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)

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

$$\Phi\left(\mathbf{y}_j, \mathbf{x}_i\right) = \sum_{m=0}^{p} a_m(\mathbf{x}_i, \mathbf{x}_*) f_m\left(\mathbf{y}_j - \mathbf{x}_*\right) + Error(p, \mathbf{x}_i, \mathbf{x}_*, \mathbf{y}_j)$$

$$= \mathbf{a}(\mathbf{x}_i, \mathbf{x}_*) \bullet \mathbf{f}\left(\mathbf{y}_j - \mathbf{x}_*\right) + Error.$$

scalar product

vectors of length *p*

How about

$$v_j = \sum_{i=1}^{N} u_i e^{-\lambda_i |\mathbf{x}_i - \mathbf{y}_j|^2}$$

Some parameter depending on *i*

More general to have

$$v_j = \sum_{i=1}^{N} u_i \Phi_i\left(\mathbf{y}_j\right) \quad \text{or} \quad v(\mathbf{y}) = \sum_{i=1}^{N} u_i \Phi_i(\mathbf{y}).$$

General Forms of Factorization for Fast Summation (2)

The potential can be factorized as

$$\Phi_i(\mathbf{y}) = \mathbf{A}_i(\mathbf{x}_*) \circ \mathbf{F}(\mathbf{y} - \mathbf{x}_*)$$

Generalized product $\circ$ can be scalar product, contraction, etc. $\mathbf{A}_i$ and $\mathbf{F}$ can be real or complex vectors, tensors, etc. in p-dimensional space.

Requirements to the product (distributivity with respect to addition)

$$(\alpha\mathbf{A}_i + \beta\mathbf{A}_j) \circ \mathbf{F} = \alpha\mathbf{A}_i \circ \mathbf{F} + \beta\mathbf{A}_j \circ \mathbf{F}.$$

In this case

$$v(\mathbf{y}) = \sum_{i=1}^{N} u_i \Phi_i(\mathbf{y}) = \sum_{i=1}^{N} u_i \mathbf{A}_i(\mathbf{x}_*) \circ \mathbf{F}(\mathbf{y} - \mathbf{x}_*) = \mathbf{A}(\mathbf{x}_*) \circ \mathbf{F}(\mathbf{y} - \mathbf{x}_*)$$

$$\mathbf{A}(\mathbf{x}_*) = \sum_{i=1}^{N} u_i \mathbf{A}_i(\mathbf{x}_*)$$

We do not need commutativity of $\circ$ (i.e. we do not request $\mathbf{A}_i \circ \mathbf{F} = \mathbf{F} \circ \mathbf{A}_i$)(!).

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

$$\Phi_{ji} = \mathbf{A}_i \circ \mathbf{F}_j$$

then

$$v_j = \sum_{i=1}^{N} u_i \Phi_{ji} = \sum_{i=1}^{N} u_i (\mathbf{A}_i \circ \mathbf{F}_j) = \left(\sum_{i=1}^{N} u_i \mathbf{A}_i \right) \circ \mathbf{F}_j .$$

Complexity of Fast Summation

Let $\circ$ be a scalar product of vectors $\mathbf{A}_i$ and $\mathbf{F}_j$ 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 $j = 1, ..., M$).
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 $\mathbf{x}_* \in \mathrm{R}^d$.

