MAIT 627 Fast Multipole Methods

Lecture 13

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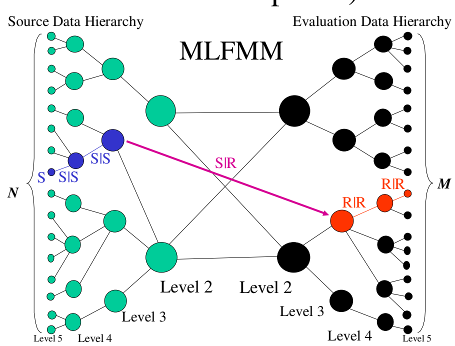
Outline

- 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

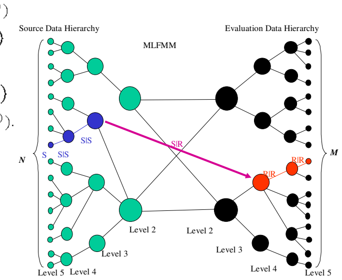
A scheme for error evaluation (1)

(How one source contributes to one evaluation points)



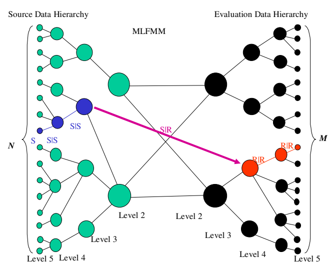
A scheme for error evaluation (2)

$$\Phi(\mathbf{y},\mathbf{x}_k) = \sum_{m=0}^{\infty} C_m^{(L)}(\mathbf{x}_k,\mathbf{x}_*^{(L)}) S_m(\mathbf{y}-\mathbf{x}_*^{(L)}) = \mathbf{C}^{(L)}(\mathbf{x}_k,\mathbf{x}_*^{(L)}) \cdot \mathbf{S}(\mathbf{y}-\mathbf{x}_*^{(L)})$$
$$= \mathbf{C}^{(L-1)}(\mathbf{x}_k,\mathbf{x}_*^{(L-1)}) \cdot \mathbf{S}(\mathbf{y}-\mathbf{x}_*^{(L-1)})$$
$$= \ldots = \mathbf{C}^{(l)}(\mathbf{x}_k,\mathbf{x}_*^{(l)}) \cdot \mathbf{S}(\mathbf{y}-\mathbf{x}_*^{(l)})$$
$$= \mathbf{D}^{(l)}(\mathbf{x}_k,\mathbf{y}_*^{(l)}) \cdot \mathbf{R}(\mathbf{y}-\mathbf{y}_*^{(l)})$$
$$= \mathbf{D}^{(l+1)}(\mathbf{x}_k,\mathbf{y}_*^{(l+1)}) \cdot \mathbf{R}(\mathbf{y}-\mathbf{y}_*^{(l+1)})$$
$$= \ldots = \mathbf{D}^{(L)}(\mathbf{x}_k,\mathbf{y}_*^{(L)}) \cdot \mathbf{R}(\mathbf{y}-\mathbf{y}_*^{(L)}).$$



A scheme for error evaluation (3)

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



A scheme for error evaluation (4)

Consider computation of the final coefficients with p-truncated matrices

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

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

So:

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

A scheme for error evaluation (5)

p-truncated functions:

