FMM CMSC 878R/AMSC 698R

Lecture 6
Outline

• General Forms of Factorization for Fast Summation
• Far Field Expansions (or S-expansions)
• Approaches for Selection Basis Functions
• Introduction to Functional Analysis
General Forms of Factorization for Fast Summation (1)

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

\[
\Phi(y_j, x_i) = \sum_{m=0}^{p} a_m(x_i, x_*) f_m(y_j - x_*) + \text{Error}(p, x_i, x_*, y_j)
\]

scalar product

\[ = a(x_i, x_*) \cdot f(y_j - x_*) + \text{Error}. \]

How about vectors of length \( p \)

\[ v_j = \sum_{i=1}^{N} u_i e^{-\lambda_j |x_i - y_j|^2} \]

Some parameter depending on \( i \)

More general to have

\[ v_j = \sum_{i=1}^{N} u_i \Phi_i(y_j) \quad \text{or} \quad v(y) = \sum_{i=1}^{N} u_i \Phi_i(y). \]
General Forms of Factorization for Fast Summation (2)

The potential can be factorized as

\[ \Phi_i(y) = A_i(x_\star) \circ F(y - x_\star) \]

Generalized product \( \circ \) can be scalar product, contraction, etc. \( A_i \) and \( F \) can be real or complex vectors, tensors, etc. in \( p \)-dimensional space.

Requirements to the product (distributivity with respect to addition)

\[ (\alpha A_i + \beta A_j) \circ F = \alpha A_i \circ F + \beta A_j \circ F. \]

In this case

\[ v(y) = \sum_{i=1}^{N} u_i \Phi_i(y) = \sum_{i=1}^{N} u_i A_i(x_\star) \circ F(y - x_\star) = A(x_\star) \circ F(y - x_\star) \]

\[ A(x_\star) = \sum_{i=1}^{N} u_i A_i(x_\star) \]

We do not need commutativity of \( \circ \) (i.e. we do not request \( A_i \circ F = F \circ A_i \)).
General Forms of Factorization for Fast Summation (3)

Actually, we even do need continuous variable y, The problem is to represent all matrix elements in the form

$$
\Phi_{ji} = A_i \circ F_j
$$

then

$$
v_j = \sum_{i=1}^{N} u_i \Phi_{ji} = \sum_{i=1}^{N} u_i (A_i \circ F_j) = \left( \sum_{i=1}^{N} u_i A_i \right) \circ F_j.
$$
Complexity of Fast Summation

Let \( \circ \) be a scalar product of vectors \( A_i \) and \( F_j \) of length \( P(p) \) (\( p \) is the truncation number). Complexity of summation over \( i \) is then \( O(PN) \).

Complexity of scalar product operation is \( P \).

Complexity of \( M \) scalar product operations is \( O(PM) \) (for \( j = 1, \ldots, M \)).

Total complexity is \( O(PM + PN) \).

Fast Method is more efficient than direct only if \( O(PM + PN) < O(MN) \), so we should have

\[
P(p) \ll \min(M, N)
\]
Far Field Expansions
(S-expansions)

Let

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

We call expansion

\[ \Phi(y, x_i) = \sum_{m=0}^{\infty} b_{m^2}(x_i, x_*) S_{m^2}(y - x_*) \]

far field expansion (or S-expansion) outside a sphere

\[ |y - x_*| > R_* \]

if the series converges for \( \forall y, |y - x_*| > R_* \).
Far Field Expansion of a Regular Potential

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

Can be like this:

\[ |x_i - x_*| > |y - x_*| > R_* \]
Local Expansion of a Regular Potential
Can be Far Field Expansion Also
(Repeat Example from Lecture 3)

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

\[ \Phi(y, x_i) = e^{-(y - x_i)^2} = \sum_{m=0}^{\infty} a_m(x_i, x_*) S_m(y - x_*). \]

We have

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

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

Choose

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

\[ S_m(y - x_*) = e^{-(y - x_*)^2} \frac{2^m}{m!} (y - x_*)^m, \quad m = 0, 1, \ldots. \]
Example of Far Field Expansion of a Regular Function (Asymptotic Series)

\[ \Phi(y, x_i) = \frac{1}{1 + (y - x_i)^2} = \sum_{m=0}^{\infty} a_m(x_i, x_*) S_m(y - x_*) \]

