Gram-Schmidt

- Procedure for constructing an orthogonal basis from a set of vectors with an inner product

In $\mathbb{R}^n$,

$$S = \{v_1, v_2, \ldots, v_k\}, \quad k \le n$$

generates an orthogonal set

$$S' = \{u_1, u_2, \ldots, u_k\}$$

$$\langle u_i | u_j \rangle = 0 \qquad i \ne j$$

orthonormal if

$$\langle u_i | u_j \rangle = \delta_{ij}$$

Ex 1 $V = \mathbb{R}^2$, $\langle v | u \rangle = v^i u^j \delta_{ij}$

$$v_1 = \begin{pmatrix} 2 \\ -1 \end{pmatrix} \qquad v_2 = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

$$\langle v_1 | v_2 \rangle = 2 \cdot 1 + (-1) \cdot 2 = 0$$

$\Rightarrow$ V is orthogonal but,

$$\langle v_1 | v_1 \rangle = 5 = \langle v_2 | v_2 \rangle$$

$\Rightarrow$ Not normalized

orthonormal set:

$$w_1 = \frac{v_1}{|\langle v_1 | v_1 \rangle|^{1/2}} \qquad w_2 = \frac{v_2}{|\langle v_2 | v_2 \rangle|^{1/2}}$$

$$\Rightarrow \quad w_1 = \begin{pmatrix} 2/\sqrt{5} \\ -1/\sqrt{5} \end{pmatrix}, \quad w_2 = \begin{pmatrix} 1/\sqrt{5} \\ 2/\sqrt{5} \end{pmatrix}$$

Ex 2 : Also true for continuous functions

$$V = C[-\pi, \pi]$$

$$\langle f | g \rangle = \int_{-\pi}^{\pi} dx\, f(x) g(x)$$

$$f_n(x) = \sin nx$$

$$\langle f_m | f_n \rangle = \int_{-\pi}^{\pi} dx \sin mx \sin nx$$

$$= \int_{-\pi}^{\pi} \frac{1}{2} \left[\cos(mx - nx) - \cos(mx + nx) \right] dx$$

$$\int_{-\pi}^{\pi} dx \cos kx = \frac{\sin kx}{k} \Big|_{-\pi}^{\pi} = 0 , \; k \in \mathbb{Z}$$

$$\text{If } k = 0 \Rightarrow \int_{-\pi}^{\pi} dx \cos kx = \int_{-\pi}^{\pi} dx = 2\pi$$

For $k = m-n$

$$\Rightarrow \langle f_m | f_n \rangle = \begin{cases} \pi & m=n \\ 0 & m \neq n \end{cases}$$

Again, orthogonal but not orthonormal

If we define

$$\widetilde{\langle f | g \rangle} = \frac{1}{\pi} \int_{-\pi}^{\pi} dx\, f(x) g(x)$$

$\Rightarrow$ orthonormal

You are used to orthonormal basis:

e.g. $\mathbb{R}^3$: $\begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\end{pmatrix}$

For an orthonormal basis

$$\langle x | y \rangle = g_{ij} x^i y^j$$

<u>Proof:</u> V_i are a set of orthonormal basis vectors for a space V

$$\langle x | y \rangle = \langle x^i g_{ij} v^j | y^k g_{kl} v^l \rangle$$

$$= x^i g_{ij} \langle v^j | y^k g_{kl} v^l \rangle$$

$$= x^i g_{ij} g_{kl} y^l \langle v^j | v^l \rangle$$

$$= x^i g_{ij} g_{kl} y^l \delta^{jl}$$

$$= g_{ij} x^i y^j \qquad \square$$

Orthogonalization / Gram-Schmidt

V is a vector space with an inner product

$\{x_1, x_2, \ldots, x_n\}$ is a basis for V.