$$\begin{aligned}
\widehat{\Phi}_L(\mathbf{y},\mathbf{x}_k) &= \widehat{C}^{(L)}(\mathbf{x}_k,\mathbf{x}_*^{(L)})\cdot S(\mathbf{y}-\mathbf{x}_*^{(L)})\\
\widehat{\Phi}_{L-1}(\mathbf{y},\mathbf{x}_k) &= \widehat{C}^{(L-1)}(\mathbf{x}_k,\mathbf{x}_*^{(L-1)})\cdot S(\mathbf{y}-\mathbf{x}_*^{(L-1)})\\
&\ldots\\
\widehat{\Phi}_l(\mathbf{y},\mathbf{x}_k) &= \widehat{C}^{(l)}(\mathbf{x}_k,\mathbf{x}_*^{(l)})\cdot S\left(\mathbf{y}-\mathbf{x}_*^{(l)}\right)\\
\widehat{\Psi}_l(\mathbf{y},\mathbf{x}_k) &= \widehat{D}^{(l)}(\mathbf{x}_k,\mathbf{y}_*^{(l)})\cdot R\left(\mathbf{y}-\mathbf{y}_*^{(l)}\right)\\
\widehat{\Psi}_{l+1}(\mathbf{y},\mathbf{x}_k) &= \widehat{D}^{(l+1)}(\mathbf{x}_k,\mathbf{y}_*^{(l+1)})\cdot R\left(\mathbf{y}-\mathbf{y}_*^{(l+1)}\right)\\
&\ldots\\
\widehat{\Psi}_L(\mathbf{y},\mathbf{x}_k) &= \widehat{D}^{(L)}(\mathbf{x}_k,\mathbf{y}_*^{(L)})\cdot R(\mathbf{y}-\mathbf{y}_*^{(L)}).
\end{aligned}$$

The error comes only from truncation operator

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

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

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

1

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:

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

$$= \left|\sum_{m=0}^{p-1} \widehat{C_m}^{(\alpha)} S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)}) - \sum_{n=0}^{p-1} \widehat{C_n}^{(\alpha+1)} S_n(\mathbf{y}-\mathbf{x}_*^{(\alpha+1)})\right|$$

$$= \left|\sum_{m=0}^{p-1}\sum_{n=0}^{p-1} (S|S)_{mn}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)})\widehat{C_n}^{(\alpha+1)} S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)})\right.$$

$$\left. - \sum_{n=0}^{p-1} \widehat{C_n}^{(\alpha+1)} \sum_{m=0}^{\infty} (S|S)_{nm}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)}) S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)})\right|$$

$$= \left|\sum_{n=0}^{p-1} \widehat{C_n}^{(\alpha+1)} \sum_{m=p}^{\infty} (S|S)_{nm}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)}) S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)})\right|$$

$$\leqslant \sum_{n=0}^{p-1}\sum_{m=p}^{\infty} \left|\widehat{C_n}^{(\alpha+1)} (S|S)_{nm}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)}) S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)})\right|$$

$$< \sum_{n=0}^{\infty}\sum_{m=p}^{\infty} \left|\widehat{C_n}^{(\alpha+1)} (S|S)_{nm}(\mathbf{x}_*^{(\alpha)} - \mathbf{x}_*^{(\alpha+1)}) S_m(\mathbf{y}-\mathbf{x}_*^{(\alpha)})\right| < \epsilon_{\max}(p).$$

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

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

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

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

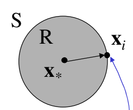
$|y - x_*| > |x_i - x_*|$:

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

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

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

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

So

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

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

S|S-operator

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

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

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

$$= (y - x_{*2})^{-n-1} \left[1 - \frac{x_{*1} - x_{*2}}{y - x_{*2}}\right]^{-n-1}$$

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

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

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

Note: this is correct, but usually we use $t = x_{*1} - x_{*2}$, in which case we need to change the sign of t.

S|S-operator (2)

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

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

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

Note: this is correct, but usually we use $t = x_{*1} - x_{*2}$, in which case we need to change the sign of t.

R|R-operator

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

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

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

Note: this is correct, but usually we use $t = x_{*1} - x_{*2}$, in which case we need to change the sign of t.

R|R-operator(2)

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

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

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

Note: this is correct, but usually we use $t = x_{*1} - x_{*2}$, in which case we need to change the sign of t.

