

# FMM CMSC 878R/AMSC 698R

## Lecture 3

# Outline

- Factorization – One of key parts of the FMM.
  - Necessary for fast summation
    - Today's class: Discuss strategies for creating factored series representations
- Types of Functions  $\Phi$ 
  - The function  $\Phi$  is also called a “field” or a “potential”
  - Singular and Regular Fields
  - Far Field and Near Field
- Local Expansions (R-expansions)
  - Local Expansions of Regular and Singular Potentials
  - Power Series
  - Taylor Series

# Matrix-Vector Multiplication

Compute matrix-vector product

$$\mathbf{v} = \Phi \mathbf{u},$$

If

$$\Phi_{ji} = \Phi(\mathbf{y}_j, \mathbf{x}_i), \quad j = 1, \dots, M, \quad i = 1, \dots, N,$$

or

$$\Phi = \begin{pmatrix} \Phi_{11} & \Phi_{12} & \dots & \Phi_{1N} \\ \Phi_{21} & \Phi_{22} & \dots & \Phi_{2N} \\ \dots & \dots & \dots & \dots \\ \Phi_{M1} & \Phi_{M2} & \dots & \Phi_{MN} \end{pmatrix} = \begin{pmatrix} \Phi(\mathbf{y}_1, \mathbf{x}_1) & \Phi(\mathbf{y}_1, \mathbf{x}_2) & \dots & \Phi(\mathbf{y}_1, \mathbf{x}_N) \\ \Phi(\mathbf{y}_2, \mathbf{x}_1) & \Phi(\mathbf{y}_2, \mathbf{x}_2) & \dots & \Phi(\mathbf{y}_2, \mathbf{x}_N) \\ \dots & \dots & \dots & \dots \\ \Phi(\mathbf{y}_M, \mathbf{x}_1) & \Phi(\mathbf{y}_M, \mathbf{x}_2) & \dots & \Phi(\mathbf{y}_M, \mathbf{x}_N) \end{pmatrix}.$$

we need to compute the following sums:

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

Generally we have two sets of  $d$ -dimensional points:

$$\begin{aligned} \mathbb{X} &= \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}, & \mathbf{x}_i &\in \mathbb{R}^d, & i &= 1, \dots, N, \\ \mathbb{Y} &= \{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_M\}, & \mathbf{y}_j &\in \mathbb{R}^d, & j &= 1, \dots, M. \end{aligned}$$

We call one of these sets, say  $\mathbb{X}$ , “set of sources”, while the other set, say  $\mathbb{Y}$ , “evaluation points”.

# Why Consider $\mathbf{R}^d$ ?

- Many problems are posed in higher dimensions
- $d = 1$ 
  - Scalar functions, interpolation, etc.
- $d = 2, 3$ 
  - Physical problems in 2 and 3 dimensional space
- $d = 4$ 
  - 3D Space + time, 3D grayscale images
- $d = 5$ 
  - Color 2D images, Motion of 3D grayscale images
- $d = 6$ 
  - Color 3D images
- $d = 7$ 
  - Motion of 3D color images
- $d = \textit{arbitrary}$ 
  - $d$ -parametric spaces, statistics, database search procedure

# Fields (Potentials)

$$\Phi(\mathbf{y}_j, \mathbf{x}_i) = \sum_{m=0}^{\infty} a_m(\mathbf{x}_i) f_m(\mathbf{y}_j) = \sum_{m=0}^p a_m(\mathbf{x}_i) f_m(\mathbf{y}_j) + \text{Error}(p; \mathbf{x}_i, \mathbf{y}_j)$$

where  $p$  is the truncation number.

Extension for arbitrary  $\mathbf{y}$  (turns  $\Phi$  to be a function of  $\mathbf{y}$ ):

$$\Phi(\mathbf{y}, \mathbf{x}_i) = \sum_{m=0}^{\infty} a_m(\mathbf{x}_i) f_m(\mathbf{y}) = \sum_{m=0}^p a_m(\mathbf{x}_i) f_m(\mathbf{y}) + \text{Error}(p; \mathbf{x}_i, \mathbf{y}), \quad \mathbf{y} \in \mathbb{R}^d.$$

Sum is also a function of  $\mathbf{y}$  :

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

$$v(\mathbf{y}) = \sum_{i=1}^N u_i \Phi(\mathbf{y}, \mathbf{x}_i), \quad \mathbf{y} \in \mathbb{R}^d,$$
$$v_j = v(\mathbf{y}_j), \quad j = 1, \dots, M.$$

Fields are continuous!  
(Almost everywhere)

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

# Examples of Fields (functions)

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

## Scalar Fields:

● Gravity

(singular at  $\mathbf{y}=\mathbf{x}_i$ )

$$\Phi(\mathbf{y}, \mathbf{x}_i) = \frac{1}{|\mathbf{y} - \mathbf{x}_i|}$$

● Monochromatic Wave ( $k$  is the wavenumber)