Let

$v_1 = x_1$

Want $\langle v_1 | v_2 \rangle = 0$

Let

$v_2 = x_2 + c_{12} x_1$

$$\Rightarrow \langle v_1 | v_2 \rangle = \langle v_1 | x_2 \rangle + c_{12} \langle v_1 | x_1 \rangle$$

$$= \langle v_1 | x_2 \rangle + c_{12} \langle v_1 | v_1 \rangle$$

$$= 0$$

$$\Rightarrow c_{12} = -\frac{\langle v_1 | x_2 \rangle}{\langle v_1 | v_1 \rangle}$$

$$v_2 = x_2 - \frac{\langle v_1 | x_2 \rangle}{\langle v_1 | v_1 \rangle} v_1$$

Can repeat this to get

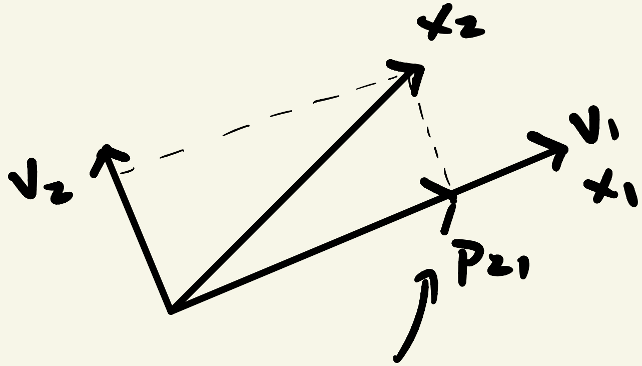
$$v_3 = x_3 - \frac{\langle v_1 | x_3 \rangle}{\langle v_1 | v_1 \rangle} v_1 - \frac{\langle v_2 | x_3 \rangle}{\langle v_2 | v_2 \rangle} v_2$$

$$\vdots$$

$$v_n = x_n - \frac{\langle v_1 | x_n \rangle}{\langle v_1 | v_1 \rangle} v_1 - \cdots - \frac{\langle v_{n-1} | x_n \rangle}{\langle v_{n-1} | v_{n-1} \rangle} v_{n-1}$$

$v_1, v_2, \ldots, v_n$ are an orthogonal basis for V

Visually:



$$\frac{\langle v_1 | x_2 \rangle}{\langle v_1 | v_1 \rangle} v_1 = p_{21}$$

Define: $$p_{ij} = \frac{\langle v_j | x_i \rangle}{\langle v_j | v_j \rangle} v_j$$

$$v_1 = x_1$$

$$v_2 = x_2 - p_{21}$$

$$v_3 = x_3 - p_{31} - p_{32}$$

$$\vdots$$

$$v_n = x_n - \sum_{i=1}^{n-1} p_{ni}$$

For an orthonormal basis just normalize:

$$u_i = \frac{v_i}{|\langle v_i | v_i \rangle|^{1/2}}$$

Ex 3

Π is a plane spanned by $x_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$ $x_2 = \begin{pmatrix} -1 \\ -1 \\ 3 \end{pmatrix}$

find an orthogonal basis

Let

$$v_1 = x_1$$

$$v_2 = x_2 - P_{21}$$

$$P_{21} = \frac{\langle v_1 | x_2 \rangle}{\langle v_1 | v_1 \rangle} v_1$$

$$\langle v_1 | v_1 \rangle = 1^2 + 1^2 + 1^2 = 3$$

$$\langle v_1 | x_2 \rangle = -1^2 - 1^2 + 3 = 1$$

$$\Rightarrow v_2 = x_2 - \frac{1}{3} x_1 = \begin{pmatrix} -4/3 \\ -4/3 \\ 8/3 \end{pmatrix}$$

Check

$$\langle v_1 | v_2 \rangle = 1\cdot(-4/3) + 1\cdot(-4/3) + 1\cdot 8/3$$
$$= 0 \quad \checkmark$$

Can normalize

$$u_1 = \frac{v_1}{|\langle v_1 | v_1 \rangle|^{1/2}} = \begin{pmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{pmatrix}$$

$$u_2 = \frac{v_2}{|\langle v_2 | v_2 \rangle|^{1/2}}$$

$$\langle v_2 | v_2 \rangle = (4/3)^2 + (4/3)^2 + (8/3)^2$$
$$= 2 \cdot \frac{16}{9} \cdot \frac{64}{9}$$
$$= \frac{96}{9} = \frac{32}{3} \Rightarrow u_2 = \sqrt{\frac{3}{32}} \begin{pmatrix} -4/3 \\ -4/3 \\ 8/3 \end{pmatrix}$$
$$= \frac{1}{\sqrt{6}} \begin{pmatrix} -1 \\ -1 \\ 2 \end{pmatrix}$$

