

Homes ①

Lecture #13: Gram-Schmidt Orthogonalization and Operators

I. Gram-Schmidt Orthogonalization

Procedure to construct an orthonormal set of functions spanning a function space

A. Sequential Construction of Orthonormal Function Set

1. Requires.
  - a. Set of functions  $\chi_i$  (not orthogonal) spanning function space
  - b. Definition of scalar product  $\langle f | g \rangle$

2. Ex: The  $\chi_n$  may be polynomials of order  $n$ . (eg,  $x^n$ )

3. Step 1: Construct first normalized function.

$$\phi_0 = \frac{\chi_0}{\langle \chi_0 | \chi_0 \rangle^{1/2}}$$

a. Thus  $\langle \phi_0 | \phi_0 \rangle = \left\langle \frac{\chi_0}{\langle \chi_0 | \chi_0 \rangle^{1/2}} \left| \frac{\chi_0}{\langle \chi_0 | \chi_0 \rangle^{1/2}} \right. \right\rangle = \frac{\langle \chi_0 | \chi_0 \rangle}{\langle \chi_0 | \chi_0 \rangle} = 1$

4. Step 2: Form (unnormalized) function orthogonal to  $\phi_0$

a. Projection of  $\chi_1$  on  $\phi_0$ :  $a_{0,1} \equiv \langle \phi_0 | \chi_1 \rangle$

b. Subtract projection from  $\chi_1$ :  $\psi_1 = \chi_1 - a_{0,1} \phi_0$

i. Thus  $\langle \phi_0 | \psi_1 \rangle = \langle \phi_0 | \chi_1 - a_{0,1} \phi_0 \rangle = \underbrace{\langle \phi_0 | \chi_1 \rangle}_{= a_{0,1}} - a_{0,1} \langle \phi_0 | \phi_0 \rangle = 0$

5. Step 3: Normalize  $\psi_1$

$$\phi_1 = \frac{\psi_1}{\langle \psi_1 | \psi_1 \rangle^{1/2}}$$

I. A. (continued)

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6. Step 4: Form function orthogonal to  $\phi_1$  &  $\phi_0$

General Projection

a.  $\psi_2 = \chi_2 - a_{0,2} \phi_0 - a_{1,2} \phi_1$

$a_{n,m} \equiv \langle \phi_n | \chi_m \rangle$

7. Step 5: Normalize  $\psi_2$

$\phi_2 = \frac{\psi_2}{\langle \psi_2 | \psi_2 \rangle^{1/2}}$

8. Generalization: To compute function  $\phi_n$ ,

a. Subtract Projection  $\psi_n = \chi_n - \sum_{i=1}^{n-1} \langle \phi_i | \chi_n \rangle \phi_i$

b. Normalize  $\phi_n = \frac{\psi_n}{\langle \psi_n | \psi_n \rangle^{1/2}}$

9. NOTE: Results depend on order in which functions  $\chi_n$  are orthonormalized using this procedure.

B. Example: Legendre Polynomials

1. a. Basis Functions:  $\chi_n = x^n$

b. Scalar Product  $\langle f | g \rangle = \int_{-1}^1 f^*(x) g(x) dx$

2.  $\chi_0 = 1$  a.  $\phi_0 = \frac{1}{\langle 1 | 1 \rangle^{1/2}} = \frac{1}{\left[ \int_{-1}^1 dx \right]^{1/2}} = \frac{1}{\sqrt{2}}$   $\Rightarrow \phi_0 = \frac{1}{\sqrt{2}}$   
 $= 1 - (-1) = 2$

Proj:

3. a.  $a_{0,1} = \langle \phi_0 | x \rangle = \int_{-1}^1 (1/x) dx = \frac{x^2}{2} \Big|_{-1}^1 = 0$  (odd function / even interval)

b.  $\psi_1 = \chi_1 - a_{0,1} \phi_0 = x$

4. Normalize:  $\phi_1(x) = \frac{x}{\langle x | x \rangle^{1/2}} = \frac{x}{\left[ \int_{-1}^1 x^2 dx \right]^{1/2}} = \sqrt{\frac{3}{2}} x$   $\phi_1 = \sqrt{\frac{3}{2}} x$   
 $= \frac{1}{3} x^3 \Big|_{-1}^1 = \frac{2}{3}$

