

Gram-Schmidt Process

- * Inner Products
- * Orthogonality
- * G-S Procedure

Logistics: MIT 7/17?
 \Rightarrow Piazza post

I. Inner Products

Informally, an operation in a vector space that "multiplies" two vectors together.

① Linearity

$$a) \langle \vec{x} + \vec{y}, \vec{z} \rangle = \langle \vec{x}, \vec{z} \rangle + \langle \vec{y}, \vec{z} \rangle$$

Additivity in 1st argument

$$b) \langle \alpha \vec{x}, \vec{y} \rangle = \alpha \langle \vec{x}, \vec{y} \rangle$$

Scaling in the 1st argument

$$A(\vec{x} + \vec{y}) = A\vec{x} + A\vec{y}$$

$$\textcircled{2} \quad \overline{\langle x, y \rangle} = \langle y, x \rangle$$

Conjugate Symmetry

$$\textcircled{3} \quad \langle x, x \rangle \geq 0 \quad \text{with} \quad \langle x, x \rangle = 0 \iff \vec{x} = \vec{0}$$

positive definiteness

a) dot product in \mathbb{R}^N

$$\langle \vec{x}, \vec{y} \rangle = \vec{x} \cdot \vec{y} = \vec{x}^T \vec{y} = \sum x_i y_i$$

↳ linear in both arguments

↳ symmetric

② Complex Inner Product

$$\langle \vec{u}, \vec{v} \rangle = \vec{u}^T \vec{v} = \vec{v}^* \vec{u}$$

$$= \sum_i \overline{v_i} u_i = \sum_i u_i \overline{v_i}$$

$\vec{v}^* =$ conjugate transpose

Why?

$$\vec{x} = \begin{bmatrix} 1 \\ j \end{bmatrix}$$

$$\vec{x} \cdot \vec{x} = 1^2 + j^2 = 0$$

But not the $\vec{0}$ vector!

$$\vec{y} = \begin{bmatrix} j \\ j \end{bmatrix}$$

$$\vec{y} \cdot \vec{y} = j^2 + j^2 = -2 < 0$$

\Rightarrow Fix by adding complex conjugate

(c) Functions?

\hookrightarrow can be vectors!

$$\langle u, v \rangle = \frac{1}{2\pi} \int_0^{2\pi} u(\theta) \overline{v(\theta)} d\theta$$

⇒ Explore in HW3!
(Q6)

related:
Fourier transform
(EE20)

II Orthogonality

a) Definitions

orthogonal: $\vec{v} \perp \vec{u} \iff \langle \vec{v}, \vec{u} \rangle = 0$

— orthogonal set of vecs: $\{\vec{v}_1, \dots, \vec{v}_n\}$

$$\langle \vec{v}_i, \vec{v}_j \rangle = \begin{cases} \neq 0 & i=j \\ 0 & i \neq j \end{cases}$$

(All pairs of distinct vectors are orthogonal)

— orthonormal set of vectors: orthogonal set where $\langle \vec{v}_i, \vec{v}_i \rangle = 1$

Set of vectors, where $\langle \vec{v}_i, \vec{v}_i \rangle = \|\vec{v}_i\|^2 = 1$

\Rightarrow orthogonal set of vectors with unit length

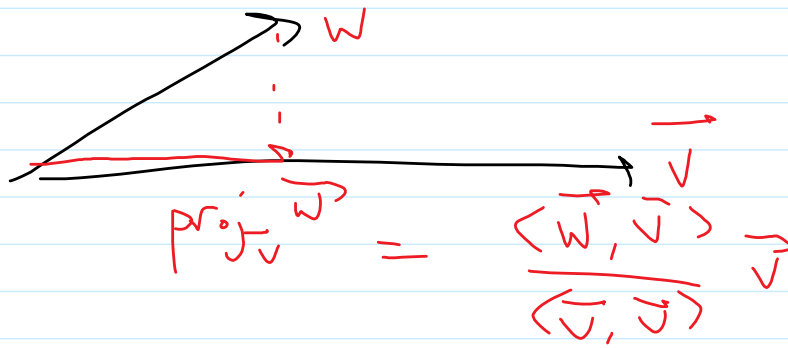
$$\langle \vec{v}_i, \vec{v}_j \rangle = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases} = \delta_{ij}$$

b) Projection (Orthogonal Projection)