(singular at  $\mathbf{y}=\mathbf{x}_i$ )

$$\Phi(\mathbf{y}, \mathbf{x}_i) = \frac{e^{ik|\mathbf{y} - \mathbf{x}_i|}}{|\mathbf{y} - \mathbf{x}_i|}$$

● Gaussian

(regular everywhere)

$$\Phi(\mathbf{y}, \mathbf{x}_i) = \{-|\mathbf{y} - \mathbf{x}_i|^2/\sigma\}$$

## Vector Field:

● 3D Velocity field:

(singular at  $\mathbf{y}=\mathbf{x}_i$ )

$$\Phi(\mathbf{y}, \mathbf{x}_i) = \nabla_{\mathbf{y}} \frac{1}{|\mathbf{y} - \mathbf{x}_i|} = \mathbf{i}_1 \frac{\partial}{\partial y_1} \frac{1}{|\mathbf{y} - \mathbf{x}_i|} + \mathbf{i}_2 \frac{\partial}{\partial y_2} \frac{1}{|\mathbf{y} - \mathbf{x}_i|} + \mathbf{i}_3 \frac{\partial}{\partial y_3} \frac{1}{|\mathbf{y} - \mathbf{x}_i|},$$
$$\mathbf{y} = (y_1, y_2, y_3) \in \mathbb{R}^3.$$

# Far Field and Near Field

Region far /near from source where there is a simplified factorization or description

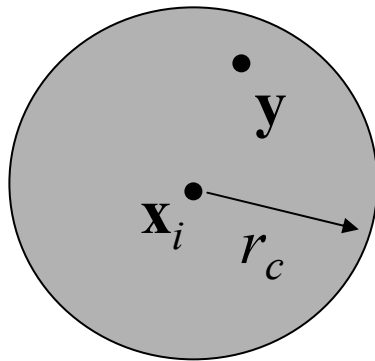
● Near Field of the  $i$ th source:

$$|\mathbf{y} - \mathbf{x}_i| < r_c.$$

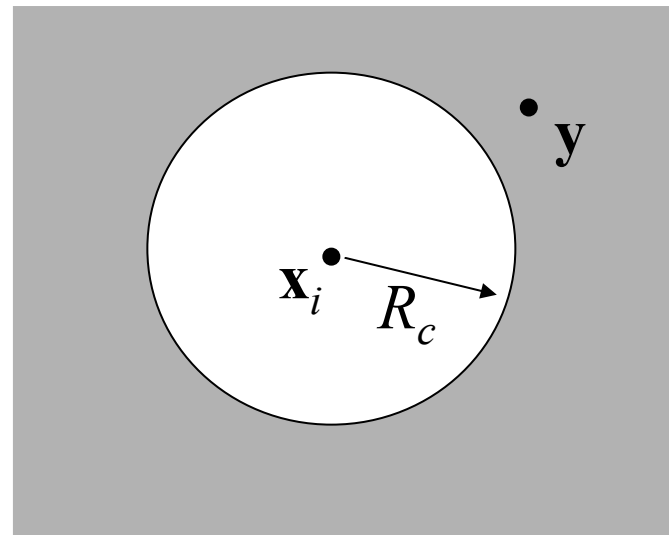
● Far Field of the  $i$ th source:

$$|\mathbf{y} - \mathbf{x}_i| > R_c.$$

Near Field



Far Field



What are these  $r_c$  and  $R_c$  ?

depends on the potential + some conventions for the terminology

# Local (Regular) Expansion

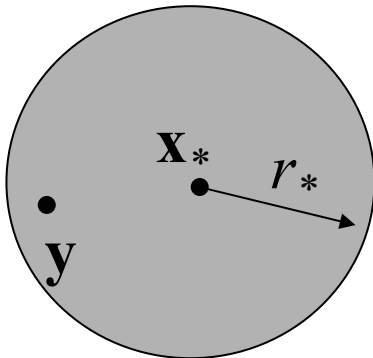
Do not confuse with the Near Field!

