## **1.3.3 Basis sets and Gram-Schmidt Orthogonalization**

Before we address the question of existence and uniqueness, we must establish one more tool for working with vectors – basis sets.

Let 
$$\underline{\mathbf{v}} \in \mathbf{R}^{\mathrm{N}}$$
, with  $\underline{\mathbf{v}} = \begin{bmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \vdots \\ \mathbf{v}_3 \end{bmatrix}$  (1.3.3-1)

We can obviously define the set of N unit vectors

$$\underline{\mathbf{e}}^{[1]} = \begin{bmatrix} 1\\0\\0\\\vdots\\0 \end{bmatrix} \qquad \underline{\mathbf{e}}^{[2]} = \begin{bmatrix} 0\\1\\0\\\vdots\\0 \end{bmatrix} \qquad \dots \qquad \underline{\mathbf{e}}^{[N]} = \begin{bmatrix} 0\\0\\0\\\vdots\\1 \end{bmatrix} \qquad (1.3.3-2)$$

so that we can write  $\underline{v}$  as

$$\underline{\mathbf{v}} = \mathbf{v}_1 \underline{\mathbf{e}}^{[1]} + \mathbf{v}_2 \underline{\mathbf{e}}^{[2]} + \dots + \mathbf{v}_N \underline{\mathbf{e}}^{[N]} \quad (\mathbf{1.3.3-3})$$

As <u>any</u>  $\underline{v} \in \mathbf{R}^{N}$  can be written in this manner, the set of vectors  $\{\underline{e}^{[1]}, \underline{e}^{[2]}, \dots, \underline{e}^{[N]}\}$  are said to form a <u>basis</u> for the vector space  $\mathbf{R}^{N}$ .

The same function can be performed by any set of mutually orthogonal vectors, i.e. a set of vectors  $\{\underline{U}^{[1]}, \underline{U}^{[2]}, ..., \underline{U}^{[N]}\}$  such that

$$\underline{U}^{[j]} \bullet \underline{U}^{[k]} = 0 \quad \text{if } j \neq k \text{ (1.3.3-4)}$$

This means that each  $\underline{U}^{[j]}$  is mutually orthogonal to all of the other vectors. We can then write any  $\underline{v} \in \mathbf{R}^{N}$  as

$$\underline{\mathbf{v}} = \mathbf{v}_{1}' \underline{\mathbf{e}}^{[1]} + \mathbf{v}_{2}' \underline{\mathbf{e}}^{[2]} + \dots + \mathbf{v}_{N}' \underline{\mathbf{e}}^{[N]} \quad (1.3.3-5)$$

Where we use a prime to denote that

$$v'_{j} \neq v_{j}$$
 (1.3.3-6)

when comparing the expansions (1.3.3-3) and (1.3.3-5)



Orthogonal basis sets are very easy to use since the coefficients of a vector  $\underline{v} \in \mathbf{R}^{N}$  in the expansion are easily determined.

We take the dot product of (1.3.3-5) with any basis vector  $\underline{U}^{[k]}$ ,  $k \in [1,N]$ ,

$$\underline{\mathbf{v}} \bullet \underline{\mathbf{U}}^{[k]} = \mathbf{v}_{1}^{'}(\underline{\mathbf{U}}^{[1]} \bullet \underline{\mathbf{U}}^{[k]}) + \dots + \mathbf{v}_{k}^{'}(\underline{\mathbf{U}}^{[k]} \bullet \underline{\mathbf{U}}^{[k]}) + \dots + \mathbf{v}_{N}^{'}(\underline{\mathbf{U}}^{[N]} \bullet \underline{\mathbf{U}}^{[k]})$$
(1.3.3-6)