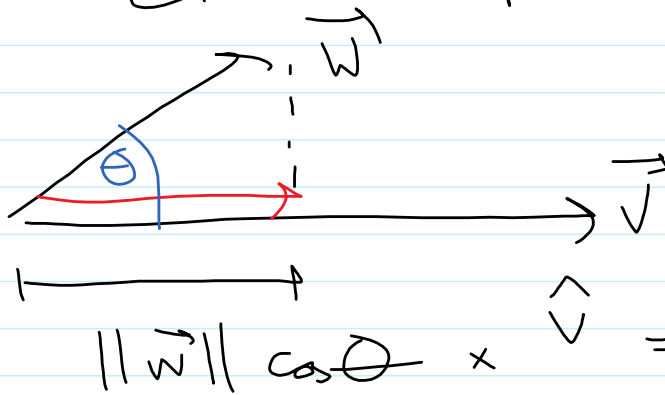
$$\text{proj}_{\vec{v}} \vec{w} = \frac{\langle \vec{w}, \vec{v} \rangle}{\langle \vec{v}, \vec{v} \rangle} \vec{v} = \frac{\langle \vec{w}, \vec{v} \rangle}{\|\vec{v}\|^2} \vec{v}$$

How to remember expression?

- $\text{proj}_{\vec{v}} \vec{w}$ should point in same direction as \vec{v}
- \vec{w} (vector being projected) only shows up once in expression



2D Euclidean space! (specific case)

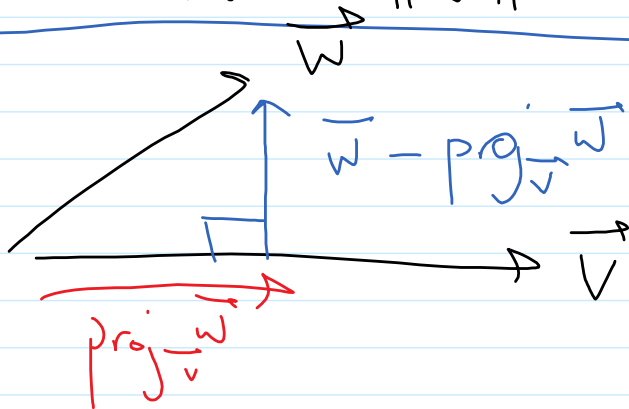


but helpful for trying to "derive" formula

$$\|w\| \cos \theta \times \frac{v}{\|v\|} = \|w\| \cos \theta \frac{v}{\|v\|}$$

$$\frac{w \cdot v}{\|v\|} = \frac{\|w\| \|v\| \cos \theta}{\|v\|}$$

$$\text{proj}_v w = \frac{w \cdot v}{\|v\|} \frac{v}{\|v\|} = \frac{\langle w, v \rangle}{\langle v, v \rangle} v$$



$$\begin{aligned}
& \langle \vec{w} - \text{proj}_{\vec{v}} \vec{w}, \vec{v} \rangle \\
&= \langle \vec{w}, \vec{v} \rangle - \langle \text{proj}_{\vec{v}} \vec{w}, \vec{v} \rangle \\
&= \langle \vec{w}, \vec{v} \rangle - \left\langle \frac{\langle \vec{w}, \vec{v} \rangle}{\langle \vec{v}, \vec{v} \rangle} \vec{v}, \vec{v} \right\rangle \\
&= \langle \vec{w}, \vec{v} \rangle - \frac{\langle \vec{w}, \vec{v} \rangle}{\langle \vec{v}, \vec{v} \rangle} \langle \vec{v}, \vec{v} \rangle \\
&= 0
\end{aligned}$$

c) Properties of Orthonormal Bases

Consider orthogonal basis

$$\{ \vec{v}_1, \dots, \vec{v}_n \}$$

$$\vec{x} = c_1 \vec{v}_1 + c_2 \vec{v}_2 + \dots + c_n \vec{v}_n$$

$$\langle \vec{x}, \vec{v}_j \rangle = \left\langle \sum_i c_i \vec{v}_i, \vec{v}_j \right\rangle$$

all terms equal to 0 unless $i=j$

$$\langle \vec{x}, \vec{v}_j \rangle = c_j \langle \vec{v}_j, \vec{v}_j \rangle$$

$$c_j = \frac{\langle \vec{x}, \vec{v}_j \rangle}{\langle \vec{v}_j, \vec{v}_j \rangle}$$

