

# CX1104: Linear Algebra for Computing

$$\underbrace{\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mn} \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}}_{x} = \underbrace{\begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}}_{b}$$

Chap. No : **6.3.2**

Lecture : **Orthogonality**

Topic : **Gram–Schmidt Process**

Concept : **Gram-Schmidt Process for QR decomposition**

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# QR Factorisation revisited

The QR decomposition can be performed by Gram–Schmidt. Given a matrix  $A$  ( $m \times n$  sized),

$$A = QR$$

$$A = [q_1 \quad q_2 \quad \dots \quad q_n] \begin{bmatrix} R_{11} & R_{12} & \dots & R_{1n} \\ 0 & R_{22} & \dots & R_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & R_{nn} \end{bmatrix}$$

## The $Q$ Factor (economy qr):

- $Q$  is  $m \times n$  with orthonormal columns and  $Q^T Q = I$  dimension  $n \times n$
- If  $A$  is square ( $m = n$ ), then  $Q$  is orthogonal, i.e,  $Q^T Q = Q Q^T = I$
- If  $A$  is tall ( $m > n$ ), then  $Q Q^T \neq I$ ,  
The matrix  $Q Q^T$  is a projection matrix of dimension  $m \times m$ , and it will project a vector  $R^m$  onto the columns space of  $A$ . In other words,  $Q Q^T y = \hat{y}$ , where  $\hat{y}$  is the least squares error approximation of  $y$  in the column space of  $A$  (see sec 7.1.4)

## The $R$ Factor:

- $R$  is  $n \times n$  upper triangular,
- If  $A$  has independent column, then  $R$  is invertible, else  $R$  is singular (not-invertible)

- Vectors  $q_1, q_2, \dots, q_n$  are orthonormal  $m$ -dimensional vectors:  $\|q_i\| = 1$  and  $q_i^T q_j = 0$  if  $i \neq j$

