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

\[ \Phi_{ji} = \Phi(y_j, x_i), \quad j = 1, \ldots, M, \quad i = 1, \ldots, N, \]

or

\[
\Phi = \begin{pmatrix}
\Phi_{11} & \Phi_{12} & \cdots & \Phi_{1N} \\
\Phi_{21} & \Phi_{22} & \cdots & \Phi_{2N} \\
& & \ddots & \vdots \\
\Phi_{M1} & \Phi_{M2} & \cdots & \Phi_{MN}
\end{pmatrix} = \begin{pmatrix}
\Phi(y_1, x_1) & \Phi(y_1, x_2) & \cdots & \Phi(y_1, x_N) \\
\Phi(y_2, x_1) & \Phi(y_2, x_2) & \cdots & \Phi(y_2, x_N) \\
& & \ddots & \vdots \\
\Phi(y_M, x_1) & \Phi(y_M, x_2) & \cdots & \Phi(y_M, x_N)
\end{pmatrix}.
\]

we need to compute the following sums:

\[ v_j = \sum_{i=1}^{N} u_i \Phi(y_j, x_i), \quad j = 1, \ldots, M. \]

Generally we have two sets of \(d\)-dimensional points:

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

We call one of these sets, say \(\mathbf{X}\), “set of sources”, while the other set, say \(\mathbf{Y}\), “evaluation points”.
Why Consider $\mathbb{R}^d$?

- 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
- $d = \text{arbitrary}$
  - d-parametric spaces, statistics, database search procedure
Fields (Potentials)

\[
\Phi(y_j, x_i) = \sum_{m=0}^{\infty} a_m(x_i)f_m(y_j) = \sum_{m=0}^{p} a_m(x_i)f_m(y_j) + Error(p; x_i, y_j)
\]

where \( p \) is the truncation number.

Extension for arbitrary \( y \) (turns \( \Phi \) to be a function of \( y \)):

\[
\Phi(y, x_i) = \sum_{m=0}^{\infty} a_m(x_i)f_m(y) = \sum_{m=0}^{p} a_m(x_i)f_m(y) + Error(p; x_i, y), \quad y \in \mathbb{R}^d.
\]

Sum is also a function of \( y \):

**Field (Potential) of a single \((i\text{th})\) unit source**

**Fields are continuous!**

\((\text{Almost everywhere})\)

**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 \( y = x_i \))

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

- **Monochromatic Wave (\( \kappa \) is the wavenumber)**
  
  (singular at \( y = x_i \))

  \[
  \Phi(y, x_i) = \frac{j\kappa|y - x_i|}{|y - x_i|}
  \]

- **Gaussian**
  
  (regular everywhere)

  \[
  \Phi(y, x_i) = \{-|y - x_i|^2/\sigma\}
  \]

Vector Field:
- **3D Velocity field**:
  
  (singular at \( y = x_i \))

  \[
  \Phi(y, x_i) = \nabla y \frac{1}{|y - x_i|} = i_1 \frac{\partial}{\partial y_1} \frac{1}{|y - x_i|} + i_2 \frac{\partial}{\partial y_2} \frac{1}{|y - x_i|} + i_3 \frac{\partial}{\partial y_3} \frac{1}{|y - x_i|},
  \]

  \[
  y = (y_1, y_2, y_3) \in \mathbb{R}^3.
  \]
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:
  \[ |y - x_i| < r_c. \]

- Far Field of the $i$th source:
  \[ |y - x_i| > R_c. \]

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

\[ x_+ \in \mathbb{R}^d. \]

We call expansion

local (regular) inside a sphere

if the series converges for \( \forall y, \ |y - x_+| < r_+ \).