Fast way to calculate coordinates in orthogonal basis

$$\vec{x}_b = B^{-1} \vec{x}_e$$

- Orthonormal Bases

$$\langle \vec{v}_j, \vec{v}_j \rangle = 1 = \|\vec{v}_j\|^2$$

$$c_j = \langle \vec{x}, \vec{v}_j \rangle$$

Even faster!

← Orthogonal Matrix

A square matrix $U \in \mathbb{R}^{n \times n}$

st. the columns form an orthonormal basis

It can be shown that $U^T = U^{-1}$, i.e.,

$$U^T U = U U^T = I$$

- Unitary Matrix

⇒ complex analogue of orthogonal matrix

A square matrix $U \in \mathbb{C}^{N \times N}$ s.t.

the columns form an orthonormal basis

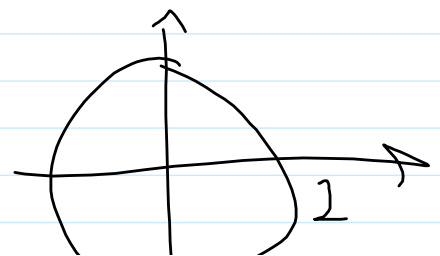
$$U^* = U^{-1}$$

(* here means conjugate transpose, aka adjoint)

Lots of interesting properties, which you will see in HW3 (Q4)

One interesting property:

$$|\det U| = 1$$



$$| \det U | = 1 \quad \left[\begin{array}{c} \text{Diagram of a unit circle in the complex plane} \end{array} \right]$$

$$\det \underline{I} = \det U^* U$$

$$\det AB = \det A \det B = \det B \det A$$

$$= \det U^* \det U = \det BA$$

$$\det U^T = \det U$$

$$\Rightarrow \det U^* = (\det U^T) = \det U$$

$$\overline{z z} = \overline{\det U} \det U$$

$$= |z|^2 = |\det U|^2 = \det \underline{I} = 1$$

$$\therefore |\det U| = 1$$

IF U is orthogonal, $\det U \in \mathbb{R}$
 then $\Rightarrow \det U = \pm 1$

Consider orthogonal matrices!
 $U^T = U^{-1}$

Rotations!

$$R(\theta) = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$$

$$R(-\theta) = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} = R(\theta)^T$$

$$\det R = \cos^2 \theta + \sin^2 \theta = 1$$

Let I orthogonal matrices correspond to rotations!

\Rightarrow Subgroup of group of orthogonal transformations $O(n)$ that can be represented by $n \times n$ orthogonal matrices

\Rightarrow Subgroup where $\det = 1$;
Special orthogonal group $SO(n)$

In physics, very important!

In physics, ...
classical mechanics $SO(3)$

\Rightarrow "3D rotation group"

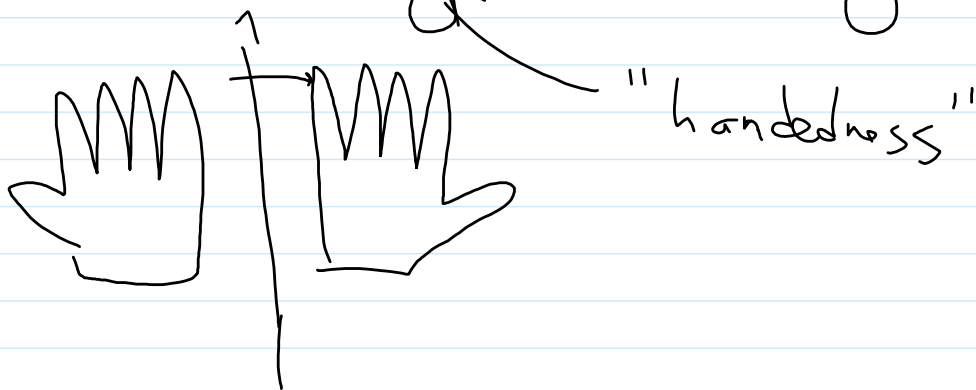
But what about $\det = -1$?