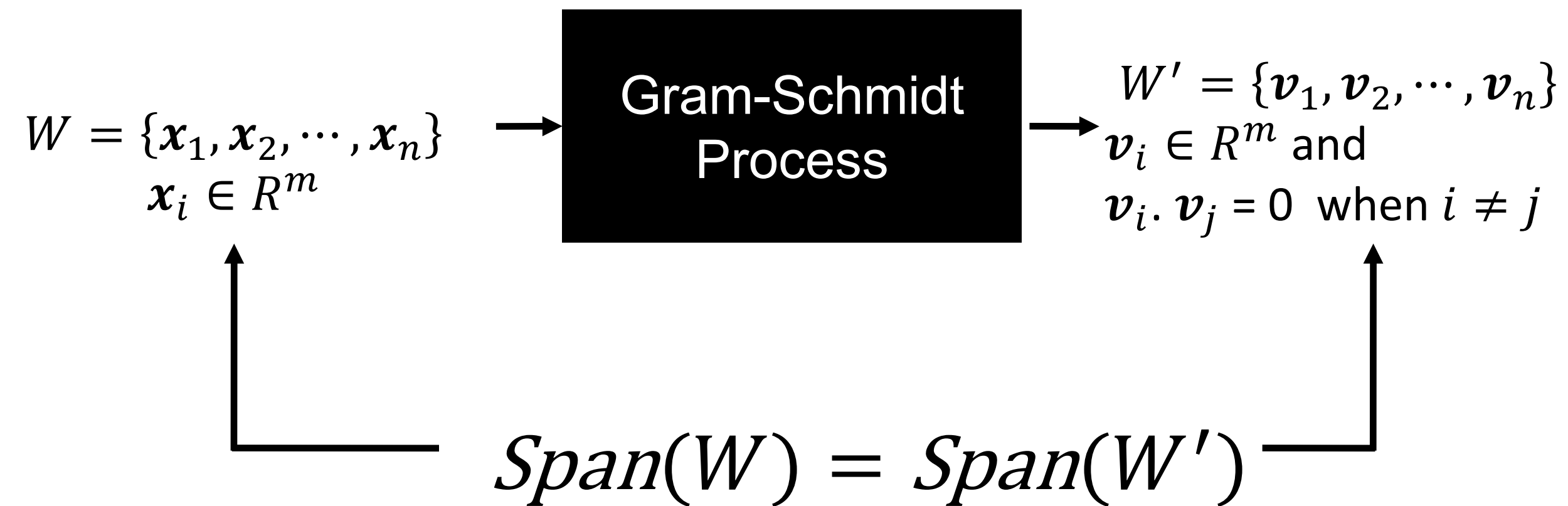
**NOTE:**

**$Q$  is obtained by performing GS Process on  $A$**

# The Gram Schmidt Process

## What does Gram-Schmidt Process Do?

It orthogonalises a set of vectors!



Typically, we are  
give a matrix  
 $A$ , and these  $x_i$  are  
columns of  $A$ .

# The Gram Schmidt Process

In basic Gram-Schmidt, we assume that  $\{x_1, x_2, \dots\}$  are independent columns,

## THEOREM 11

### The Gram–Schmidt Process

Given a basis  $\{x_1, \dots, x_p\}$  for a nonzero subspace  $W$  of  $\mathbb{R}^n$ , define

$$v_1 = x_1$$

$$v_2 = x_2 - \frac{x_2 \cdot v_1}{v_1 \cdot v_1} v_1$$

$$v_3 = x_3 - \frac{x_3 \cdot v_1}{v_1 \cdot v_1} v_1 - \frac{x_3 \cdot v_2}{v_2 \cdot v_2} v_2$$

$$\vdots$$

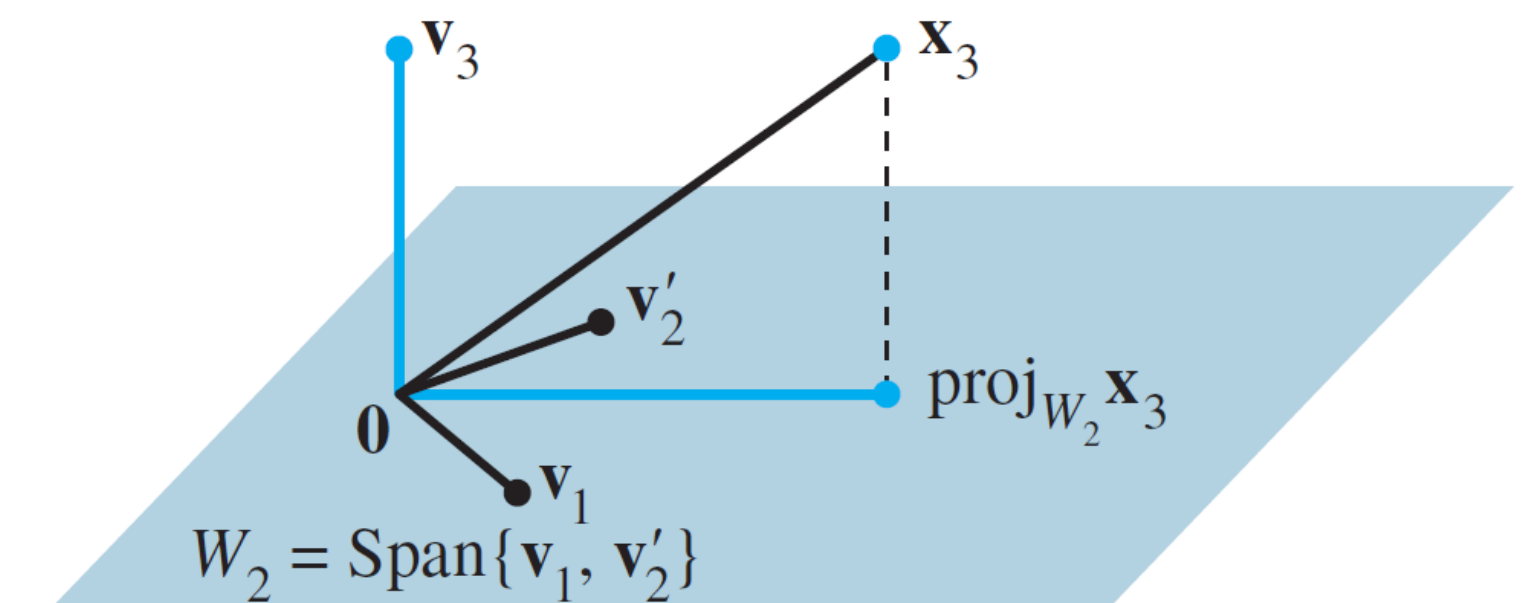
$$v_p = x_p - \frac{x_p \cdot v_1}{v_1 \cdot v_1} v_1 - \frac{x_p \cdot v_2}{v_2 \cdot v_2} v_2 - \dots - \frac{x_p \cdot v_{p-1}}{v_{p-1} \cdot v_{p-1}} v_{p-1}$$