S-Expansion Error

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

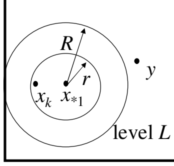
$$b_m(x_k, x_{*1}) = (x_k - x_{*1})^m, \quad m = 0, 1, \dots,$$

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

Assume

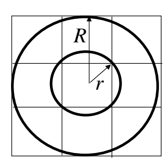
$$|x_k - x_{*1}| \leqslant r, \quad |y - x_{*1}| \geqslant R.$$

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

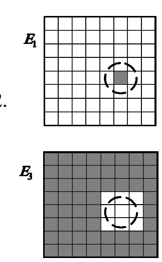


S-Expansion Error

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



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



S|S-Translation Error

Translation from level α+1 to α:

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

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

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

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!

Note: this is correct, but usually we use $t = x_{*1} - x_{*2}$, in which case we need to change the sign of t.

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:

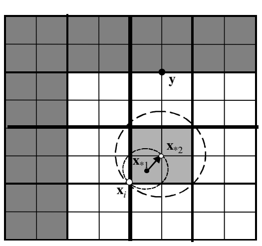
$$\left|\Phi(\mathbf{y},\mathbf{x}_k) - \widehat{\Phi}_\alpha(\mathbf{y},\mathbf{x}_k)\right| \leqslant \left(\frac{2^{L-\alpha}r}{2^{L-\alpha}R}\right)^p \frac{1}{2^{L-\alpha}(R-r)}$$
$$\leqslant \left(\frac{r}{R}\right)^p \frac{1}{(R-r)} = ExpansionError(p,R,r)$$

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

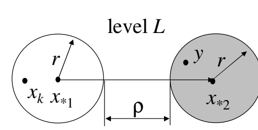
Note that in result of S|S-translations, first p coefficients are exact!

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

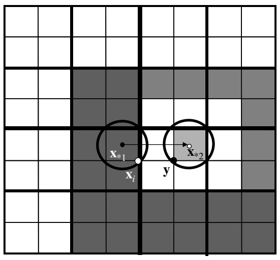
$$|x_k - x_{*1}| \leqslant 2^{L-l}r, \quad |y-x_{*2}| \leqslant 2^{L-l}r, \quad |x_{*2} - x_{*1}| \geqslant 2^{L-l}r + 2^{L-l}r + 2^{L-l}\rho$$

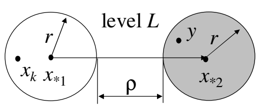
Translation with p –truncated operator $(S|R)_{mn}^{(p)}(t)$ yields

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



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)

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

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

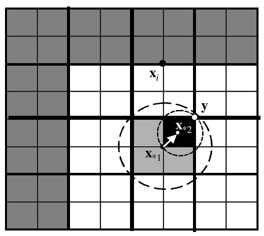
$$= \frac{2}{2^{L-l}r(1 + \frac{\rho}{r})^{p+1}} \frac{1}{1 - \frac{1}{1+\rho/r}} = \frac{2}{2^{L-l}r(1 + \frac{\rho}{r})^{p+1}} \frac{r}{\rho}\left(1 + \frac{\rho}{r}\right)$$

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

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)

$$
\begin{aligned}
&\left|\widehat{\Psi}_{\alpha}(\mathbf{y},\mathbf{x}_k)-\widehat{\Psi}_{\alpha+1}(\mathbf{y},\mathbf{x}_k)\right| \\
&=\left|\sum_{n=0}^{p-1}\widehat{D_n}^{(\alpha)}R_n(\mathbf{y}-\mathbf{y}_*^{(\alpha)})-\sum_{m=0}^{p-1}\widehat{D_m}^{(\alpha+1)}R_m(\mathbf{y}-\mathbf{y}_*^{(\alpha+1)})\right| \\
&=\left|\sum_{n=0}^{p-1}\sum_{m=0}^{\infty}(R|R)_{mn}(\mathbf{y}_*^{(\alpha+1)}-\mathbf{y}_*^{(\alpha)})\widehat{D_n}^{(\alpha)}R_m(\mathbf{y}-\mathbf{y}_*^{(\alpha+1)})\right. \\
&\qquad\left.-\sum_{m=0}^{p-1}\sum_{n=0}^{p-1}(R|R)_{mn}(\mathbf{y}_*^{(\alpha+1)}-\mathbf{y}_*^{(\alpha)})\widehat{D_n}^{(\alpha)}R_m(\mathbf{y}-\mathbf{y}_*^{(\alpha+1)})\right| \\
&=\left|\sum_{n=0}^{p-1}\sum_{m=p}^{\infty}(R|R)_{mn}(\mathbf{y}_*^{(\alpha+1)}-\mathbf{y}_*^{(\alpha)})\widehat{D_n}^{(\alpha)}R_m(\mathbf{y}-\mathbf{y}_*^{(\alpha+1)})\right| = 0.
\end{aligned}
$$