Let

We call expansion

local (regular) inside a sphere

if the series converges for  $\forall \mathbf{y}, |\mathbf{y} - \mathbf{x}_*| < r_*$ .



$$\mathbf{x}_* \in \mathbb{R}^d.$$

Basis  
Functions

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

$$|\mathbf{y} - \mathbf{x}_*| < r_*,$$

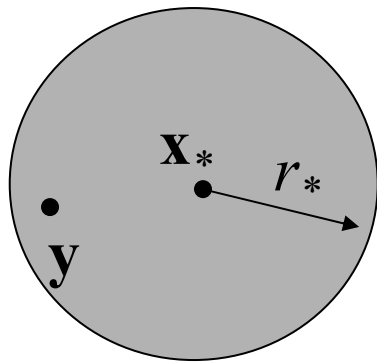
Expansion  
Coefficients

**We also call this R-expansion,**  
since basis functions  $R_m$  should be *regular*  
Regular functions are “finite” functions

# Local Expansion of a Regular Function

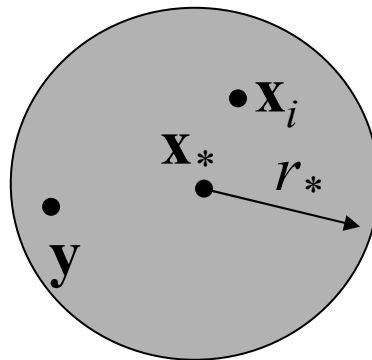
- Region of validity

Can be like this:  $\bullet \mathbf{x}_i$



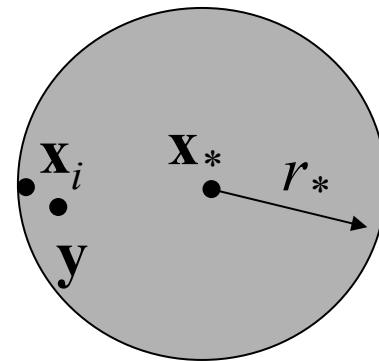
$$|\mathbf{y} - \mathbf{x}_*| < r_* < |\mathbf{x}_i - \mathbf{x}_*|$$

...or like this:



$$r_* > |\mathbf{y} - \mathbf{x}_*| > |\mathbf{x}_i - \mathbf{x}_*|$$

...or like this:



$$r_* > |\mathbf{x}_i - \mathbf{x}_*| > |\mathbf{y} - \mathbf{x}_*|$$

# Local Expansion of a Regular Function (Example)

$$x, y \in \mathbb{R}^1.$$

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

$$\Phi(y, x_i) = e^{-(y-x_i)^2}.$$

Looking for factorization:

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

We have

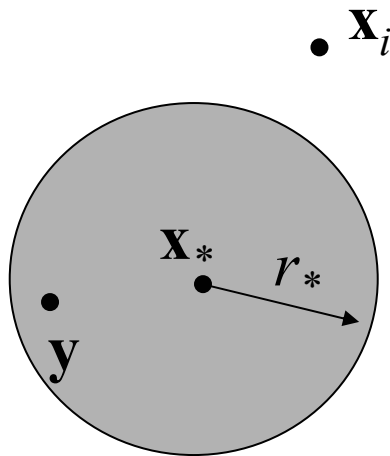
$$\begin{aligned} e^{-(y-x_i)^2} &= e^{-(y-x_* - (x_i-x_*))^2} = e^{-(y-x_*)^2} e^{-(x_i-x_*)^2} e^{2(x_i-x_*)(y-x_*)} \\ &= e^{-(y-x_*)^2} e^{-(x_i-x_*)^2} \sum_{m=0}^{\infty} \frac{2^m (x_i - x_*)^m (y - x_*)^m}{m!}. \end{aligned}$$

Choose

$$\begin{aligned} a_m(x_i - x_*) &= e^{-(x_i-x_*)^2} \sqrt{\frac{2^m}{m!}} (x_i - x_*)^m, \quad m = 0, 1, \dots, \\ R_m(y - x_*) &= e^{-(y-x_*)^2} \sqrt{\frac{2^m}{m!}} (y - x_*)^m, \quad m = 0, 1, \dots \end{aligned}$$

# Local Expansion of a Singular Potential

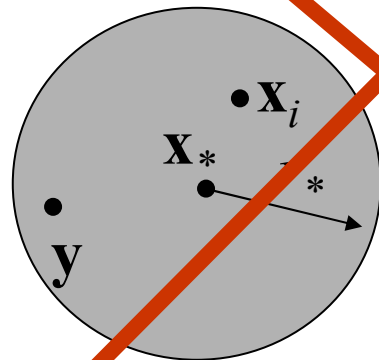
Can be like this:



$$|\mathbf{y} - \mathbf{x}_*| < r_* \leq |\mathbf{x}_i - \mathbf{x}_*|$$

Like this only!

...or like this:

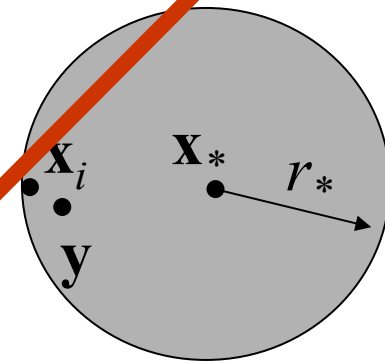


$$r_* > |\mathbf{y} - \mathbf{x}_*| > |\mathbf{x}_i - \mathbf{x}_*|$$

Never ever!