Then  $\{v_1, \dots, v_p\}$  is an orthogonal basis for  $W$ . In addition

$$\text{Span}\{v_1, \dots, v_k\} = \text{Span}\{x_1, \dots, x_k\} \quad \text{for } 1 \leq k \leq p \quad (1)$$

Watch these worked out examples:

1. GramSchmidt: <https://www.youtube.com/watch?v=Aslf3KGq2UE>
2. QR: <https://www.youtube.com/watch?v=6DybLNNkWyE>
3. MIT Gram Schmidt: <https://www.youtube.com/watch?v=TRktLuAktBQ&t=17s>



**FIGURE 2** The construction of  $v_3$  from  $x_3$  and  $W_2$ .



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Instructor: Ana Rita Pires  
View the complete course: <http://ocw.mit.edu/18-06SCF11>



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# Proof Theorem 11: Span of vectors generated by GS is same as original set of vectors

**PROOF** For  $1 \leq k \leq p$ , let  $W_k = \text{Span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$ . Set  $\mathbf{v}_1 = \mathbf{x}_1$ , so that  $\text{Span}\{\mathbf{v}_1\} = \text{Span}\{\mathbf{x}_1\}$ . Suppose, for some  $k < p$ , we have constructed  $\mathbf{v}_1, \dots, \mathbf{v}_k$  so that  $\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$  is an orthogonal basis for  $W_k$ . Define

$$\mathbf{v}_{k+1} = \mathbf{x}_{k+1} - \text{proj}_{W_k} \mathbf{x}_{k+1} \quad (2)$$

By the Orthogonal Decomposition Theorem,  $\mathbf{v}_{k+1}$  is orthogonal to  $W_k$ . Note that  $\text{proj}_{W_k} \mathbf{x}_{k+1}$  is in  $W_k$  and hence also in  $W_{k+1}$ . Since  $\mathbf{x}_{k+1}$  is in  $W_{k+1}$ , so is  $\mathbf{v}_{k+1}$  (because  $W_{k+1}$  is a subspace and is closed under subtraction). Furthermore,  $\mathbf{v}_{k+1} \neq \mathbf{0}$  because  $\mathbf{x}_{k+1}$  is not in  $W_k = \text{Span}\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$ . Hence  $\{\mathbf{v}_1, \dots, \mathbf{v}_{k+1}\}$  is an orthogonal set of nonzero vectors in the  $(k+1)$ -dimensional space  $W_{k+1}$ . By the Basis Theorem in Section 4.5, this set is an orthogonal basis for  $W_{k+1}$ . Hence  $W_{k+1} = \text{Span}\{\mathbf{v}_1, \dots, \mathbf{v}_{k+1}\}$ . When  $k+1 = p$ , the process stops. ■

Theorem 11 shows that any nonzero subspace  $W$  of  $\mathbb{R}^n$  has an orthogonal basis, because an ordinary basis  $\{\mathbf{x}_1, \dots, \mathbf{x}_p\}$  is always available (by Theorem 11 in Section 4.5), and the Gram–Schmidt process depends only on the existence of orthogonal projections onto subspaces of  $W$  that already have orthogonal bases.



# Example:

**EXAMPLE 2** Let  $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$ ,  $\mathbf{x}_2 = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix}$ , and  $\mathbf{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$ . Then  $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3\}$  is

clearly linearly independent and thus is a basis for a subspace  $W$  of  $\mathbb{R}^4$ . Construct an orthogonal basis for  $W$ .