Asymptotic Expansion:

\[
\frac{1}{1 + (y - x_i)^2} = \frac{1}{1 + [y - x_* - (x_i - x_*)]^2} \\
= \frac{1}{1 + (y - x_*)^2} \left[ 1 - \frac{2(x_i - x_*)(y - x_*)}{1 + (y - x_*)^2} + \frac{(x_i - x_*)^2}{1 + (y - x_*)^2} \right]^{-1} \\
= \frac{1}{1 + (y - x_*)^2} \left\{ 1 + \frac{2(x_i - x_*)(y - x_*)}{1 + (y - x_*)^2} - \frac{(x_i - x_*)^2}{1 + (y - x_*)^2} \left[ 1 - 4\frac{(y - x_*)^2}{1 + (y - x_*)^2} \right] \right\} \\
+ O \left( \left( \frac{x_i - x_*}{\sqrt{1 + (y - x_*)^2}} \right)^3 \right) \]

Converges, if \(|x_i - x_*| < \sqrt{1 + (y - x_*)^2}\).
Example of Far Field Expansion of a Regular Function (continuation)

\[ \Phi(y, x_i) = \frac{1}{1 + (y - x_i)^2} = \sum_{m=0}^{\infty} a_m(x_i, x_\star) S_m(y - x_\star). \]

Choose

\[ a_m(x_i, x_\star) = (x_i - x_\star)^m, \quad m = 0, 1, \ldots. \]

\[ S_0(y - x_\star) = \frac{1}{1 + (y - x_\star)^2}, \]

\[ S_1(y - x_\star) = \frac{2(y - x_\star)}{[1 + (y - x_\star)^2]^2}, \]

\[ S_2(y - x_\star) = \frac{1 - 3(y - x_\star)^2}{[1 + (y - x_\star)^2]^3}, \]

\[ \vdots \]

\[ S_m(y - x_\star) = O\left(\left[1 + (y - x_\star)^2\right]^{-1-m/2}\right), \]

\[ \vdots \]
Far Field Expansion of a Singular Potential

\[ |y - x*| > R* > |x_i - x*| \]

\[ y - x* > R* \geq |x_i - x*| \]

This case only!
Example For S-expansion of Singular Potential

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

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

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

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

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

\[ S_m(y - x_*) = (y - x_*)^{-m-1}, \quad m = 0, 1, \ldots \]
Let us compare with the R-expansion of the same function

\[ |y - x_*| < |x_i - x_*| : \]

**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!
What Do We Need For Real FMM
(that provides spatial grouping)

We need S-expansion for \(|y - x_*| > R_* > |x_i - x_*|\)
We need R-expansion for \(|y - x_*| < r_* < |x_i - x_*|\)
Basis Functions

- Power series are great, but do they provide the best approximation? (sometimes yes!)
- Other approaches to factorization:
  - Asymptotic Series (Can be divergent!);
  - Orthogonal Bases in $L_2$;
  - Eigen Functions of Differential Operators;
  - Functions Generated by Differentiation or Other Linear Operators.
- Some of this approaches will be considered in this course.
Introduction to Functional Analysis

Source: I. Stakgold: “Green’s Functions and Boundary Value problems” Wiley Interscience, 1979

Goal: Introduce terminology and issues involved.
Linear/Vector Spaces

• Motivation: We have to deal with questions such as
  – What does it mean when an approximation is close to the true value?
  – What basis functions can be used to approximate a function?
  – What is a basis function?
  – How does the approximation converge?
• In the physical world we live in we are endowed with the concept of vectors and distances
• Goal of vector space theory is to imbue functions with this kind of abstract structure
  – Understand functions and their transformations using this structure
Vectors