Might be Singular (at $\mathbf{y} = \mathbf{x}_*$) Basis Functions

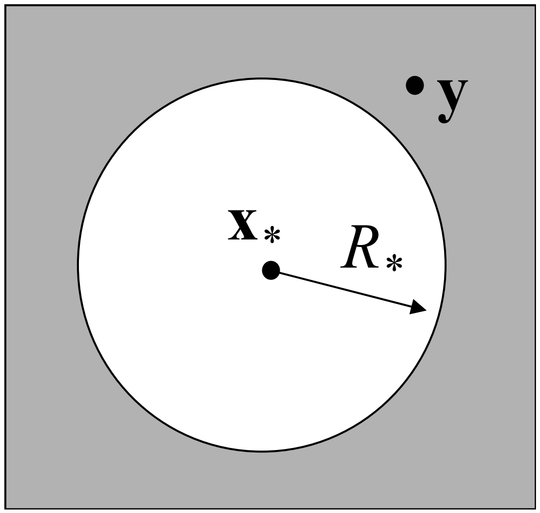
We call expansion

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

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

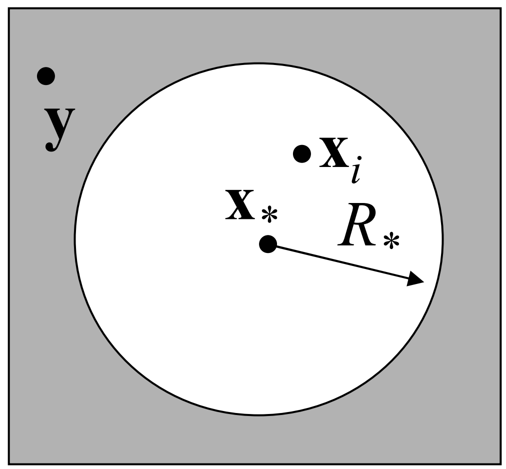
$$|\mathbf{y} - \mathbf{x}_*| > R_*,$$

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



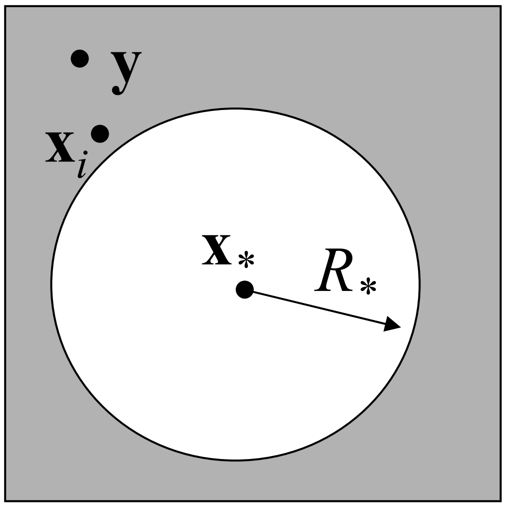
Far Field Expansion of a Regular Potential

Can be like this:



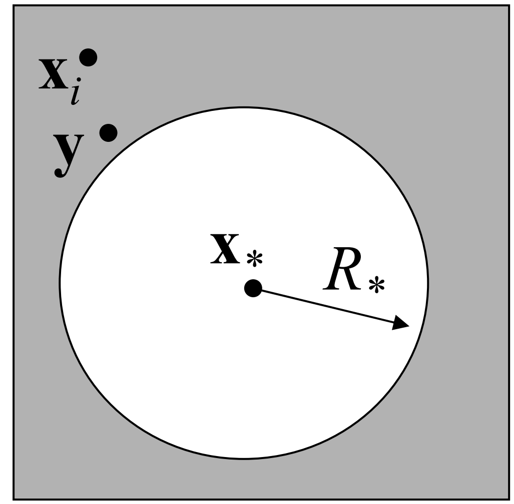
$|\mathbf{y} - \mathbf{x}_*| > R_* > |\mathbf{x}_i - \mathbf{x}_*|$

…sometimes like this:



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

…sometimes like this:



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

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:

$$\frac{1}{1+(y-x_i)^2} = \frac{1}{1+[y-x_*-(x_i-x_*)]^2}$$

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

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

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

Converges, if $|x_i-x_*| < \sqrt{1+(y-x_*)^2}$.