5. Proj: a.  $a_{1,2} = \langle \phi_1 | x^2 \rangle = \int_{-1}^1 \left( \sqrt{\frac{3}{2}} x \right) x^2 dx = \sqrt{\frac{3}{2}} \frac{x^4}{4} \Big|_{-1}^1 = 0$  (odd function / even interval)

Z.B.5. (Continued)

Howes (3)

$$b. a_{0,2} = \langle \phi_0 | x^2 \rangle = \int_{-1}^1 \left(\frac{1}{\sqrt{2}}\right) x^2 dx = \frac{x^3}{3\sqrt{2}} \Big|_{-1}^1 = \frac{\sqrt{2}}{3}$$

$$c. \phi_2 = x^2 - a_{1,2} \phi_1 - a_{0,2} \phi_0 = x^2 - \frac{\sqrt{2}}{3} \left(\frac{1}{\sqrt{2}}\right) = x^2 - \frac{1}{3}$$

6. Normalize:

$$a. \phi_2(x) = \frac{x^2 - \frac{1}{3}}{\langle x^2 - \frac{1}{3} | x^2 - \frac{1}{3} \rangle^{1/2}}$$

$$b. \langle x^2 - \frac{1}{3} | x^2 - \frac{1}{3} \rangle = \int_{-1}^1 \left(x^2 - \frac{1}{3}\right)^2 dx = \int_{-1}^1 \left(x^4 - \frac{2x^2}{3} + \frac{1}{9}\right) dx$$

$$= \left[ \frac{x^5}{5} - \frac{2x^3}{9} + \frac{x}{9} \right]_{-1}^1 = \frac{2}{5} - \frac{4}{9} + \frac{2}{9} = \frac{18-10}{45} = \frac{8}{45}$$

$$c. \phi_2(x) = \frac{3\sqrt{5}}{2\sqrt{2}} \left(x^2 - \frac{1}{3}\right) = \boxed{\sqrt{\frac{5}{2}} \left(\frac{3x^2}{2} - \frac{1}{2}\right) = \phi_2(x)}$$

7. In general  $\phi_n(x) = \sqrt{\frac{2n+1}{2}} P_n(x)$

where  $P_n(x)$  is  $n$ th order Legendre Polynomial (not unit normalization)

C. General Orthogonal Polynomial Sets  $U_n = x^n \quad n=0, 1, 2, \dots$

1. a. Many different sets (Legendre, Chebyshev, Laguerre, Hermite, ...)

are generated by Gram-Schmidt process.

b. Scalar Product definition covers key differences

$$\int_a^b f^*(x) g(x) w(x) dx \quad \begin{array}{l} \text{Limits } [a, b] \\ \text{Weight } w(x) \end{array}$$

2. Table 5.1 in text provides different polynomials sets and associated scalar product definition.

b. Many of these are not normalized to unity.

D. Orthonormalization of Physical Vectors

1. Gram-Schmidt Orthonormalization can be used to generate orthonormal basis vectors: scalar product is dot product!

## I. D. (Continued)

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2a. Consider a space spanned by two (not necessarily orthogonal) vectors  $\underline{a}_1$  and  $\underline{a}_2 \Rightarrow |\underline{a}_1\rangle$  &  $|\underline{a}_2\rangle$

$$b. |\underline{b}_1\rangle = \frac{|\underline{a}_1\rangle}{\langle \underline{a}_1 | \underline{a}_1 \rangle^{1/2}} \Leftrightarrow \underline{b}_1 = \frac{\underline{a}_1}{|\underline{a}_1|}$$

$$c. \text{Project: } |\underline{b}'_2\rangle = |\underline{a}_2\rangle - \langle \underline{b}_1 | \underline{a}_2 \rangle |\underline{b}_1\rangle \Leftrightarrow \underline{b}'_2 = \underline{a}_2 - (\underline{a}_2 \cdot \underline{a}_1) \underline{b}_1$$

$$d. \text{Normalize } |\underline{b}_2\rangle = \frac{|\underline{b}'_2\rangle}{\langle \underline{b}'_2 | \underline{b}'_2 \rangle^{1/2}}$$

## II. Operators

### A. Basics

1a. Operator maps between functions in its domain and functions in its range

b. We focus on operators where domain & range is in same Hilbert space.