**SOLUTION**

**Step 1.** Let  $\mathbf{v}_1 = \mathbf{x}_1$  and  $W_1 = \text{Span}\{\mathbf{x}_1\} = \text{Span}\{\mathbf{v}_1\}$ .

**Step 2.** Let  $\mathbf{v}_2$  be the vector produced by subtracting from  $\mathbf{x}_2$  its projection onto the subspace  $W_1$ . That is, let

$$\begin{aligned} \mathbf{v}_2 &= \mathbf{x}_2 - \text{proj}_{W_1} \mathbf{x}_2 \\ &= \mathbf{x}_2 - \frac{\mathbf{x}_2 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 \quad \text{Since } \mathbf{v}_1 = \mathbf{x}_1 \\ &= \begin{bmatrix} 0 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \frac{3}{4} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -3/4 \\ 1/4 \\ 1/4 \\ 1/4 \end{bmatrix} \end{aligned}$$

As in Example 1,  $\mathbf{v}_2$  is the component of  $\mathbf{x}_2$  orthogonal to  $\mathbf{x}_1$ , and  $\{\mathbf{v}_1, \mathbf{v}_2\}$  is an orthogonal basis for the subspace  $W_2$  spanned by  $\mathbf{x}_1$  and  $\mathbf{x}_2$ .

Note:  $v'_2 = v_2 * 4$  to get rid of denominator in  $v_2$

**Step 3.** Let  $\mathbf{v}_3$  be the vector produced by subtracting from  $\mathbf{x}_3$  its projection onto the subspace  $W_2$ . Use the orthogonal basis  $\{\mathbf{v}_1, \mathbf{v}'_2\}$  to compute this projection onto  $W_2$ :