Example of Far Field Expansion of a Regular Function (continuation)

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

Choose

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

$$S_0(y-x_*) = \frac{1}{1+(y-x_*)^2},$$

$$S_1(y-x_*) = \frac{2(y-x_*)}{\left[1+(y-x_*)^2\right]^2},$$

$$S_2(y-x_*) = \frac{1-3(y-x_*)^2}{\left[1+(y-x_*)^2\right]^3},$$

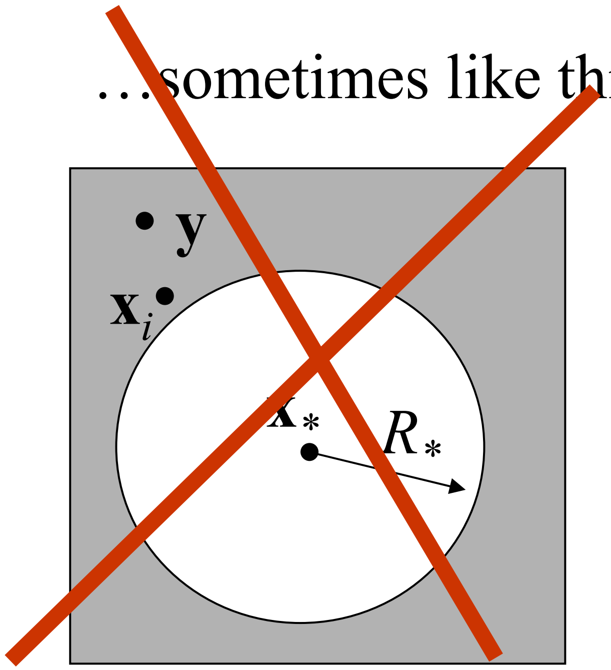
$$\ldots$$

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

$$\ldots$$

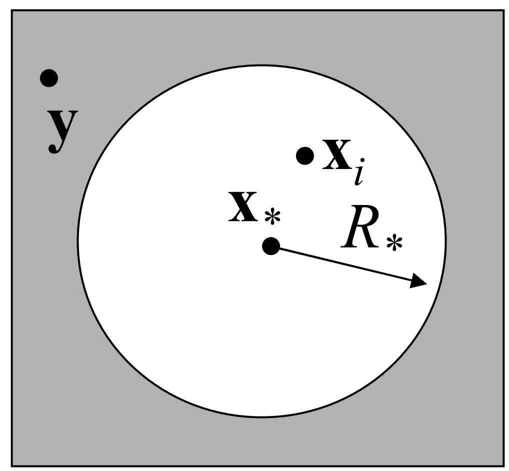
Far Field Expansion of a Singular Potential

…sometimes like this:



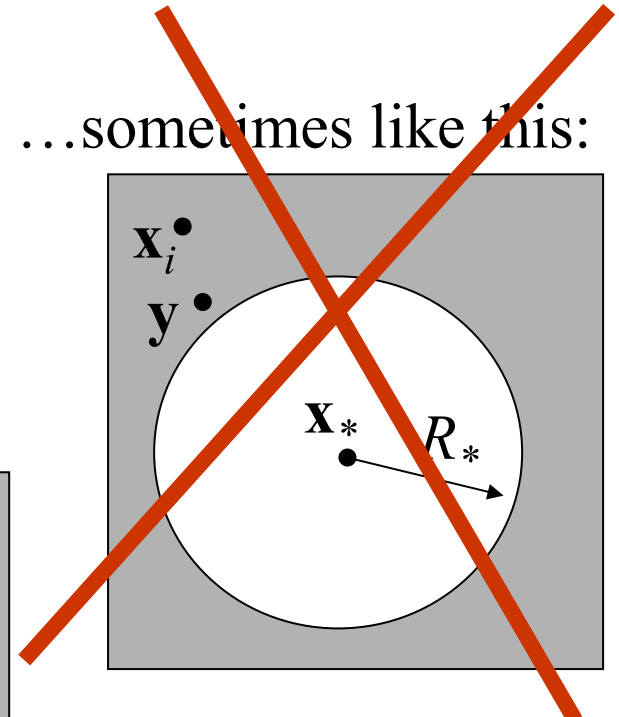
$|\mathbf{y} - \mathbf{x}_*| > R_* > |\mathbf{x}_i - \mathbf{x}_*|$

Can be like this:



