac{1}{(2+\frac{\rho}{r})^{m}}\frac{1}{\left(1-\frac{1}{2+\rho/r}\right)^{m+1}}$$

continued →

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

S|R-Translation Error (5)

$$= \frac{2}{2^{L-l} r (2+\frac{\rho}{r})} \sum_{m=p}^{\infty} \frac{1}{(2+\frac{\rho}{r})^m} \frac{1}{(1+\frac{\rho}{r})^{m+1}} \left(2+\frac{\rho}{r}\right)^{m+1}$$

$$= \frac{2}{2^{L-l} r} \sum_{m=p}^{\infty} \frac{1}{(1+\frac{\rho}{r})^{m+1}} = \frac{2}{2^{L-l} r (1+\frac{\rho}{r})^{p+1}} \sum_{m=0}^{\infty} \frac{1}{(1+\frac{\rho}{r})^{m}}$$

$$= \frac{2}{2^{L-l} r (1+\frac{\rho}{r})^{p+1}} \frac{1}{1-\frac{1}{1+\rho/r}} = \frac{2}{2^{L-l} r (1+\frac{\rho}{r})^{p+1}} \frac{r}{\rho}\left(1+\frac{\rho}{r}\right)$$

$$= \frac{2}{2^{L-l}\rho}\left(\frac{r}{r+\rho}\right)^p \leqslant \frac{2}{\rho}\left(\frac{r}{r+\rho}\right)^p.$$

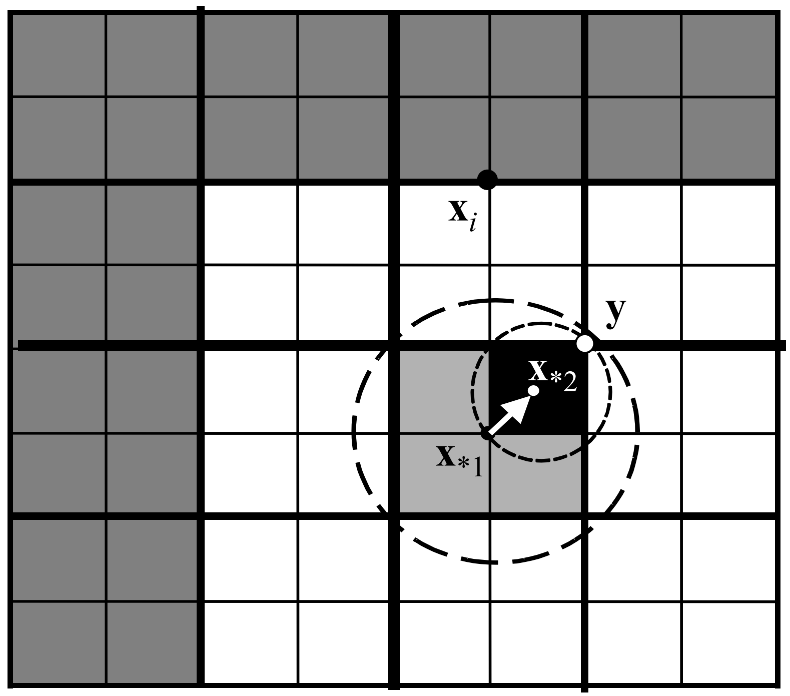
That's it!

$d = 1$: $\rho/r = 2$,

$d = 2$: $\rho/r = 2(2 - \sqrt{2})/\sqrt{2}$

$= 2(\sqrt{2} - 1) > 0.8$

R|R-Translation Error



R|R-Translation Error(2)

$$\left|\widehat{\Psi}_{\alpha}(\mathbf{y},\mathbf{x}_k) - \widehat{\Psi}_{\alpha+1}(\mathbf{y},\mathbf{x}_k)\right|$$

$$= \left|\sum_{n=0}^{p-1} \widehat{D_n}^{(\alpha)} R_n(\mathbf{y}-\mathbf{y}_*^{(\alpha)}) - \sum_{m=0}^{p-1} \widehat{D_m}^{(\alpha+1)} R_m(\mathbf{y}-\mathbf{y}_*^{(\alpha+1)})\right|$$

$$= \left|\sum_{n=0}^{p-1}\sum_{m=0}^{\infty} (R|R)_{mn}(\mathbf{y}_*^{(\alpha+1)}-\mathbf{y}_*^{(\alpha)})\widehat{D_n}^{(\alpha)} R_m(\mathbf{y}-\mathbf{y}_*^{(\alpha+1)})\right.$$

