Howes 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 χ_i (not orthogonal) spanning function space
   b. Definition of scalar product $\langle f | g \rangle$

2. Ex: The χ_n may be polynomials of order n. (eg; x^n)

3. Step 1: Construct first normalized function.

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

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

4. Step 2: Form (unnormalized) function orthogonal to ϕ_0

a. Projection of χ_1 on ϕ_0: $a_{0,1} \equiv \langle \phi_0 | \chi_1 \rangle$

b. Subtract projection from χ_1: $\boxed{\psi_1 = \chi_1 - a_{0,1} \phi_0}$

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

5. Step 3: Normalize ψ_1 $\boxed{\phi_1 = \frac{\psi_1}{\langle \psi_1 | \psi_1 \rangle^{\frac{1}{2}}}}$

I. A. (Continued)

6. Step 4: Form function orthogonal to ϕ_1 & ϕ_0

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

General Projection

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

7. Step 5: Normalize ψ_2 $\boxed{\phi_2 = \dfrac{\psi_2}{\langle \psi_2 | \psi_2 \rangle^{\frac{1}{2}}}}$

8. Generalization: To compute function ϕ_n,

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

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

9. NOTE: Results depend on order in which functions χ_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. $\phi_0 = \dfrac{1}{\langle 1 | 1 \rangle^{\frac{1}{2}}} = \dfrac{1}{\Big[\underbrace{\int_{-1}^{1} dx}_{=1-(-1)=2}\Big]^{\frac{1}{2}}} = \dfrac{1}{\sqrt{2}} \Rightarrow \boxed{\phi_0 = \frac{1}{\sqrt{2}}}$

Project:

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

4. Normalize: $\phi_1(x) = \dfrac{x}{\langle x | x \rangle^{\frac{1}{2}}} = \dfrac{x}{\Big[\underbrace{\int_{-1}^{1} x^2 dx}_{=\frac{x^3}{3}\big|_{-1}^{1} = \frac{2}{3}}\Big]^{\frac{1}{2}}} = \sqrt{\frac{3}{2}}\, x$ $\boxed{\phi_1 = \sqrt{\tfrac{3}{2}}\, x}$

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

I. 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. $\psi_2 = x_2 - \cancel{a_{1,2}}^{0} \phi_1 - a_{0,2}\phi_0 = x^2 - \frac{\sqrt{2}}{3}\left(\frac{1}{\sqrt{2}}\right) = x^2 - \frac{1}{3}$

6. <u>Normalize:</u>

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

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. <u>General Orthogonal Polynomial Sets</u> $u_n = x^n \quad n = 0, 1, 2, \ldots$

1. a. Many different sets (Legendre, Chebyshev, Laguerre, Hermite, ...) are generated by Gram-Schmidt process.

b. Scalar Product definition creates key differences

$$\int_a^b f^*(x)\, g(x)\, w(x)\, dx$$

Limits $[a, b]$
Weight $w(x)$

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

b. Many of these are <u>not</u> normalized to unity.

D. <u>Orthonormalization of Physical Vectors</u>

1. Gram-Schmidt Orthogonalization can be used to generate orthonormal basis vectors: Scalar product is <u>dot product</u>!

I. D. (Continued)

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

b. $|\underset{\sim}{b}_1\rangle = \dfrac{|\underset{\sim}{a}_1\rangle}{\langle \underset{\sim}{a}_1|\underset{\sim}{a}_1\rangle^{\frac{1}{2}}} \Leftrightarrow \underset{\sim}{b}_1 = \dfrac{\underset{\sim}{a}_1}{|\underset{\sim}{a}_1|}$

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

d. Normalize $|\underset{\sim}{b}_2\rangle = \dfrac{|\underset{\sim}{b}_2'\rangle}{\langle \underset{\sim}{b}_2'|\underset{\sim}{b}_2'\rangle^{\frac{1}{2}}}$

II. Operators

A. Basics

1. a. 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. Multiplication by 2: $f \Rightarrow 2f$
   b. Differentiation, $\frac{d}{dx}$: $f \Rightarrow \frac{df}{dx}$
   c. Integral operator: $Af(x) \equiv \int G(x,x') f(x') dx'$

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

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

II A. (Continued)

5. <u>Commutator</u>:

a. Differential operators act on functions to their right
$\Rightarrow$ they don't necessarily commute.

b. <u>Define</u>: Commutator: $\boxed{[A,B] = AB - BA}$

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

i. $[x,p]f(x) = xpf(x) - pxf(x) = -ix\frac{\partial f}{\partial x} - \left[-i\frac{d}{dx}(xf(x))\right]$

$= \cancel{-ix\frac{df}{dx}} + if(x) + \cancel{ix\frac{df}{dx}} = if(x)$

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

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

ii. $[A, B+C] = [A,B] + [A,C]$

iii. $k[A,B] = [kA, B] = [A, kB]$

6. <u>Identity Operator</u>: a. I, or 1 b. $\boxed{If = f}$

7. <u>Inverse</u>: a. A^{-1} b. $\boxed{A^{-1}A = AA^{-1} = 1}$

8. <u>Adjoint</u>: a. $A^{\dagger}$ b. $\boxed{\langle f | Ag \rangle = \langle A^{\dagger} f | g \rangle}$

c. <u>Hermitian (Self-Adjoint) Operator</u>: $\boxed{A^{\dagger} = A}$

9. <u>Unitary Operator</u>: $\boxed{U^{\dagger} = U^{-1}}$ If U is real $\Rightarrow$ <u>orthogonal</u>.