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

…sometimes like this:



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

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

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

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

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

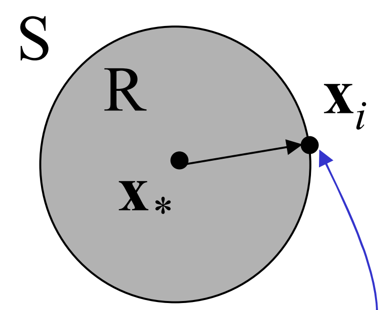
$|y - x_*| > |x_i - x_*|$:

S-expansion

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

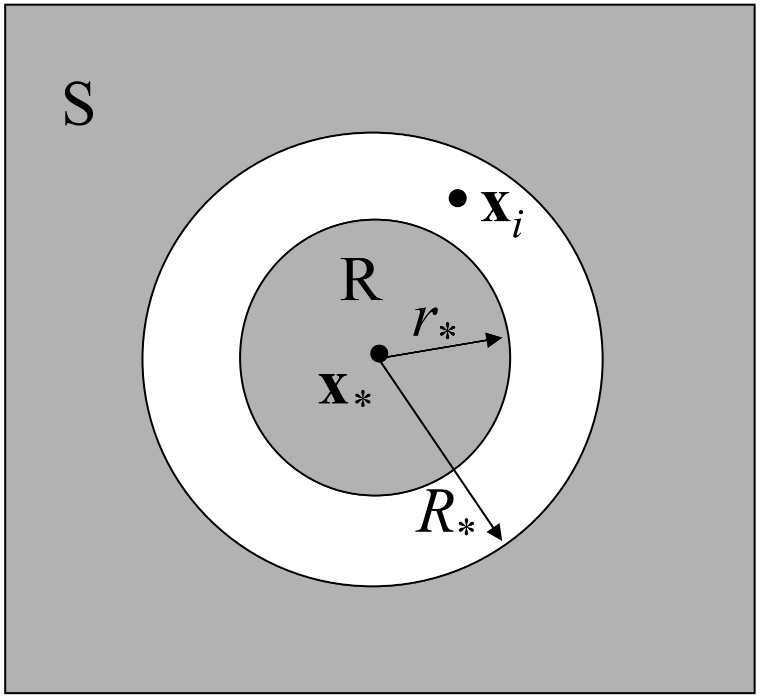
$$b_m(x_i, x_*) = (x_i - x_*)^m, \quad m = 0, 1, \ldots,$$

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



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)



$r_* < R_*$

We need S-expansion for $|\mathbf{y} - \mathbf{x}_*| > R_* > |\mathbf{x}_i - \mathbf{x}_*|$

We need R-expansion for $|\mathbf{y} - \mathbf{x}_*| < r_* < |\mathbf{x}_i - \mathbf{x}_*|$

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 **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