\Rightarrow reflections

$$\det \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} = -1$$

\Rightarrow "parity" in physics and chemistry, i.e. flip the sign of one coordinate

\Rightarrow test of symmetry, e.g. chirality in chemistry



For unitary matrices \Rightarrow unitary group $U(n)$

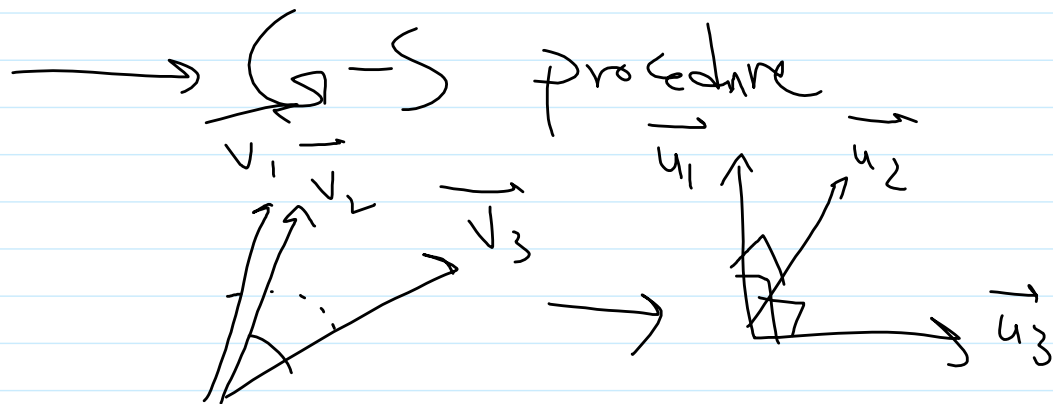
$|U| = 1 \Rightarrow$ special unitary

$\det U = 1 \implies$ special unitary
group $SU(n)$

group theory: abstract algebra?
(not sure) Math 113?

III. Gram-Schmidt

→ how do we make orthonormal
sets of vectors?



Dis 3C Worksheet

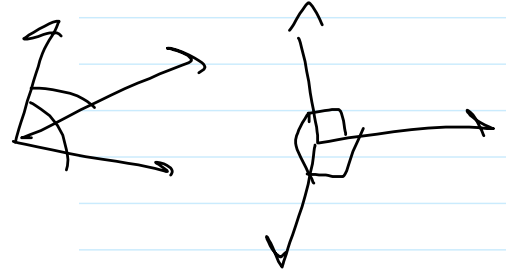
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3 Gram-Schmidt Algorithm

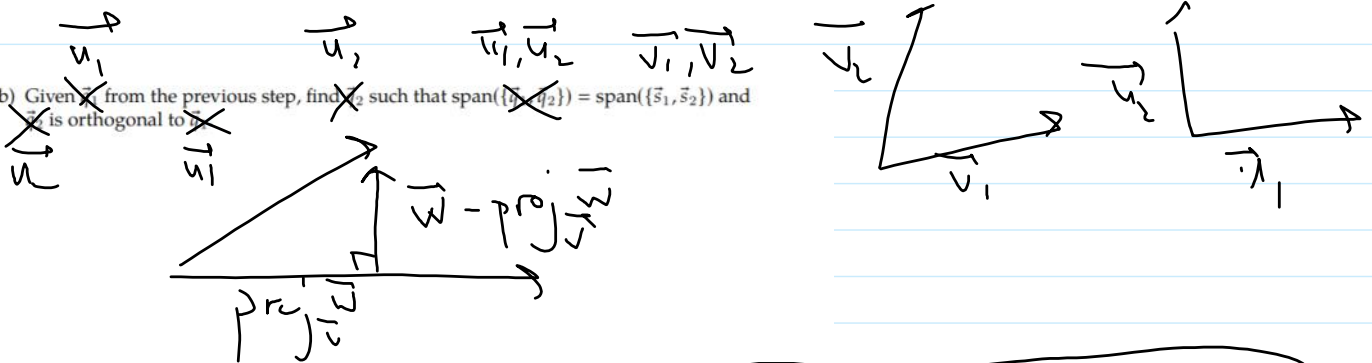
Let's apply Gram-Schmidt orthonormalization to a set of three linearly independent vectors $\{s_1, s_2, s_3\}$.