Because

$$\underline{\mathbf{U}}^{[j]} \bullet \underline{\mathbf{U}}^{[k]} = (\underline{\mathbf{U}}^{[k]} \bullet \underline{\mathbf{U}}^{[k]}) \delta_{jk} = \left| \underline{\mathbf{U}}^{[k]} \right|^2 \delta_{jk} \quad (1.3.3-7)$$

with

$$\delta_{jk} = \begin{cases} 1, j = k \\ 0, j \neq k \end{cases}$$
 (1.3.3-8)

then (1.3.3-6) becomes

$$\underline{\mathbf{v}} \bullet \underline{\mathbf{U}}^{[k]} = \mathbf{v}_{k}^{'} \left| \underline{\mathbf{U}}^{[k]} \right|^{2} \Rightarrow \mathbf{v}_{k}^{'} = \frac{\underline{\mathbf{v}} \bullet \underline{\mathbf{U}}^{[k]}}{\left| \underline{\mathbf{U}}^{[k]} \right|^{2}} \quad \textbf{(1.3.3-9)}$$

In the special case that all basis vectors are <u>normalized</u>, i.e.  $|\underline{U}^{[k]}|=1$  for all  $k \in [1,N]$ , we have an <u>orthonormal</u> basis set, and the coefficients of  $\underline{v} \in \mathbf{R}^N$  are simply the dot products with each basis set vector.

Exmaple 1.3.3-1

Consider the orthogonal basis for  $\mathbf{R}^3$ 

$$\underline{U}^{[1]} = \begin{bmatrix} 1\\1\\0 \end{bmatrix} \qquad \underline{U}^{[2]} = \begin{bmatrix} 1\\-1\\0 \end{bmatrix} \qquad \underline{U}^{[3]} = \begin{bmatrix} 0\\0\\1 \end{bmatrix} \quad (1.3.3-10)$$
  
for any  $\underline{v} \in \mathbf{R}^3$ ,  $\underline{v} = \begin{bmatrix} v_1\\v_2\\v_3 \end{bmatrix}$  what are the coefficients of the expansion

$$\underline{\mathbf{v}} = \mathbf{v}_1^{'} \underline{\mathbf{U}}^{[1]} + \mathbf{v}_2^{'} \underline{\mathbf{U}}^{[2]} + \mathbf{v}_3^{'} \underline{\mathbf{U}}^{[3]} \qquad \textbf{(1.3.3-11)}$$

First, we check the basis set for orthogonality  $\begin{bmatrix} r & r \end{bmatrix}$ 

$$\underline{\mathbf{U}}^{[2]} \bullet \underline{\mathbf{U}}^{[2]} = \begin{bmatrix} 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} = (1)(1) + (1)(-1) + (0)(0) = 0$$

$$\underline{\mathbf{U}}^{[1]} \bullet \underline{\mathbf{U}}^{[3]} = \begin{bmatrix} 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = (1)(0) + (1)(0) + (0)(1) = 0 \quad \textbf{(1.3.3-12)}$$

$$\underline{\mathbf{U}}^{[2]} \bullet \underline{\mathbf{U}}^{[3]} = \begin{bmatrix} 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = (1)(0) + (-1)(0) + (0)(1) = 0$$

We also have

$$\left|\underline{U}^{[1]}\right|^{2} = \begin{bmatrix} 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = 2$$
$$\left|\underline{U}^{[2]}\right|^{2} = \begin{bmatrix} 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} = 2$$
$$\left|\underline{U}^{[3]}\right|^{2} = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = 1$$

(1.3.3-13)

So the coefficients of  $\underline{\mathbf{v}} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$  are

$$\mathbf{v}_{1}^{'} = \frac{\underline{\mathbf{v}} \bullet \underline{\mathbf{U}}^{[1]}}{\left|\underline{\mathbf{U}}^{[1]}\right|^{2}} = \frac{1}{2} \begin{bmatrix} \mathbf{v}_{1} & \mathbf{v}_{2} & \mathbf{v}_{3} \end{bmatrix} \begin{bmatrix} 1\\1\\0 \end{bmatrix} = \frac{1}{2} (\mathbf{v}_{1} + \mathbf{v}_{2})$$
$$\mathbf{v}_{2}^{'} = \frac{\underline{\mathbf{v}} \bullet \underline{\mathbf{U}}^{[2]}}{\left|\underline{\mathbf{U}}^{[2]}\right|^{2}} = \frac{1}{2} \begin{bmatrix} \mathbf{v}_{1} & \mathbf{v}_{2} & \mathbf{v}_{3} \end{bmatrix} \begin{bmatrix} 1\\-1\\0 \end{bmatrix} = \frac{1}{2} (\mathbf{v}_{1} - \mathbf{v}_{2})$$
$$\mathbf{v}_{3}^{'} = \frac{\underline{\mathbf{v}} \bullet \underline{\mathbf{U}}^{[3]}}{\left|\underline{\mathbf{U}}^{[3]}\right|^{2}} = \frac{1}{1} \begin{bmatrix} \mathbf{v}_{1} & \mathbf{v}_{2} & \mathbf{v}_{3} \end{bmatrix} \begin{bmatrix} 0\\0\\1 \end{bmatrix} = \mathbf{v}_{3}$$