- A vector \( \mathbf{x} \) of dimension \( d \) represents a point in a \( d \)-dimensional space
- Examples
  - A point in 3D space \([x, y, z]\) or 2D image space \([u, v]\)
  - Point in color space \([r, g, b]\) or \([y, u, v]\)
  - Point in an infinite dimensional functional space on a Fourier basis (coefficients)
  - Point in expansion in terms of power series (coefficients)
- Essentially a short-hand notation to denote a grouping of points
  - No special structure yet
  - Will add structure to it.
• In 3D/2D we have additional structure
  – Distances
  – Angles
  – Geometry …

• We want to understand if there is a way to give high dimensional spaces and infinite dimensional spaces, the same structure so that these questions can be answered.
Linear/Vector Space

- A collection of points that obey certain rules
  - Commutative, existence of a zero element
    \[ u + v = v + u; \quad u + (v + w) = (u + v) + w \]
    \[ \exists 0, \; u + 0 = u \quad \forall u; \quad u + (\neg u) = 0 \]
  - Scalar multiplication
    \[ \alpha (\beta u) = (\alpha \beta) u; \quad 1u = u \]
    \[ (\alpha + \beta) u = \alpha u + \beta u; \quad \alpha (u + v) = \alpha u + \alpha v \]

- Let \( u_1, \ldots, u_k \) be a set of vectors:
  Linear combination
  \[ \alpha_1 u_1 + \cdots + \alpha_k u_k \]
  Manifold spanned by \( u \)
Dependency, dimension, Basis

• Let $\alpha_1 u_1 + \cdots + \alpha_k u_k = 0$
  – if this is true for a set of non zero $\alpha$ the set is dependent
  – If the set is dependent, at least one of the vectors is a linear combination of the others
  – If 0 is a part of the set the set is dependent

• Dimension of a space is the maximum size of an independent set

• Basis: A set of functions $\{h_1, h_2, \ldots, h_k\}$ is a basis for a space if every vector in the space can be expressed as a sum of these vectors in one and only one way
  – The basis functions are independent
  – In an $n$ dimensional space, any set of $n$ independent vectors form a basis
Dependence and dimensionality

• A set of vectors is dependent if for some scalars $\alpha_1, \ldots, \alpha_k$ not all zero we can write

$$\alpha_1 u_1 + \cdots + \alpha_k u_k = 0$$

  - If the zero vector is part of a set of vectors that set is dependent. If a set of vectors is dependent so is any larger set which contains it.

• A linear space is $n$ dimensional if it possesses a set of $n$ independent vectors but every $n+1$ dimensional set is dependent.

• A set of vectors $b_1, \ldots, b_k$ is a basis for a $k$ dimensional space $X$ if each vector in $X$ can be expressed in one and only one way as a linear combination of $b_1, \ldots, b_k$.

• One example of a basis are the vectors $(1,0,\ldots,0)$, $(0,1,\ldots,0)$, $\ldots$, $(0,0,\ldots,1)$.
Lengths and Norms

- We would like to measure distances and directions in the vector space the same way that we do it in Euclidean 3D.
Metric space

- Distance function \(d(u,v)\) makes a vector space a metric space if it satisfies
  - \(d(u,v)>0\) for \(u,v\) different
  - \(d(u,u)=0, \quad d(u,v)=d(v,u)\)
  - \(d(u,w)\leq d(u,v)+d(v,w)\) (triangle inequality)

- Norm ("length").
  - \(\|u\|>0\) for \(u\) not 0, \(\|0\|=0\)
  - \(\|\alpha u\|=|\alpha| \|u\|, \quad \|u+v\| \leq \|u\| + \|v\|\)

- Normed linear space is a metric space with the metric defined by \(d(u,v)=\|u-v\|\) and \(\|u\|=d(u,0)\)
**Limits and Completeness**

- Can use this distance function to define limits of sequences of functions

\[ \lim_{k \to \infty} u_k = u \]

there exists an index \( N \) such that

\[ d(u, u_k) \leq \varepsilon \quad \text{for} \quad k > N \]

- Limit can lie within the space or outside it. IF limits of all convergent sequences inside converge to an element of the space, it is complete.