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

a. $\langle f | Ag \rangle = \int_{-\infty}^{\infty} f^*(x)\left[x\frac{dg(x)}{dx}\right]dx = \cancel{xf^*(x)g(x)\Big|_{-\infty}^{\infty}} - \int \frac{d}{dx}\left[xf^*(x)\right]g(x)\,dx$

$u = xf^*(x)$ $\quad dv = \frac{dg}{dx}dx$

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

$= \langle -\frac{d}{dx}xf | g \rangle$

II. A. 10. (Continued)

b. Thus $\boxed{A^{\dagger} = -\frac{d}{dx} x}$ $A \neq A^{\dagger} \Rightarrow$ not Hermitian.

B. <u>Basis Expansion of Operators</u>

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

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

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

$$= \langle A^{\dagger}\phi_m | \phi_n \rangle$$

2. a. 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

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

3. Thus, <u>operator A is determined by its matrix elements.</u>

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

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

5. <u>Adjoint Basis Expansion</u>

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 $\boxed{A^{\dagger} = \sum_{mn} |\phi_n\rangle a_{mn}^* \langle \phi_m |}$

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

$$\boxed{\text{If } \underset{\approx}{A} \text{ is a matrix representing an operator } A\text{, then } \underset{\approx}{A}^\dagger \text{ is the matrix representing the adjoint operator } A^\dagger}$$

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 $B\alpha = 0$ $\quad B\beta = \alpha$

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

$$\boxed{\underset{\approx}{B} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}}$$

NOTE: $\underset{B}{\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}} \underset{\alpha}{\begin{pmatrix} 1 \\ 0 \end{pmatrix}} = \underset{0}{\begin{pmatrix} 0 \\ 0 \end{pmatrix}}$ $\quad \underset{B}{\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}} \underset{\beta}{\begin{pmatrix} 0 \\ 1 \end{pmatrix}} = \underset{\alpha}{\begin{pmatrix} 1 \\ 0 \end{pmatrix}}$

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

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

C. Self-Adjoint Operators (Hermitian)

1. In quantum mechanics, observables are associated with Hermitian operators
2. Def: Expectation Value $\boxed{\langle A\rangle = \langle\psi|A|\psi\rangle}$
   a. $\langle A\rangle$ is real, even if A & ψ are complex.
   b. $\langle A\rangle^* = \langle\psi|A|\psi\rangle^* = \langle A^\dagger\psi|\psi\rangle = \langle A\psi|\psi\rangle$ $(A = A^\dagger)$

3. a. Coefficients of Hermitian matrix: $\boxed{a_{nm} = a_{mn}^*}$
   b. Diagonal elements of Hermitian matrix are real.
   ↳ expectation values for basis functions!

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

$$\langle A\rangle = \langle\psi|A|\psi\rangle = \left\langle \sum_n c_n\phi_n \middle| A \middle| \sum_m c_m\phi_m \right\rangle = \sum_{nm} c_n^* \langle\phi_n|A|\phi_m\rangle c_m$$

$$= \sum_{nm} c_n^* a_{nm} c_m \iff \underset{\sim}{c}^\dagger \underset{\approx}{A} \underset{\sim}{c}$$

4. Ex: Self-Adjoint Operator $p = -i\frac{d}{dx}$ $\qquad \langle f|g\rangle = \int_{-\infty}^{\infty} f^*(x) g(x)\, dx$

a. $\langle f|p|g\rangle = \int_{-\infty}^{\infty} f^*(x)\left(-i\frac{dg}{dx}\right) dx = \cancel{-i f^*(x) g(x)\Big|_{-\infty}^{\infty}}^{\,0} + \int_{-\infty}^{\infty} i \frac{df^*}{dx} g(x)\, dx$

$u = -i f^*$, $du = -i\frac{df^*}{dx}dx$, $dv = \frac{dg}{dx}dx$, $v = g$

II C 4. (Continued)

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

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

a. $\langle\psi|AB|\phi\rangle = \langle \underset{A=A^\dagger}{A}\psi|B\phi\rangle = \langle \underset{B=B^\dagger}{B}A\psi|\phi\rangle$

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

D. Unitary Operators

1. Describe transformations between orthonormal bases.

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

b. In a basis ϕ':

i. Expand basis ϕ_m in ϕ_n': $\phi_m = \sum_n U_{nm}\phi_n' = \Big(\sum_n|\phi_n'\rangle\langle\phi_n'|\Big)|\phi_m\rangle$

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

c. Insert expansion for ϕ_m:

$\psi = \sum_m c_m\Big[\sum_n U_{nm}\phi_n'\Big] = \sum_n\Big(\sum_m U_{nm}c_m\Big)\phi_n' = \sum_n c_n'\phi_n'$

d. Thus $c_n' = \sum_m U_{nm}c_m \Rightarrow \boxed{\underset{\sim}{c}' = \underset{\approx}{U}\,\underset{\sim}{c}}$

3. For inverse transformation from ϕ_m' to ϕ_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 $V_{nm} = \langle\phi_n|\phi_m'\rangle = \langle\phi_m'|\phi_n\rangle^* = U_{mn}^* = U_{nm}^\dagger$

$\Rightarrow \underset{\approx}{V} = \underset{\approx}{U}^\dagger$ Inverse transformation is just adjoint!

c. So $\underset{\sim}{c} = \underset{\approx}{V}\,\underset{\approx}{U}\,\underset{\sim}{c} = \underset{\approx}{U}^\dagger\underset{\approx}{U}\,\underset{\sim}{c} \Rightarrow \boxed{\underset{\approx}{U}^\dagger\underset{\approx}{U} = 1}$ Unitary Matrix

4 a. $\boxed{\text{Transformation between orthonormal bases is unitary}}$

b. Analogous to Rotations by orthogonal matrix $\underset{\approx}{S} \Rightarrow$ $\boxed{\text{Unitary is generalization to complex space of orthogonality}}$