Although orthogonal basis sets are very convenient to use, a set of N vectors  $B = \{\underline{b}^{[1]}, \underline{b}^{[2]}, \dots, \underline{b}^{[N]}\}$  need not be mutually orthogonal to be used as a basis – they need merely be linearly independent.

Let us consider a set of  $M \le N$  vectors  $\underline{b}^{[1]}, \underline{b}^{[2]}, \dots, \underline{b}^{[M]} \in \mathbf{R}^{N}$ . This set of M vectors is said to be <u>linearly independent</u> if

$$c_1\underline{b}^{[1]} + c_2\underline{b}^{[2]} + \dots + c_M\underline{b}^{[M]} = 0$$
 implies  $c_1 = c_2 = \dots = c_M = 0$  (1.3.3-16)

This means that no  $\underline{b}^{[j]}$ ,  $j \in [1,M]$  can be written as a linear combination of the other M-1 basis vectors.

For example, the set of 3 vectors for  $\mathbf{R}^3$ 

$$\underline{\mathbf{b}}^{[1]} = \begin{bmatrix} 2\\0\\0 \end{bmatrix} \quad \underline{\mathbf{b}}^{[2]} = \begin{bmatrix} 1\\1\\0 \end{bmatrix} \quad \underline{\mathbf{b}}^{[3]} = \begin{bmatrix} 1\\-1\\0 \end{bmatrix} \quad (\mathbf{1.3.3-17})$$

is <u>not</u> linearly independent because we can write  $\underline{b}^{[3]}$  as a linear combination of  $\underline{b}^{[1]}$  and  $\underline{b}^{[2]}$ ,

$$\underline{\mathbf{b}}^{[1]} \cdot \underline{\mathbf{b}}^{[2]} = \begin{bmatrix} 2\\0\\0 \end{bmatrix} - \begin{bmatrix} 1\\1\\0 \end{bmatrix} = \begin{bmatrix} 1\\-1\\0 \end{bmatrix} = \underline{\mathbf{b}}^{[3]} \quad (\mathbf{1.3.3-18})$$

Here, a vector  $\underline{v} \in \mathbf{R}^{N}$  is said to be a <u>linear combination</u> of the vectors  $\underline{b}^{[1]}, \dots, \underline{b}^{[M]} \in \mathbf{R}^{N}$  if it can be written as

$$\underline{\mathbf{v}} = \mathbf{v}'_{1}\underline{\mathbf{b}}^{[1]} + \mathbf{v}'_{2}\underline{\mathbf{b}}^{[2]} + \dots + \mathbf{v}'_{M}\underline{\mathbf{b}}^{[M]}$$
 (1.3.3-19)

We see that the 3 vectors of (1.3.3-17) do <u>not</u> form a basis for  $\mathbf{R}^3$  since we cannot express any vector  $\underline{v} \in \mathbf{R}^3$  with  $v_3 \neq 0$  as a linear combination of  $\{\underline{b}^{[1]}, \underline{b}^{[2]}, \underline{b}^{[3]}\}$  since

$$\underline{\mathbf{v}} = \mathbf{v}_{1}^{'} \begin{bmatrix} 2\\0\\0 \end{bmatrix} + \mathbf{v}_{2}^{'} \begin{bmatrix} 1\\1\\0 \end{bmatrix} + \mathbf{v}_{3}^{'} \begin{bmatrix} 1\\-1\\0 \end{bmatrix} = \begin{bmatrix} 2\mathbf{v}_{1}^{'} - \mathbf{v}_{2}^{'} + \mathbf{v}_{3}^{'} \\ \mathbf{v}_{2}^{'} - \mathbf{v}_{3}^{'} \\ 0 \end{bmatrix}$$
(1.3.3-20)