### 2. Examples of operators:

$$a. \text{ Multiplication by } 2: f \Rightarrow 2f$$

$$b. \text{ Differentiation, } \frac{d}{dx}: f \Rightarrow \frac{df}{dx}$$

$$c. \text{ Integral operator: } Af(x) = \int G(x, x') f(x') dx'$$

3. We restrict our focus to linear operators:

$$a. (A+B)f = Af + Bf$$

$$b. A(f+g) = Af + Ag$$

$$c. Ak = kA$$

4. Ex: Differential operators

$$a. \mathcal{L}(x) = (1-x^2) \frac{d^2}{dx^2} - 2x \frac{d}{dx}$$

$$b. \text{ Legendre's Equation } (1-x^2) \frac{d^2 y}{dx^2} - 2x \frac{dy}{dx} + \lambda y = 0$$

$$\text{can be written } \boxed{\mathcal{L}(x)y = -\lambda y}$$

## II A. (Continued)

Haves (5)

### 5. Commutator:

a. Differential operators act on functions to their right  
 $\Rightarrow$  they do not necessarily commute.

b. Define: Commutator:  $[A, B] = AB - BA$

c. Ex: Consider operators  $x$  and  $p = -i \frac{d}{dx}$

$$\begin{aligned} \text{i. } [x, p] f(x) &= xp f(x) - px f(x) = -ix \frac{df}{dx} - \left[ -i \frac{d}{dx} (x f(x)) \right] \\ &= -ix \frac{df}{dx} + i f(x) + ix \frac{df}{dx} = i f(x) \end{aligned}$$

$$\text{ii. Thus } [x, p] = i$$

d. Commutator Algebra: i.  $[A, B] = -[B, A]$

$$\text{ii. } [A, B+C] = [A, B] + [A, C]$$

$$\text{iii. } k[A, B] = [kA, B] = [A, kB]$$

6. Identity Operator: a.  $I$ , or  $1$

$$\text{b. } [I f = f]$$

7. Inverse: a.  $A^{-1}$

$$\text{b. } [A^{-1} A = A A^{-1} = 1]$$

8. Adjoint: a.  $A^\dagger$

$$\text{b. } [\langle f | A g \rangle = \langle A^\dagger f | g \rangle]$$

c. Hermitian (Self-Adjoint) Operator:  $[A^\dagger = A]$

9. Unitary Operator:

$$[U^\dagger = U^{-1}]$$

If  $U$  is real  $\Rightarrow$  orthogonal.

10. Ex: Computing Adjoint,  $A = x \frac{d}{dx}$ ,  $\langle f | g \rangle = \int_{-\infty}^{\infty} f^*(x) g(x) dx$

$$\begin{aligned} \text{a. } \langle f | A g \rangle &= \int_{-\infty}^{\infty} f^*(x) \left[ x \frac{d}{dx} g(x) \right] dx = x f^*(x) g(x) \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{d}{dx} [x f^*(x)] g(x) dx \\ &= \int_{-\infty}^{\infty} \left[ -\frac{d}{dx} x f(x) \right] g(x) dx \\ &= \langle -\frac{d}{dx} x f | g \rangle \end{aligned}$$

$u = x f^*(x) \quad dv = \frac{d}{dx} g(x)$   
 $du = \frac{d}{dx} [x f^*(x)] \quad v = g(x)$

## II. A. 10. (Continued)

Haves (6)

b. Thus  $A^\dagger = -\frac{d}{dx} x$

$A \neq A^\dagger \rightarrow$  not Hermitian.