    $$u+v=v+u; \qquad u+(v+w)=(u+v)+w$$

    $$\exists 0,\ u+0=u\ \ \forall u; \qquad u+(-u)=0$$

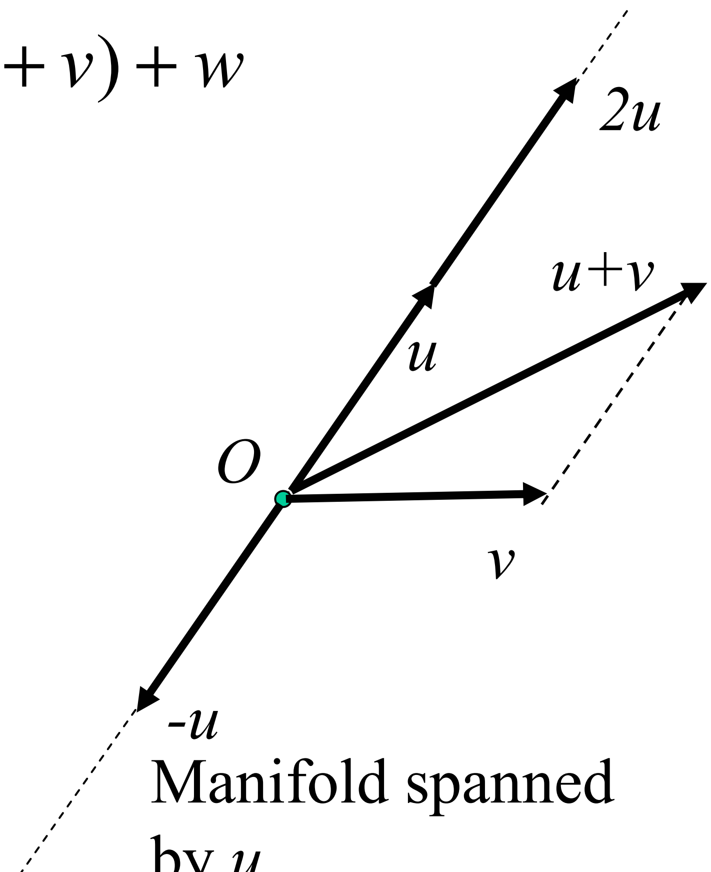
  - Scalar multiplication

    $$\alpha(\beta u)=(\alpha\beta)u; \quad 1u=u$$

    $$(\alpha+\beta)u=\alpha u+\beta u;\ \alpha(u+v)=\alpha u+\alpha v$$

- Let $\mathbf{u_1}$, …, $\mathbf{u_k}$ be a set of vectors:
  Linear combination

$$\alpha_1\mathbf{u}_1+\cdots+\alpha_k\mathbf{u}_k$$



Manifold spanned by u

Dependency, dimension, Basis

- Let $\alpha_1 \mathbf{u}_1 + \cdots + \alpha_k \mathbf{u}_k = 0$
  - if this is true for a set of non zero α 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 α_1, ..., α_k not all zero we can write

$$\alpha_1 \mathbf{u}_1 + \cdots + \alpha_k \mathbf{u}_k = 0$$

  - 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 $\mathbf{b_1}$, …, $\mathbf{b_k}$ 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 $\mathbf{b_1}$, …, $\mathbf{b_k}$
- One example of a basis are the vectors (1,0,…,0), (0,1,…,0), …, (0,0, …, 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 $d(\mathbf{u},\mathbf{v})$ makes a vector space a metric space if it satisfies
  - $d(\mathbf{u},\mathbf{v})>0$ for $\mathbf{u},\mathbf{v}$ different
  - $d(\mathbf{u},\mathbf{u})=0$, $d(\mathbf{u},\mathbf{v})=d(\mathbf{v},\mathbf{u})$
  - $d(\mathbf{u},\mathbf{w})\leq d(\mathbf{u},\mathbf{v})+d(\mathbf{v},\mathbf{w})$ *(triangle inequality)*
- Norm ("length").
  - $||\mathbf{u}|| >0$ for $\mathbf{u}$ not 0, $||\mathbf{0}||=0$
  - $|| \alpha \mathbf{u}||=| \alpha| \ ||\mathbf{u}||$, $||\mathbf{u}+\mathbf{v}|| \leq ||\mathbf{u}|| + ||\mathbf{v}||$
- Normed linear space is a metric space with the metric defined by $d(\mathbf{u},\mathbf{v})=||\mathbf{u}-\mathbf{v}||$ and $||\mathbf{u}||=d(\mathbf{u},0)$

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

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

- 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
  - Transcedentals can be defined as limits of rational sequences

Normed space

- A normed linear space possesses a norm with following properties

$$||u|| > 0, \qquad u \neq 0$$

$$||0|| = 0$$

$$||\alpha u|| = |\alpha|\ ||u||$$

$$||u+v|| \leq ||u|| + ||v||$$

- 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

  $$\langle \mathbf{x},\mathbf{y}\rangle = \quad \mathbf{x}^t\mathbf{y} = \sum_{i=1}^{d} x_i y_i = \mathbf{y}^t\mathbf{x}.$$