We see however that if we instead had the set of 3 linearly independent vectors

$$\underline{\mathbf{b}}^{[1]} = \begin{bmatrix} 2\\0\\0 \end{bmatrix} \qquad \underline{\mathbf{b}}^{[2]} = \begin{bmatrix} 1\\1\\0 \end{bmatrix} \qquad \underline{\mathbf{b}}^{[3]} = \begin{bmatrix} 0\\0\\2 \end{bmatrix} \qquad (1.3.3-21)$$

then we could write any  $\underline{\mathbf{v}} \in \mathbf{R}^3$  as

$$\underline{\mathbf{v}} = \begin{bmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \mathbf{v}_3 \end{bmatrix} = \mathbf{v}_1 \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix} + \mathbf{v}_2 \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} + \mathbf{v}_3 \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix} = \begin{bmatrix} 2\mathbf{v}_1' + \mathbf{v}_2' \\ \mathbf{v}_2' \\ 2\mathbf{v}_3' \end{bmatrix}$$
(1.3.3-22)

(1.3.3-22) defines a set of 3 simultaneous linear equations

$$2v'_{1} + v'_{2} = v_{1}$$
  
 $v'_{2} = v_{2}$   
 $2v'_{3} = v_{3}$  (1.3.3-23)

 $\begin{bmatrix} 2 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 2 \end{bmatrix} \begin{bmatrix} v_1' \\ v_2' \\ v_3' \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$ 

that we must solve for  $v'_1, v'_2, v'_3$ ,

$$\mathbf{v}'_1 = \frac{\mathbf{v}_3}{2}, \qquad \mathbf{v}'_2 = \mathbf{v}_2, \qquad \mathbf{v}'_1 = \frac{(\mathbf{v}_1 - \mathbf{v}'_2)}{2}$$
 (1.3.3-24)

We therefore make the following statement:

Any set B of N <u>linearly independent</u> vectors  $\underline{b}^{[1]}, \underline{b}^{[2]}, ..., \underline{b}^{[N]} \in \mathbf{R}^{N}$  can be used as a basis for  $\mathbf{R}^{N}$ .

We can pick any M subset of the linearly independent basis B, and define the <u>span</u> of this subset  $\{\underline{b}^{[1]}, \underline{b}^{[2]}, \dots, \underline{b}^{[M]}\} \subset B$  as the space of all possible vectors  $\underline{v} \in \mathbf{R}^N$  that can be written as

$$\underline{\mathbf{v}} = c_1 b^{[1]} + c_2 \underline{b}^{[2]} + \dots + c_M \underline{b}^{[M]} \quad \textbf{(1.3.3-25)}$$

For the basis set (1.3.3-21), we choose  $\underline{b}^{[1]} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}$  and  $\underline{b}^{[3]} = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$ .(1.3.3-26)

Then, span  $\{\underline{b}^{[1]}, \underline{b}^{[3]}\}$  is the set of all vectors  $\underline{v} \in \mathbf{R}^3$  that can be written as

$$\underline{\mathbf{v}} = \begin{bmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \mathbf{v}_3 \end{bmatrix} = \mathbf{c}_1 \mathbf{b}^{[1]} + \mathbf{c}_3 \mathbf{b}^{[3]} = \mathbf{c}_1 \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix} + \mathbf{c}_3 \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix} = \begin{bmatrix} 2c_1 \\ 0 \\ 2c_3 \end{bmatrix} \quad (1.3.3-27)$$

Therefore, for this case it is easy to see that  $\underline{v} \in \text{span} \{ \underline{b}^{[1]}, \underline{b}^{[3]} \}$ , if and only if ("iff")  $v_2 = 0$ .