### B. Basis Expansion of Operators

1. The effect of a linear operator  $A$  on an arbitrary function can be written in terms of its effect on basis functions  $\phi_n$ ,

$$A\phi_n = \sum_{mn} a_{mn} \phi_m$$

where  $a_{mn} = \langle \phi_m | A\phi_n \rangle \equiv \langle \phi_m | A | \phi_n \rangle$   
 $= \langle A^\dagger \phi_m | \phi_n \rangle$

2. Let a function be expressed  $\psi = \sum_m c_m \phi_m$   $c_m = \langle \phi_m | \psi \rangle$

b. Thus  $A\psi = \sum_m c_m A\phi_m = \sum_m c_m \sum_n a_{nm} \phi_n = \sum_n \left( \sum_m a_{nm} c_m \right) \phi_n$

c. If  $\chi = A\psi$ , where  $\chi = \sum_n b_n \phi_n$ , then

$$b_n = a_{nm} c_m \xrightarrow[\text{multiplication}]{\text{matrix}} b \approx A c$$

3. Thus, operator  $A$  is determined by its matrix elements.

4. In Dirac notation,  $A\psi = \sum_{mn} |\phi_n\rangle \underbrace{\langle \phi_n | A | \phi_m \rangle}_{= a_{nm}} \underbrace{\langle \phi_m | \psi \rangle}_{= c_m}$ , so

$$A = \sum_{mn} |\phi_n\rangle \langle \phi_n | A | \phi_m \rangle \langle \phi_m | \Rightarrow A = \sum_{mn} |\phi_n\rangle a_{nm} \langle \phi_m |$$

### 5. Adjoint Basis Expansion

a. NOTE:  $\langle \psi | A | \chi \rangle = \langle A^\dagger \psi | \chi \rangle = \langle \chi | A^\dagger | \psi \rangle^*$

b. So  $\langle \chi | A^\dagger | \psi \rangle = \langle \psi | A | \chi \rangle^* = \left[ \langle \psi | \left( \sum_{mn} |\phi_n\rangle a_{nm} \langle \phi_m | \right) | \chi \rangle \right]^*$   
 $= \sum_{mn} \langle \psi | \phi_n \rangle^* a_{nm}^* \langle \phi_m | \chi \rangle^* = \sum_{mn} \langle \chi | \phi_m \rangle a_{nm}^* \langle \phi_n | \psi \rangle$

c. Thus  $A^\dagger = \sum_{mn} |\phi_n\rangle a_{nm}^* \langle \phi_m |$

## II. B5 (Continued)

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d. Thus adjoint operator  $A^\dagger$  has  $a_{mn}^*$ , whereas  $A$  has  $a_{nm}$ .

If  $A$  is a matrix representing an operator  $A$ , then  $A^\dagger$  is the matrix representing the adjoint operator  $A^\dagger$

6. Ex. Adjoint of Spin Operator  $\langle \alpha | \alpha \rangle = \langle \beta | \beta \rangle = 1$ ,  $\langle \alpha | \beta \rangle = \langle \beta | \alpha \rangle = 0$ .

a. Operator  $B\alpha = 0$   $B\beta = \alpha$

b. Thus  $\langle \alpha | B\alpha \rangle = 0$   $\langle \beta | B\alpha \rangle = 0$   $\langle \alpha | B\beta \rangle = 1$   $\langle \beta | B\beta \rangle = 0$

$$B = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{NOTE: } \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

c. Adjoint:  $\langle B^\dagger \alpha | \alpha \rangle = 0$   $\langle B^\dagger \beta | \alpha \rangle = 0$   $\langle B^\dagger \alpha | \beta \rangle = 1$   $\langle B^\dagger \beta | \beta \rangle = 0$

$$\Rightarrow B^\dagger \alpha = \beta, \quad B^\dagger \beta = 0 \quad \Rightarrow B^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

## C. Self-Adjoint Operators (Hermitian)

1. In quantum mechanics, observables are associated with Hermitian operators

2. Def. Expectation Value  $\langle A \rangle = \langle \psi | A | \psi \rangle$

a.  $\langle A \rangle$  is real, even if  $A$  &  $\psi$  are complex.

b.  $\langle A \rangle^* = \langle \psi | A | \psi \rangle^* = \langle A^\dagger \psi | \psi \rangle = \langle A \psi | \psi \rangle$  ( $A = A^\dagger$ )

3a. Coefficients of Hermitian matrix:  $a_{nm} = a_{mn}^*$

b. Diagonal elements of Hermitian matrix are real.  
 $\rightarrow$  expectation values for basis functions!