a) Find unit vectors u_1 such that $\text{span}(\{u_1\}) = \text{span}(\{s_1\})$

$$u_1 = \frac{v_1}{\|v_1\|}$$



b) Given u_1 from the previous step, find u_2 such that $\text{span}(\{u_1, u_2\}) = \text{span}(\{s_1, s_2\})$ and u_2 is orthogonal to u_1 .



$$z_2 = v_2 - \text{proj}_{u_1} v_2 = v_2 - \frac{\langle v_2, u_1 \rangle}{\|u_1\|^2} u_1$$

$$u_2 = \frac{z_2}{\|z_2\|}$$

c) Now given u_1 and u_2 in the previous steps, find u_3 such that $\text{span}(\{u_1, u_2, u_3\}) = \text{span}(\{s_1, s_2, s_3\})$.

$$z_3 = v_3 - \text{proj}_{u_1} v_3 - \text{proj}_{u_2} v_3$$

$$\begin{aligned} \vec{z}_3 &= \vec{v}_3 - \text{prj}_{\vec{u}_1} \vec{v}_3 - \text{prj}_{\vec{u}_2} \vec{v}_3 \\ &= \vec{v}_3 - \langle \vec{v}_3, \vec{u}_1 \rangle \vec{u}_1 - \langle \vec{v}_3, \vec{u}_2 \rangle \vec{u}_2 \\ \vec{u}_3 &= \frac{\vec{z}_3}{\|\vec{z}_3\|} \end{aligned}$$

d) Let's extend this algorithm to n linearly independent vectors. That is, given an input $\{\vec{s}_1, \dots, \vec{s}_n\}$, write the algorithm to calculate the orthonormal set of vectors $\{\vec{q}_1, \dots, \vec{q}_n\}$, where $\text{span}(\{\vec{s}_1, \dots, \vec{s}_n\}) = \text{span}(\{\vec{q}_1, \dots, \vec{q}_n\})$. Hint: How would you calculate the i^{th} vector, \vec{q}_i ?

Input: $\{\vec{v}_1 \dots \vec{v}_n\}$ (lin ind)
 Output: $\{\vec{u}_1 \dots \vec{u}_n\}$ (orthonormal)

$$\vec{u}_1 = \frac{\vec{v}_1}{\|\vec{v}_1\|}$$

for $i=2, \dots, n$ $i++$

$$\vec{z}_i = \vec{v}_i - \sum_{j=1}^{i-1} \langle \vec{v}_i, \vec{u}_j \rangle \vec{u}_j$$

Semicolons (I'm bad at writing)

$$\vec{u}_i = \frac{\vec{z}_i}{\|\vec{z}_i\|} \quad j=1$$

4 The Order of Gram-Schmidt

a) If we are performing the Gram-Schmidt method on a set of vectors, does the order in which we take the vectors matter? Consider the set of vectors

$$\{\vec{v}_1, \vec{v}_2, \vec{v}_3\} = \left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \right\} \quad (4)$$

Perform Gram-Schmidt on these vectors first in the order $\vec{v}_1, \vec{v}_2, \vec{v}_3$.