Note that if  $\underline{v} \in \text{span}\{\underline{b}^{[1]}, \underline{b}^{[3]}\}\$  and  $\underline{w} \in \text{span}\{\underline{b}^{[1]}, \underline{b}^{[3]}\}\$ , then automatically  $\underline{v} + \underline{w} \in \text{span}\{\underline{b}^{[1]}, \underline{b}^{[3]}\}\$ .

We see then that span { $\underline{b}^{[1]}$ ,  $\underline{b}^{[3]}$ } itself satisfies all the properties of a vector space identified in section 1.3.1.

Since span {  $\underline{b}^{[1]}$ ,  $\underline{b}^{[3]}$  }  $\subset \mathbf{R}^3$  (i.e. it is a subset of  $\mathbf{R}^3$ ), we call span {  $\underline{b}^{[1]}$ ,  $\underline{b}^{[3]}$  } a subspace of  $\mathbf{R}^3$ .

This concept of basis sets also lets us formally identify the meaning of dimension – this will be useful in the establishment of criteria for existence/uniqueness of solutions.

Let us consider a vector space V that satisfies all the properties of a vector space identified in section 1.3.1.

We say that the dimension of V is N if every set of N+1 vectors  $\underline{v}^{[1]}, \underline{v}^{[2]}, \dots, \underline{v}^{[N+1]} \in V$  is linearly independent and if there exists some set of N linearly independent vectors  $\underline{b}^{[1]}, \dots, \underline{b}^{[N]} \in V$  that forms a basis for V. We say then that dim(V) = N. (1.3.3-28)

While linearly independent basis sets are completely valid, they are more difficult to use than orthogonal basis sets because one must solve a set of N linear algebraic equations to find the coefficients of the expansion

$$\underline{\mathbf{v}} = \mathbf{v}_{1}^{'} \underline{\mathbf{b}}^{[1]} + \mathbf{v}_{2}^{'} \underline{\mathbf{b}}^{[2]} + \dots + \mathbf{v}_{N}^{'} \underline{\mathbf{b}}^{[N]}$$
(1.3.3-29)

 $\begin{bmatrix} b_1^{[1]} & b_1^{[2]} & \dots & b_1^{[N]} \\ b_2^{[1]} & b_2^{[2]} & \dots & b_2^{[N]} \\ \vdots & \vdots & \ddots & \vdots \\ b_N^{[1]} & b_N^{[2]} & \dots & b_N^{[N]} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_N \end{bmatrix} \bullet O(N^3) \text{ effort to solve for all } v_j \text{'s} \qquad (1.3.3-30)$ 

This requires more effort for an orthogonal basis  $\{\underline{U}^{[1]}, \dots, \underline{U}^{[N]}\}$  as

$$\mathbf{v}'_{j} = \frac{\underline{\mathbf{v}} \bullet \underline{\mathbf{U}}^{[j]}}{\underline{\mathbf{U}}^{[j]} \bullet \underline{\mathbf{U}}^{[j]}} \bullet \mathbf{U}^{[j]} \bullet \mathbf{U}^{[j]$$

This provides an impetus to perform <u>Gramm-Schmidt orthogonalization</u>. We start with a linearly independent basis set  $\{\underline{b}^{[1]}, \underline{b}^{[2]}, ..., \underline{b}^{[N]}\}$  for  $\mathbf{R}^{N}$ . From this set, we construct an orthogonal basis set  $\{\underline{U}^{[1]}, \underline{U}^{[2]}, ..., \underline{U}^{[N]}\}$  through the following procedure:

1. First, set  $\underline{U}^{[1]} = \underline{b}^{[1]}$  (1.3.3-31)

2. Next, we construct  $\underline{U}^{[2]}$  such that  $\underline{U}^{[2]} \bullet \underline{U}^{[1]} = 0$ . Since  $\underline{U}^{[1]} = \underline{b}^{[1]}$ , and  $\underline{b}^{[2]}$  and  $\underline{b}^{[1]}$  are linearly independent, we can form an orthogonal vector  $\underline{U}^{[2]}$  from  $\underline{b}^{[2]}$  by the following procedure:



We write  $\underline{U}^{[2]} = \underline{b}^{[2]} + c\underline{U}^{[1]}$  (1.3.3-32)