4. For  $\psi = \sum_n c_n \phi_n$ ,

$$\begin{aligned} \langle A \rangle &= \langle \psi | A | \psi \rangle = \langle \sum_n c_n \phi_n | A | \sum_m c_m \phi_m \rangle = \sum_{nm} c_n^* \langle \phi_n | A | \phi_m \rangle c_m \\ &= \sum_{nm} c_n^* a_{nm} c_m \iff \underline{\underline{c^\dagger A c}} \end{aligned}$$

4. Ex. Self-Adjoint Operator  $p = -i \frac{d}{dx}$

$$\langle f | p | g \rangle = \int_{-\infty}^{\infty} f^*(x) \left( -i \frac{dg}{dx} \right) dx = -i f^*(x) g(x) \Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} i \frac{df^*}{dx} g(x) dx$$

## II C 4. (Continued)

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$$b. = + \int_{-\infty}^{\infty} \left[ -i \frac{d}{dx} \right]^* g(x) dx = \langle p^{\dagger} | g \rangle = \langle f | p^{\dagger} g \rangle \Rightarrow \boxed{p = p^{\dagger}}$$

5. If A & B are self-adjoint, is AB self-adjoint?

$$a. \langle \psi | AB | \phi \rangle = \langle A \psi | B \phi \rangle = \langle BA \psi | \phi \rangle$$

$A = A^{\dagger}$                        $B = B^{\dagger}$

b. Thus, only self-adjoint if  $[A, B] = 0$  ( $AB = BA$ ).

## D. Unitary Operators

1. Describe transformations between orthonormal bases.

2a. Consider  $\psi$  in basis  $\phi$ :  $\psi = \sum_m c_m \phi_m = \underbrace{\left( \sum_m |\phi_m\rangle \langle \phi_m| \right)}_{\text{Identity}} \psi$

b.  $\psi$  in basis  $\phi'$ :

i. Expand basis  $\phi_m$  in  $\phi'_n$ :  $\phi_m = \sum_n U_{nm} \phi'_n = \left( \sum_n |\phi'_n\rangle \langle \phi'_n| \right) |\phi_m\rangle$

$$= \sum_n \underbrace{\langle \phi'_n | \phi_m \rangle}_{= U_{nm}} \phi'_n$$

c. Insert expansion for  $\phi_m$ :

$$\psi = \sum_m c_m \left[ \sum_n U_{nm} \phi'_n \right] = \sum_n \left( \sum_m U_{nm} c_m \right) \phi'_n = \sum_n c'_n \phi'_n$$

d. Thus  $c'_n = \sum_m U_{nm} c_m \Rightarrow \boxed{c' = U c}$

3. For inverse transformation from  $\phi'_m$  to  $\phi_n$ :

a.  $\phi'_m = \sum_n V_{nm} \phi_n = \sum_n \underbrace{\langle \phi_n | \phi'_m \rangle}_{= V_{nm}} \phi_n$

b. So  $V_{nm} = \langle \phi_n | \phi'_m \rangle = \langle \phi'_m | \phi_n \rangle^* = U_{mn}^* = U_{nm}^{\dagger}$

$$\Rightarrow \underline{V} = \underline{U}^{\dagger} \quad \text{Inverse transformation is just adjoint!}$$

c. So  $\underline{c} = \underline{V} \underline{c} = \underline{U}^{\dagger} \underline{U} \underline{c} \Rightarrow \boxed{\underline{U}^{\dagger} \underline{U} = \underline{1}}$  Unitary Matrix

4. Transformation between orthonormal bases is unitary

b. Analogous to Rotations by orthogonal matrix  $\underline{O} \Rightarrow$  Unitary is generalization to complex space of orthogonality