- Rational numbers are incomplete
  - Transcendentals can be defined as limits of rational sequences
Normed space

- A normed linear space possesses a norm with following properties

\[ ||u|| > 0, \quad u \neq 0 \]
\[ ||0|| = 0 \]
\[ ||\alpha u|| = |\alpha| ||u|| \]
\[ ||u+v|| \leq ||u|| + ||v|| \]

- Knowing norm, we can define a distance function \( d \)

\[ d(u,v) = ||u-v||, \]

- Called “natural metric”

- If space is complete in its natural metric it is called a “Banach” space
• Have not yet define what the “norm” is
• Have a notion of length of vector
• No notion of angle between vectors
  – Inner or “dot” product
Dot Product

- Dot product of two vectors with same dimension
  Recall dot product of two vectors
  \[ \langle x, y \rangle = \sum_{i=1}^{d} x_i y_i = y^t x. \]
- Dot product space behaves like Euclidean \( \mathbb{R}^3 \)
- Dot product defines a norm and a metric.
  \[ \langle u, v \rangle = \langle v, u \rangle \]
  \[ \langle \alpha u, v \rangle = \alpha \langle u, v \rangle \]
  \[ \langle u + v, w \rangle = \langle u, w \rangle + \langle v, w \rangle \]
  \[ \langle u, u \rangle > 0 \text{ for } u \neq 0 \]
- Parallelogram law
  \[ ||u+v||^2 + ||u-v||^2 = 2||u||^2 + 2 ||v||^2 \]
- Orthogonal vectors \( \langle u, v \rangle = 0 \)
- Angle between vectors
  \[ \cos \theta = \frac{\langle x, y \rangle}{||x|| ||y||} \]
• Orthonormal basis -- elements have norm 1 and are perpendicular to each other

• Hilbert space
  – Space that is complete in this inner product

• Other distances and products can also define a space:
  – Mahalanobis distance in statistics
  – Sobolev spaces in FEM
  – RKHS in learning theory
Gram Schmidt Orthogonalization

- Given a basis and this definition can now construct an orthonormal basis
- Gram Schmidt Orthogonalization
- Given a set of basis vectors \((b_1, b_2, \ldots, b_n)\)
  construct an orthonormal basis \((e_1, e_2, \ldots, e_n)\) from it.
  - Set \(e_1 = b_1 / ||b_1||\)
  - \(g_2 = b_2 - <b_2, e_1>e_1, \quad e_2 = g_2 / ||g_2||\)
  - For \(k=3, \ldots, n\)
    \(g_k = b_k - \sum_j <b_k, e_j>e_j, \quad e_k = g_k / ||g_k||\)
Matrices as operators

• Matrix is an operator that takes a vector to another vector.
  – Square matrix takes it to a vector in the space of the same dimension.

• Dot product provides a tool to examine matrix properties
  – Adjoint matrix \( <Au,v> = <u,A^*v> \)
  – Square Matrix fully defined as result of its operation on members of a basis.
    \[
    A_{ij} = <Ab_j,b_i>
    \]
Infinite Operators

- Function, Transformation, Operator, Mapping: synonyms
- A function takes elements $x$ defined on its “Domain” $D$ to elements $y$ in its “Range” $R$ which is part of $E$

IF for each $y$ in $R$ there is exactly one $x$ in $D$ the function is one-to-one. In this case an inverse exists whose domain is $R$ and whose range is $D$

- Here interested in functions that go from a given Hilbert space to itself.
• Operators are like infinite dimensional matrices
• Can be characterized by their action on basis elements
• Norm of an operator
  • $\forall x \quad \frac{||Ax||}{||x||}$
Eigenvalues and Eigenvectors

- Square matrix possesses its own natural basis.
- Eigen relation

\[ Au = \lambda u \]

- Matrix \( A \) acts on vector \( u \) and produces a scaled version of the vector.
- Eigen is a German word meaning “proper” or “specific”
- \( u \) is the eigenvector while \( \lambda \) is the eigenvalue.
  - If \( u \) is an eigenvector so is \( \alpha u \)
  - If \( ||u||=1 \) then we call it a normal eigenvector
  - \( \lambda \) is like a measure of the “strength” of \( A \) in the direction of \( u \)
- Set of all eigenvalues and eigenvectors of \( A \) is called the “spectrum of \( A \)”