Then, taking the dot product with  $\underline{U}^{[1]}$ ,

$$\underline{\mathbf{U}}^{[2]} \bullet \underline{\mathbf{U}}^{[1]} = \mathbf{0} = \underline{\mathbf{b}}^{[2]} \bullet \underline{\mathbf{U}}^{[1]} + \mathbf{c}\underline{\mathbf{U}}^{[1]} \bullet \underline{\mathbf{U}}^{[1]}$$
 (1.3.3-33)

Therefore

$$c = \frac{-\underline{b}^{[2]} \cdot \underline{U}^{[1]}}{\left|\underline{U}^{[1]}\right|^2} \quad (1.3.3-34)$$

And our 2<sup>nd</sup> vector in the orthogonal basis is

$$\underline{\mathbf{U}}^{[2]} = \underline{\mathbf{b}}^{[2]} - \left[ \frac{\underline{\mathbf{b}}^{[2]} \bullet \underline{\mathbf{U}}^{[1]}}{\left| \underline{\mathbf{U}}^{[1]} \right|^2} \right] \underline{\mathbf{U}}^{[1]} \quad \textbf{(1.3.3-35)}$$

3. We now form  $\underline{U}^{[3]}$  in a similar manner. Since  $\underline{U}^{[2]}$  is a linear combination of  $\underline{b}^{[1]}$  and  $\underline{b}^{[2]}$ , we can add a component from  $\underline{b}^{[3]}$ direction to form  $U^{[3]}$ ,

$$\underline{U}^{[3]} = \underline{b}^{[3]} + c_2 \underline{U}^{[2]} + c_1 \underline{U}^{[1]}$$
 (1.3.3-36)

First, we want  $\underline{U}^{[3]} \bullet \underline{U}^{[1]} = 0 = \underline{b}^{[3]} \bullet \underline{U}^{[1]} + c_2 \underline{U}^{[2]} \bullet \underline{U}^{[1]} + c_1 \underline{U}^{[1]} \bullet \underline{U}^{[1]}$  (1.3.3-37)

so

$$c_{1} = \frac{-\underline{b}^{[3]} \bullet \underline{U}^{[1]}}{\left|\underline{U}^{[1]}\right|^{2}} \quad (1.3.3-38)$$

A similar condition that  $\underline{U}^{[3]} \bullet \underline{U}^{[2]} = 0$  yields  $-\mathbf{h}^{[3]} \bullet \underline{U}^{[2]}$ 

$$c_2 = \frac{-\underline{b}^{\lfloor J \rfloor} \bullet \underline{U}^{\lfloor 2 \rfloor}}{\left| \underline{U}^{\lfloor 2 \rfloor} \right|^2} \quad (1.3.3-39)$$

so that the 3<sup>rd</sup> member of the orthogonal basis set is

$$\underline{\mathbf{U}}^{[3]} = \underline{\mathbf{b}}^{[3]} - \left[\frac{\underline{\mathbf{b}}^{[3]} \bullet \underline{\mathbf{U}}^{[2]}}{\left|\underline{\mathbf{U}}^{[2]}\right|^2}\right] \underline{\mathbf{U}}^{[2]} - \left[\frac{\underline{\mathbf{b}}^{[3]} \bullet \underline{\mathbf{U}}^{[1]}}{\left|\underline{\mathbf{U}}^{[1]}\right|^2}\right] \underline{\mathbf{U}}^{[1]} \quad (1.3.3-40)$$

4. Continue for  $\underline{U}^{[j]}$ , j = 4, 5, ..., N where

$$\underline{U}^{[j]} = \underline{b}^{[j]} - \sum_{k=1}^{j-1} \left[ \frac{\underline{b}^{[j]} \bullet \underline{U}^{[k]}}{\left| \underline{U}^{[k]} \right|^2} \right] \underline{U}^k \quad (1.3.3-41)$$

5. Normalize vectors if desired (we can do this also during construction of orthogonal basis set)

$$\underline{\underline{U}}^{[i]} \leftarrow \frac{\underline{\underline{U}}^{[i]}}{\left|\underline{\underline{U}}^{[i]}\right|} \quad \textbf{(1.3.3-42)}$$