We can extend this to a basis for $\mathbb{R}^3$ by including

$$x_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\Rightarrow v_3 = x_3 - p_{31} - p_{32}$$

$$p_{31} = \frac{\langle v_1 | x_3 \rangle}{\langle v_1 | v_1 \rangle} v_1 = \frac{1}{3} v_1$$

$$p_{32} = \frac{\langle v_2 | x_3 \rangle}{\langle v_2 | v_2 \rangle} v_2$$

$$\langle v_2 | v_2 \rangle = \frac{32}{3}$$

$$\langle v_2 | x_3 \rangle = \frac{8}{3}$$

$$\Rightarrow p_{32} = \frac{8}{32} v_2 = \frac{1}{4} v_2$$

$$\Rightarrow v_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} - \frac{1}{3}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \frac{1}{4}\begin{pmatrix} -4/3 \\ -4/3 \\ 8/3 \end{pmatrix}$$

$$= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow$$ x_3 is linearly dependant on x_1, x_2

Try $x_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

$$p_{31} = \frac{1}{3} v_1$$

$$\langle v_2 | x_3 \rangle = -\frac{4}{3} \Rightarrow p_{32} = \frac{-4}{32} v_2 = \frac{-v_2}{8}$$

$$\Rightarrow v_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} - \frac{1}{3}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + \frac{1}{8}\begin{pmatrix} -4/3 \\ -4/3 \\ 8/3 \end{pmatrix}$$

$$= \begin{pmatrix} -1/2 \\ 1/2 \\ 0 \end{pmatrix}$$

$\Rightarrow \{v_1, v_2, v_3\}$ are an orthogonal basis

Ex 4 $\quad V = P[-1,1]$

$$f_n = x^n \quad , n = \{0, 1, 2, \dots\}$$

$$\langle f_m | f_n \rangle = \int_{-1}^{1} dx\, f_m(x) f_n(x)$$

$$\underline{P_0(x) = f_0(x) = 1}$$

$$P_1(x) = f_1(x) - \frac{\langle f_1 | P_0 \rangle}{\langle P_0 | P_0 \rangle} P_0(x)$$

$$\langle P_0 | P_0 \rangle = \langle f_0 | f_0 \rangle$$

$$= \int_{-1}^{1} dx = 2$$

$$\langle f_1 | P_0 \rangle = \int_{-1}^{1} dx\, x = \frac{1}{2} x^2 \Big|_{-1}^{1} = 0$$

$$\Rightarrow P_1(x) = f_1(x) = x$$

$$P_2(x) = f_2(x) - \frac{\langle f_2 | P_1 \rangle}{\langle P_1 | P_1 \rangle} P_1 - \frac{\langle f_2 | P_0 \rangle}{\langle P_0 | P_0 \rangle} P_0$$

$\langle P_0 | P_0 \rangle = 2$,

$$\langle f_2 | P_0 \rangle = \int_{-1}^{1} dx\, x^2 = \frac{1}{3} x^3 \Big|_{-1}^{1} = \underline{\frac{2}{3}}$$

$$\langle P_1 | P_1 \rangle = \int_{-1}^{1} dx\, x^2 = \underline{\frac{2}{3}}$$

$$\langle f_2 | P_1 \rangle = \int_{-1}^{1} dx\, x^3 = \frac{1}{4} x^4 \Big|_{-1}^{1} = 0$$

$$\Rightarrow P_2(x) = x^2 - \frac{1}{3}$$

$\vdots$

If we choose $P(1) = 1$ for a normalization,

$\Rightarrow$ Generates <u>Legendre Polynomials</u>

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = \frac{1}{2}(3x^2 - 1)$$

$$\vdots$$

- Important in QM
- orbitals of atoms