$$\left. - \sum_{m=0}^{p-1}\sum_{n=0}^{p-1} (R|R)_{mn}(\mathbf{y}_*^{(\alpha+1)}-\mathbf{y}_*^{(\alpha)})\widehat{D_n}^{(\alpha)} R_m(\mathbf{y}-\mathbf{y}_*^{(\alpha+1)})\right|$$

$$= \left|\sum_{n=0}^{p-1}\sum_{m=p}^{\infty} (R|R)_{mn}(\mathbf{y}_*^{(\alpha+1)}-\mathbf{y}_*^{(\alpha)})\widehat{D_n}^{(\alpha)} R_m(\mathbf{y}-\mathbf{y}_*^{(\alpha+1)})\right| = 0.$$

$$\text{since } (R|R)_{mn}(t) = 0, \quad m > n$$

This is something, but why?

R|R-Translation Error(3)

Indeed, in our case the regular basis functions are polynomials up to order p-1, which are obviously can be expressed via other polynomial basis up to order p-1 near arbitrary expansion center.

Zero error is provided due to domains of validity are includes hierarchically to larger validity domains.

Total Error

$$
\begin{aligned}
AbsSingleSourceError &\leqslant MaxExpansionError(p,R,r) + MaxSRTranslationError(p,r,\rho) \\
&= \left(\frac{r}{R}\right)^p \frac{1}{R-r} + \frac{2}{\rho}\left(\frac{r}{r+\rho}\right)^p. \\
AbsTotalError &= N \cdot AbsSingleSourceError \\
&= N\left[\left(\frac{r}{R}\right)^p \frac{1}{R-r} + \frac{2}{\rho}\left(\frac{r}{r+\rho}\right)^p\right].
\end{aligned}
$$

since $R > r + \rho$,

$$
AbsTotalError < \frac{3N}{\rho}\left(\frac{r}{r+\rho}\right)^p.
$$

Total Error(2)

$$d = 1 : \quad \rho = 2^{-L}, \quad r = 0.5 \cdot 2^{-L},$$

$$AbsTotalError < 3 \frac{2^L N}{3^p}.$$

$$d = 2 : \quad \rho = \left(2 - \sqrt{2}\right) 2^{-L}, \quad r = 0.5\sqrt{2} \cdot 2^{-L},$$

$$AbsTotalError < 3 \frac{2^L N}{2 - \sqrt{2}} \left(\frac{\sqrt{2}}{2\left(\sqrt{2}/2 + 2 - \sqrt{2}\right)} \right)^p$$

$$= 3 \frac{2^L N}{2 - \sqrt{2}} \left(\frac{\sqrt{2}}{4 - \sqrt{2}} \right)^p < 5.2(0.6)^p \cdot 2^L N.$$

Both formulae can be described as

$$AbsTotalError < C\alpha^p 2^L N = \epsilon(p, N, L, d).$$

Total Error(3)

$$AbsTotalError < C\alpha^p 2^L N = \epsilon(p,N,L,d).$$

Example: $N = 10^4,\ L = 10,\ d = 1$:

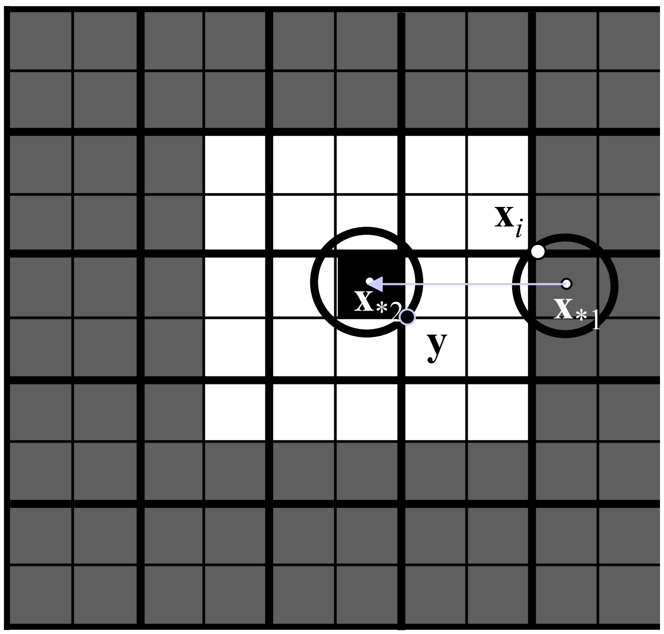
p	10	20	30	40
$\epsilon,<$	$6\cdot10^{2}$	$9\cdot10^{-3}$	$2\cdot10^{-7}$	$3\cdot10^{-12}$