As an example, let us use this method to generate an orthogonal basis for  $\mathbf{R}^3$  such that the  $1^{st}$  member of the basis set is

$$\underline{\mathbf{U}}^{[1]} = \begin{bmatrix} 1\\1\\0 \end{bmatrix} \quad (\mathbf{1.3.3-43})$$

First, we write a linearly independent basis that is not, in general, orthogonal. For example, we could choose

$$\underline{\mathbf{b}}^{[1]} = \begin{bmatrix} 1\\1\\0 \end{bmatrix} \qquad \underline{\mathbf{b}}^{[2]} = \begin{bmatrix} 1\\0\\0 \end{bmatrix} \qquad \underline{\mathbf{b}}^{[3]} = \begin{bmatrix} 0\\0\\1 \end{bmatrix} \qquad (1.3.3-44)$$

We now perform Gram-Schmidt orthogonalization,

1. 
$$\underline{\mathbf{U}}^{[1]} = \underline{\mathbf{b}}^{[1]} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$
 (1.3.3-45)

2. We next set

$$\underline{U}^{[2]} = \underline{b}^{[2]} - \left[\frac{\underline{b}^{[2]} \cdot \underline{U}^{[1]}}{|\underline{U}^{[1]}|^2}\right] \underline{U}^{[1]} \quad (1.3.3-35, \text{ repeated})$$
$$\left|\underline{U}^{[1]}\right|^2 = \begin{bmatrix} 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = 2 \quad (1.3.3-46)$$

$$\underline{\mathbf{b}}^{[2]} \bullet \underline{\mathbf{U}}^{[1]} = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = 1 \quad \textbf{(1.3.3-47)}$$

so

$$\underline{U}^{[2]} = \begin{bmatrix} 1\\0\\0 \end{bmatrix} - \frac{1}{2} \begin{bmatrix} 1\\1\\0 \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\\-\frac{1}{2}\\0 \end{bmatrix} \quad (1.3.3-48)$$
  
Note  $\underline{U}^{[2]} \bullet \underline{U}^{[1]} = \begin{bmatrix} 1/2 & -1/2 & 0 \end{bmatrix} \begin{bmatrix} 1\\1\\0 \end{bmatrix} = \frac{1}{2} - \frac{1}{2} = 0 \quad (1.3.3-49)$ 

We now calculate

$$\underline{U}^{[3]} = \underline{b}^{[3]} \cdot \left[ \frac{\underline{b}^{[3]} \cdot \underline{U}^{[2]}}{|\underline{U}^{[2]}|^2} \right] \underline{U}^{[2]} - \left[ \frac{\underline{b}^{[3]} \cdot \underline{U}^{[1]}}{|\underline{U}^{[1]}|^2} \right] \underline{U}^{[1]}$$
(1.3.3-41, repeated)
$$\left| \underline{U}^{[2]} \right|^2 = \begin{bmatrix} 1/2 & -1/2 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ 0 \\ 0 \end{bmatrix} = \left( \frac{1}{2} \right)^2 + \left( -\frac{1}{2} \right)^2 = \frac{1}{4} + \frac{1}{4} = \frac{1}{2}$$
(1.3.3-50)
$$\underline{b}^{[3]} \cdot \underline{U}^{[2]} = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ 0 \\ 0 \end{bmatrix} = 0$$
(1.3.3-51)
$$\underline{b}^{[3]} \cdot \underline{U}^{[1]} = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} = 0$$
(1.3.3-52)

We therefore have merely  $\underline{U}^{[3]} = \underline{b}^{[3]} = \begin{bmatrix} 0\\0\\1 \end{bmatrix}$  (1.3.3-53)

Our orthogonal basis set is therefore

$$\underline{\mathbf{U}}^{[1]} = \begin{bmatrix} 1\\1\\0 \end{bmatrix} \qquad \underline{\mathbf{U}}^{[2]} = \begin{bmatrix} \frac{1}{2}\\-\frac{1}{2}\\0 \end{bmatrix} \qquad \underline{\mathbf{U}}^{[3]} = \begin{bmatrix} 0\\0\\1 \end{bmatrix} \quad (\mathbf{1.3.3-54})$$