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

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: $x_i$

...or like this:

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

...or like this:

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

$r_* > |y - x_*| > |x_i - x_*|$
Local Expansion of a Regular Function (Example)

Valid for any \( r_* < \infty \), and \( x_i \):

\[
\Phi(y, x_i) = e^{-\psi - x_i y}.
\]

Looking for factorization:

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

We have

\[
es^{-y-x_i} = e^{-(y-x_*)} e^{-(x_i-x_*)} = e^{-(y-x_*)} e^{-(x_i-x_*)} e^{2(y-x_*) (y-x_*)}
\]

\[
= e^{-(y-x_*)} e^{-(x_i-x_*)} \sum_{m=0}^{\infty} \frac{2^m (x_i - x_*)^m (y - x_*)^m}{m!}.
\]

Choose

\[
\alpha_m(x_i - x_*) = e^{-(x_i-x_*)} \sqrt{\frac{2^m}{m!}} (x_i - x_*)^m, \quad m = 0, 1, \ldots,
\]

\[
R_m(y-x_*) = e^{-\psi - x_i y} \sqrt{\frac{2^m}{m!}} (y - x_*)^m, \quad m = 0, 1, \ldots
\]
Local Expansion of a Singular Potential

Can be like this:

\[ |y - x_*| < r_* \leq |x_i - x_*| \]

Like this only!

\[ r_* > |y - x_*| > |x_i - x_*| \]

Never ever!

Because \( x_i \) is a singular point!
Local Expansion of a Singular Potential (Example)

Looking for factorization:

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

We have

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

Geometric progression:

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

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

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

$$\mathcal{R}_m(y-x_*) = (y-x_*)^m, \quad m = 0, 1, ...$$
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 $r_*$.

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

\[
f(y) = f(x_*) + f'(x_*)(y - x_*) + \frac{1}{2!}f''(x_*)(y - x_*)^2 + \ldots + \frac{1}{(r_*)!}f^{(r_*)}(x_*)(y - x_*)^{r_*} + \text{Residual}_n(y).
\]

Cauchy’s evaluation:

\[
|\text{Residual}_n(y)| \leq \frac{|y - x_*|^n}{r_*!} \int_{x_*}^{y} f^{(r_*)}(x) \, dx.
\]

Lagrange evaluation:

\[
\text{Residual}_n(y) = \int_{x_*}^{y} dx \int_{x_*}^{x} dx \ldots \int_{x_*}^{x} f^{(r_*)}(x) \, dx = \frac{1}{r_*!} f^{(r_*)}(X)(y - x_*)^{r_*},
\]

where \( X \in (x_*, x_* + r_*). \)

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

\[
\lim_{n \to \infty} \text{Residual}_n(y) = 0,
\]

Then

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

It converges to \( f(y) \) for any \( |y - x_*| < q \), where \( 0 \leq q \leq r \).
Local 1D Taylor Expansion

Looking for a local expansion

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

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

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

\[
R_m(y-x_*) = (y-x_*)^m, \quad m = 0, 1, \ldots
\]
Local 1D Taylor Expansion (Example)

- Creating a factorization of a function using a Taylor series
  \[ \Phi(y, x_i) = e^{xy}. \]

- Evaluate error bound
  \[ \frac{\partial^m \Phi(y, x_i)}{\partial y^m} (y, x_i) = x_i^m e^{xy}, \quad \frac{\partial^m \Phi(x_*, x_i)}{\partial y^m} (x_*, x_i) = x_i^m e^{x_*}, \]

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

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

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

\[ |\text{Residuals}(y)| \leq \frac{|y - x_*|^n}{n!} \bigg|_{x_+ - \alpha < y < x_* + \alpha} \frac{\partial^n \Phi}{\partial y^n} (y, x_i) \leq \frac{\alpha^n}{n!} x_i^n e^{x_*(x_+ + \alpha)}. \]

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

\[ |\text{Residuals}(y)| \leq \frac{e}{25 \cdot 5!} < \frac{3}{32 \cdot 120} = \frac{1}{1280} < 10^{-3}. \]
Multidimensional Taylor Series

Let $f(y)$ be a real function,

\[ f(y) \in D^\infty(U_{x_+}), \quad y = (y_1, ..., y_d) \in U_{x_+} \subset \mathbb{R}^d, \quad x_+ = (x_{+1}, ..., x_{+d}) \subset \mathbb{R}^d \]

Then we can write

\[ f(y) = f(y_1, y_2, ..., y_d) \]

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