- Dot product space behaves like Euclidean R^3
- Dot product defines a norm and a metric.

  $$\langle u,v\rangle = \langle v,u\rangle \qquad \langle \alpha u, v\rangle = \alpha \langle u,v\rangle$$

  $$\langle u+v,w\rangle = \langle u,w\rangle + \langle v,w\rangle \qquad \langle u,u\rangle > 0 \text{ for } u \neq 0$$

- Parallelogram law

  $$\|\mathbf{u}+\mathbf{v}\|^2 + \|\mathbf{u}-\mathbf{v}\|^2 = 2\|\mathbf{u}\|^2 + 2\,\|\mathbf{v}\|^2$$

- Orthogonal vectors $\langle \mathbf{u},\mathbf{v}\rangle = 0$
- Angle between vectors

  $$\cos\theta = \langle \mathbf{x},\mathbf{y}\rangle / \|x\|\,\|y\|$$

- 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:
  - Mahalnobis 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 $(\mathbf{b}_1,\mathbf{b}_2, \ldots, \mathbf{b}_n)$ construct an orthonormal basis $(\mathbf{e}_1,\mathbf{e}_2, \ldots, \mathbf{e}_n)$ from it.
  - Set $\mathbf{e}_1 = \mathbf{b}_1/\|\mathbf{b}_1\|$
  - $\mathbf{g}_2 = \mathbf{b}_2 - \langle \mathbf{b}_2, \mathbf{e}_1 \rangle \mathbf{e}_1$, $\quad \mathbf{e}_2 = \mathbf{g}_2/\|\mathbf{g}_2\|$
  - For k=3, …,n
    $\mathbf{g}_k = \mathbf{b}_k - \Sigma_j \langle \mathbf{b}_k, \mathbf{e}_j \rangle \mathbf{e}_j$, $\quad \mathbf{e}_k = \mathbf{g}_k/\|\mathbf{g}_k\|$

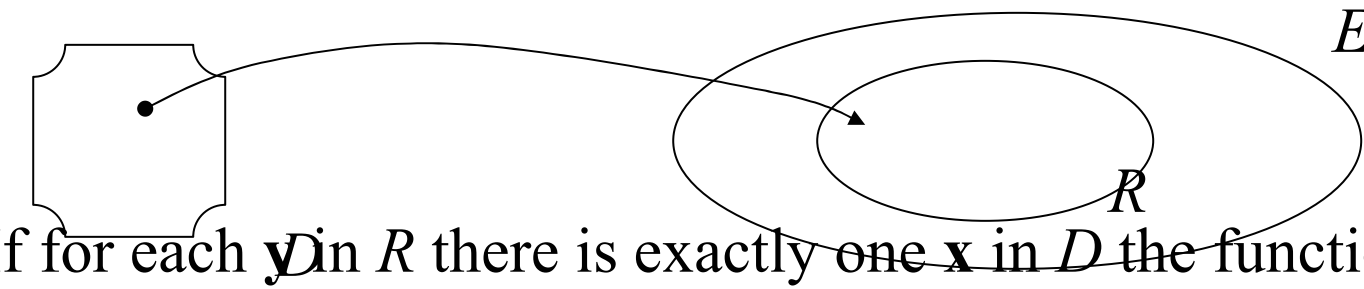
Matrices as operators

- 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 $< \mathbf{Au},\mathbf{v}> = <\mathbf{u},\mathbf{A}^{*}\mathbf{v}>$
  - Square Matrix fully defined as result of its operation on members of a basis.

$$A_{ij} = < \mathbf{Ab}_j,\mathbf{b}_i>$$

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
    - $\forall x \qquad ||Ax||/||x||$

Eigenvalues and Eigenvectors

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

$$\mathbf{Au} = \lambda \mathbf{u}$$

- 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 λ is the eigenvalue.
  - If **u** is an eigenvector so is $\alpha\mathbf{u}$
  - If $||\mathbf{u}||=1$ then we call it a normal eigenvector
  - λ 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”