$$\vec{u}_1 = \frac{\vec{v}_1}{\|\vec{v}_1\|} = \vec{v}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\begin{aligned} \vec{z}_2 &= \vec{v}_2 - \langle \vec{v}_2, \vec{u}_1 \rangle \vec{u}_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} - \left(\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \end{aligned}$$

$$\vec{u}_2 = \vec{z}_2 / \|\vec{z}_2\| = \vec{z}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\vec{z}_3 = \vec{v}_3 - \text{proj}_{\vec{u}_1} \vec{v}_3 - \text{proj}_{\vec{u}_2} \vec{v}_3$$

$$\begin{aligned}
 \vec{z}_3 &= \vec{v}_3 - \text{proj}_{\vec{u}_1} \vec{v}_3 - \text{proj}_{\vec{u}_2} \vec{v}_3 \\
 &= \vec{v}_3 - \langle \vec{v}_3, \vec{u}_1 \rangle \vec{u}_1 - \langle \vec{v}_3, \vec{u}_2 \rangle \vec{u}_2 \\
 &= \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \left(\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} - \left(\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right) \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \\
 &= \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - 1 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} - 1 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}
 \end{aligned}$$

$$\vec{u}_3 = \vec{z}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\left\{ \vec{u}_1, \vec{u}_2, \vec{u}_3 \right\} = \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\}$$

b) Now perform Gram-Schmidt on these vectors in the order $\vec{v}_3, \vec{v}_2, \vec{v}_1$. Do you get the same result?

$$\vec{z}_3 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\vec{u}_3 = \frac{\vec{z}_3}{\|\vec{z}_3\|} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{1^2+1^2+1^2}} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\vec{z}_2 = \vec{v}_2 - \text{proj}_{\vec{u}_3} \vec{v}_2 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} - \langle \vec{v}_2, \vec{u}_3 \rangle \vec{u}_3$$

$$= \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} - \left(\frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \right) \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} - \frac{1}{3} (2) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1/3 \\ 1/3 \\ -2/3 \end{pmatrix}$$

$$\vec{u}_2 = \begin{pmatrix} 1/3 \\ 1/3 \\ -2/3 \end{pmatrix} \frac{1}{\sqrt{\frac{1}{9} + \frac{1}{9} + \frac{4}{9}}} = \sqrt{\frac{3}{2}} \begin{pmatrix} 1/3 \\ 1/3 \\ -2/3 \end{pmatrix}$$

$$\vec{z}_1 = \vec{v}_1 - \text{proj}_{\vec{u}_3} \vec{v}_1 - \text{proj}_{\vec{u}_2} \vec{v}_1$$

$$= \vec{v}_1 - \langle \vec{v}_1, \vec{u}_3 \rangle \vec{u}_3 - \langle \vec{v}_1, \vec{u}_2 \rangle \vec{u}_2$$

$$= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} - \left(\frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right) \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$- \left(\sqrt{\frac{3}{2}} \begin{pmatrix} 1/3 \\ 1/3 \\ -2/3 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right) \sqrt{\frac{3}{2}} \begin{pmatrix} 1/3 \\ 1/3 \\ -2/3 \end{pmatrix}$$

$$= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} - \frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \frac{3}{2} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 1/3 \\ 1/3 \\ -2/3 \end{pmatrix}$$

$$= \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} - \frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} - \frac{3}{2} \cdot \frac{1}{3} \begin{pmatrix} 1/3 \\ 1/3 \\ -2/3 \end{pmatrix}$$

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

$$\vec{u}_3 = \begin{pmatrix} 1/2 \\ -1/2 \\ 0 \end{pmatrix} \frac{1}{\sqrt{\frac{1}{4} + \frac{1}{4}}} = \sqrt{2} \begin{pmatrix} 1/2 \\ -1/2 \\ 0 \end{pmatrix}$$

$$\left\{ \vec{u}_1, \vec{u}_2, \vec{u}_3 \right\} = \left\{ \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \sqrt{\frac{3}{2}} \begin{pmatrix} 1/3 \\ 1/3 \\ -2/3 \end{pmatrix}, \sqrt{2} \begin{pmatrix} 1/2 \\ -1/2 \\ 0 \end{pmatrix} \right\}$$

Spans same space, but different basis!