Because  $\mathbf{x}_i$  is a singular point!

...or like this:



$$r_* \geq |\mathbf{x}_i - \mathbf{x}_*| > |\mathbf{y} - \mathbf{x}_*|$$

# Local Expansion of a Singular Potential (Example)

$$x, y \in \mathbb{R}^1.$$

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

Looking for factorization:

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

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

We have

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

Geometric progression:

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

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

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

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

# Power Series

- Classic example of local regular expansions
- Monomials form a basis

Power series relative to real or complex variable  $y$  is a series of type

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

where  $a_m$  are real or complex numbers.

# Properties of Power Series

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

For any number  $q$ , such that  $0 < q < r_*$ , the power series uniformly converges at  $|y - x_*| < q$ .

# Properties of Power Series

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

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

The power series can be differentiated term by term at  $|y-x_*| < r_*$  and integrated over any closed interval included in  $|y-x_*| < r_*$ .

Differentiated or integrated series (if integration is taken from  $x_*$  to  $y-x_*$ ) have the same convergence radius  $r_*$ .

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

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

Cauchy's rule



$$\left[ \sum_{m=0}^{\infty} a_m (y-x_*)^m \right] \left[ \sum_{m=0}^{\infty} b_m (y-x_*)^m \right] = \sum_{n=0}^{\infty} \left[ \sum_{m=0}^n a_m b_{n-m} \right] (y-x_*)^n$$

# Properties of Power Series

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

# For those who love proofs

Prove the above properties!

(Not a course formal requirement, but a good exercise)

# Taylor Series (Finite)

- Definition for a function which possesses a known finite number of derivatives

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

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

Cauchy's evaluation:

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

Lagrange evaluation:

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

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

# Taylor Series (Infinite)

- Extended definition for a function with infinite number of derivatives

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

$$\lim_{n \rightarrow \infty} \text{Residual}_n(y) = 0,$$

Then

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

$T_n$  converges to  $f(y)$  for any  $|y - x_*| \leq q$ , where  $0 \leq q \leq r$ .

# Local 1D Taylor Expansion

Looking for a local expansion

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

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

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

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

# Local 1D Taylor Expansion (Example)

- Creating a factorization of a function using a Taylor series

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

- Evaluate error bound

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

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

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

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

$$|\text{Residual}_n(y)| \leq \frac{|y - x_*|^n}{n!} \max_{x_* - \alpha < y < x_* + \alpha} \left| \frac{\partial^n \Phi}{\partial y^n}(y, x_i) \right| < \frac{\alpha^n}{n!} x_i^n e^{x_i(x_* + \alpha)}.$$

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

$$|\text{Residual}_5(y)| < \frac{e}{2^5 5!} < \frac{3}{32 \cdot 120} = \frac{1}{1280} < 10^{-3}.$$

# Multidimensional Taylor Series

Let  $f(\mathbf{y})$  be a real function,

$$f(\mathbf{y}) \in D^\infty(\mathbf{U}_{\mathbf{x}_*}), \quad \mathbf{y} = (y_1, \dots, y_d) \in \mathbf{U}_{\mathbf{x}_*} \subset \mathbb{R}^d, \quad \mathbf{x}_* = (x_{*1}, \dots, x_{*d}) \in \mathbb{R}^d$$

Then we can write

$$f(\mathbf{y}) = f(y_1, y_2, \dots, y_d)$$

$$\begin{aligned} f(y_1, y_2, \dots, y_d) &= \sum_{m_1=0}^{\infty} \frac{1}{m_1!} \frac{\partial^{m_1} f}{\partial y_1^{m_1}}(x_{*1}, y_2, \dots, y_d) (y_1 - x_{*1})^{m_1} \\ &= \sum_{m_1=0}^{\infty} \frac{1}{m_1!} \sum_{m_2=0}^{\infty} \frac{1}{m_2!} \frac{\partial^{m_1}}{\partial y_1^{m_1}} \frac{\partial^{m_2}}{\partial y_2^{m_2}} f(x_{*1}, x_{*2}, \dots, y_d) (y_1 - x_{*1})^{m_1} (y_2 - x_{*2})^{m_2} \\ &= \dots \\ &= \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \dots \sum_{m_d=0}^{\infty} \frac{\partial^{m_1}}{\partial y_1^{m_1}} \frac{\partial^{m_2}}{\partial y_2^{m_2}} \dots \frac{\partial^{m_d}}{\partial y_d^{m_d}} f(x_{*1}, x_{*2}, \dots, x_{*d}) \prod_{i=1}^d \frac{1}{m_i!} (y_i - x_{*i})^{m_i}. \end{aligned}$$