Example: $N = 10^4,\ L = 10,\ d = 2$:

p	40	50	60	70
$\epsilon,<$	$8\cdot10^{-2}$	$5\cdot10^{-4}$	$3\cdot10^{-6}$	$2\cdot10^{-8}$

Total Error(4). 5-Neighborhood.

5-neighborhood



$$d = 1: \quad \rho = 2 \cdot 2^{-L}, \quad r = 0.5 \cdot 2^{-L},$$

$$AbsTotalError < 3\frac{2^L N}{5^p}.$$

$$d = 2: \quad \rho = \left(3 - \sqrt{2}\right)2^{-L}, \quad r = 0.5\sqrt{2} \cdot 2^{-L},$$

$$AbsTotalError < 3\frac{2^L N}{3 - \sqrt{2}}\left(\frac{\sqrt{2}}{2\left(\sqrt{2}/2 + 3 - \sqrt{2}\right)}\right)^p$$

$$= 3\frac{2^L N}{3 - \sqrt{2}}\left(\frac{\sqrt{2}}{6 - \sqrt{2}}\right)^p < 2(0.31)^p \cdot 2^L N.$$

$$AbsTotalError < C\alpha^p 2^L N = \epsilon(p, N, L, d).$$

Total Error(5). 5-Neighborhood.

$$AbsTotalError < C\alpha^p 2^L N = \epsilon(p, N, L, d).$$

Example: $N = 10^4$, $L = 10$, $d = 1$:

p	10	15	20	25
$\epsilon, <$	4	$2 \cdot 10^{-3}$	$4 \cdot 10^{-7}$	$2 \cdot 10^{-10}$

Example: $N = 10^4$, $L = 10$, $d = 2$:

p	15	20	25	30
$\epsilon, <$	$5 \cdot 10^{-1}$	$2 \cdot 10^{-3}$	$4 \cdot 10^{-6}$	$2 \cdot 10^{-8}$

Optimization of MLFMM within error bounds

In the example considered, the FMM error depends on:

- Truncation number, *p;*
- Max level of space subdivision, *L*;
- Size of the neighborhood (3,5, or maybe other);
- Number of sources, *N;*
- Problem dimensionality, *d*.

For fixed (given) *N* and *d* parameters *p,L,*and *Neighborhood Size* can be optimized.

MLFMM Complexity

$$CostMLFMM = (M+N)P + 2^d(P_4(d)+2)\frac{N}{s}CostTranslation(P) + P_2(d)sMCostFunc,$$

$$N = 2^{L_* d}, \quad s = 2^{L_s d}, \quad L = L_* - L_s = \frac{1}{d}\log\frac{N}{s}.$$

Consider

$$\epsilon(p,N,L,d) = C\alpha^p 2^L N = C\alpha^p\left(\frac{N}{s}\right)^{1/d} N < \epsilon_0$$

$$p > \frac{1}{\log\frac{1}{\alpha}}\log\frac{CN^{1+1/d}}{\epsilon_0 s^{1/d}} \sim a\log N - b\log s + c$$

$$CostMLFMM(s) = (M+N)p(N,s) + 2^d(P_4(d)+2)\frac{N}{s}p^2(N,s) + P_2(d)sM$$

$$0 = \frac{dCostMLFMM(s)}{ds} \sim -b\frac{M+N}{s} - 2^d(P_4(d)+2)\frac{N}{s^2}(a\log N - b\log s + c)^2$$
$$- 2^{d+1}(P_4(d)+2)\frac{bN}{s^2}(a\log N - b\log s + c) + P_2(d)M$$

MLFMM Complexity(2)

For asymptotic optimum s we can consider $a\log N - b\log s \sim a\log N$, so

$$s_{opt} \sim \left[\frac{2^d (P_4(d) + 2) a^2 \log N}{P_2(d) M} \right]^{1/2} \sim \left[\frac{N \log^2 N}{M} \right]^{1/2} \sim \log N.$$

$$CostMLFMM_{opt} \sim O(N \log N).$$

Different schemes for error estimate are possible.