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)

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

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

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

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

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

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

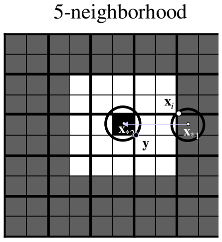
p	10	20	30	40
$\epsilon, <$	$6 \cdot 1\bar{0}^{2}$	$9 \cdot 10^{-3}$	$2 \cdot 10^{-7}$	$3 \cdot 10^{-12}$

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

p	40	50	60	70
$\epsilon, <$	$8 \cdot 10^{-2}$	$5 \cdot 10^{-4}$	$3 \cdot 10^{-6}$	$2 \cdot 10^{-8}$

Total Error(4). 2-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). 2-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 (1,2, 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)

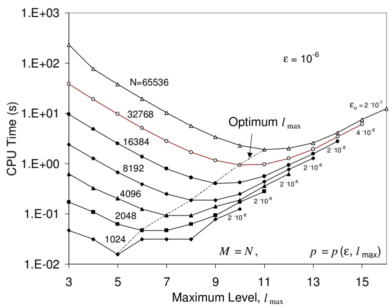
For asymptotic optimum s we can consider $a\log N - b\log s \sim a\log N$, so

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

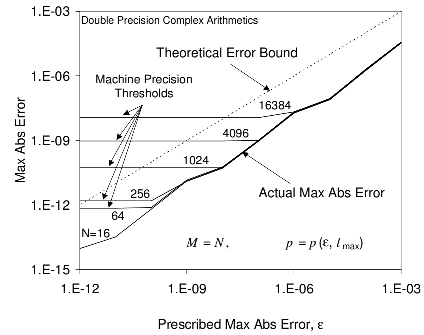
$$CostMLFMM_{opt} \sim O(N\log N).$$

Different schemes for error estimate are possible.

Optimum max level (experiment)



Effects of Machine Precision (1)

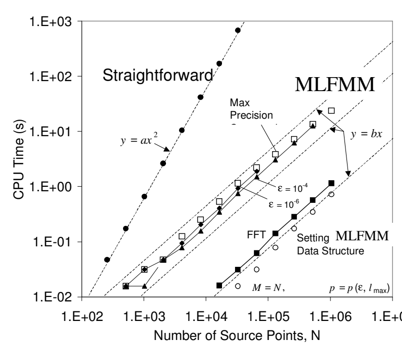


Effects of Machine Error (2)

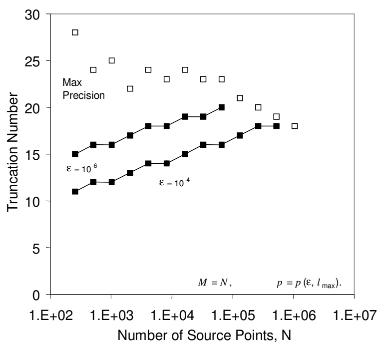
Two different computational problems:

1) Compute with a given prescribed accuracy;
2) Compute with a machine precision for a given type of float numbers.

Effects of Machine Error (3)



Effects of Machine Error (4)



Effects of Machine Error (5)

If the cost of search is $O(1)$,
then for computations with fixed machine precision

$$CostMLFMM_{opt} = O(N)$$