Projection of  
 $\mathbf{x}_3$  onto  $\mathbf{v}_1$   
↓

Projection of  
 $\mathbf{x}_3$  onto  $\mathbf{v}'_2$   
↓

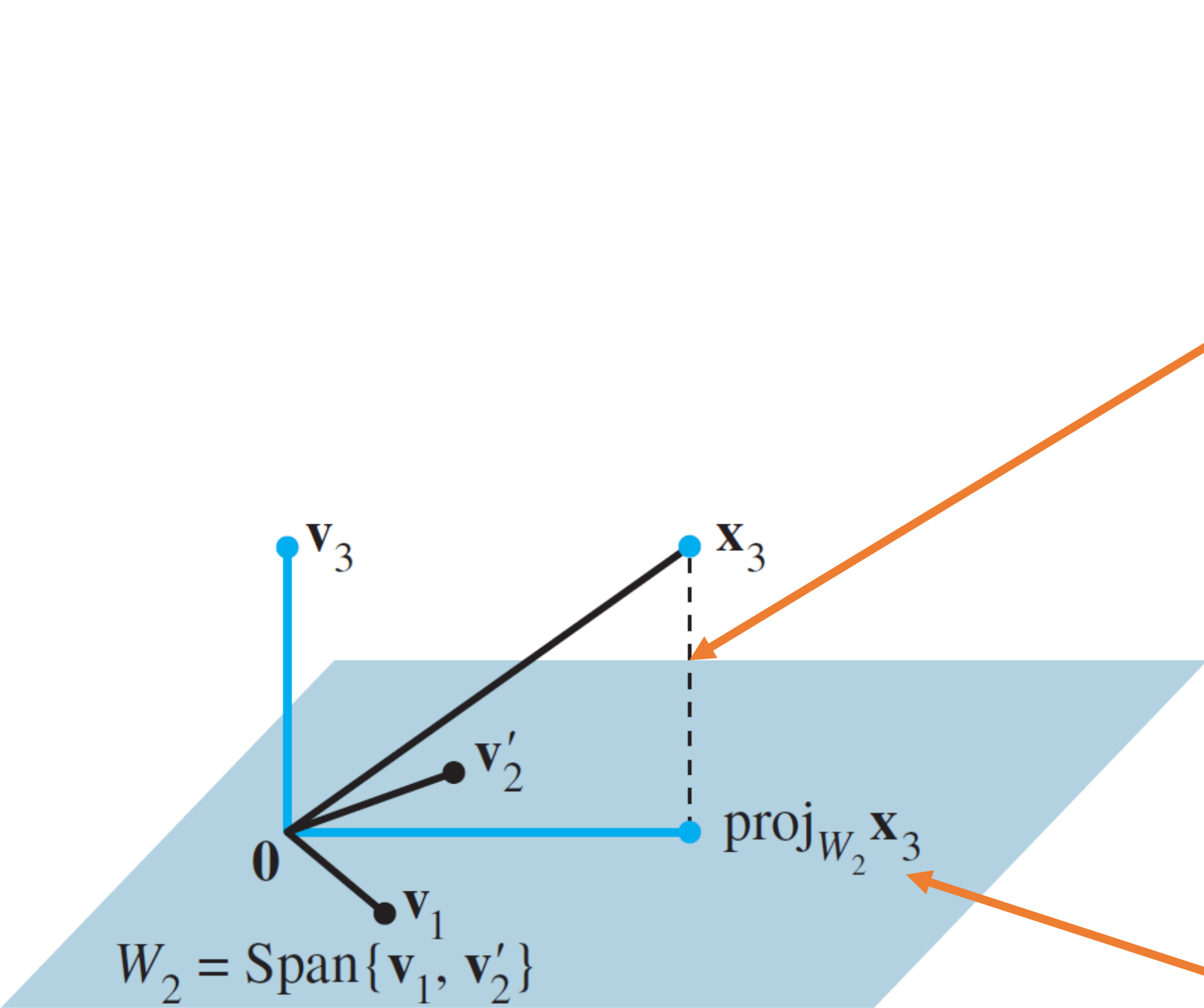
$$\text{proj}_{W_2} \mathbf{x}_3 = \frac{\mathbf{x}_3 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1 + \frac{\mathbf{x}_3 \cdot \mathbf{v}'_2}{\mathbf{v}'_2 \cdot \mathbf{v}'_2} \mathbf{v}'_2 = \frac{2}{4} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} + \frac{2}{12} \begin{bmatrix} -3 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 2/3 \\ 2/3 \\ 2/3 \end{bmatrix}$$

Then  $\mathbf{v}_3$  is the component of  $\mathbf{x}_3$  orthogonal to  $W_2$ , namely,

$$\mathbf{v}_3 = \mathbf{x}_3 - \text{proj}_{W_2} \mathbf{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 0 \\ 2/3 \\ 2/3 \\ 2/3 \end{bmatrix} = \begin{bmatrix} 0 \\ -2/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

See Slide 3 of Chapter 6.2.5 for explanation.

# Example:



**FIGURE 2** The construction of  $\mathbf{v}_3$  from  $\mathbf{x}_3$  and  $W_2$ .

$$\mathbf{v}_3 = \mathbf{x}_3 - \text{proj}_{W_2} \mathbf{x}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 0 \\ 2/3 \\ 2/3 \\ 2/3 \end{bmatrix} = \begin{bmatrix} 0 \\ -2/3 \\ 1/3 \\ 1/3 \end{bmatrix}$$

See Fig. 2 for a diagram of this construction. Observe that  $\mathbf{v}_3$  is in  $W$ , because  $\mathbf{x}_3$  and  $\text{proj}_{W_2} \mathbf{x}_3$  are both in  $W$ . Thus  $\{\mathbf{v}_1, \mathbf{v}'_2, \mathbf{v}_3\}$  is an orthogonal set of nonzero vectors and hence a linearly independent set in  $W$ . Note that  $W$  is three-dimensional since it was defined by a basis of three vectors. Hence, by the Basis Theorem in Section 4.5,  $\{\mathbf{v}_1, \mathbf{v}'_2, \mathbf{v}_3\}$  is an orthogonal basis for  $W$ . ■

$$\text{proj}_{W_2} \mathbf{x}_3 = \underbrace{\frac{\mathbf{x}_3 \cdot \mathbf{v}_1}{\mathbf{v}_1 \cdot \mathbf{v}_1} \mathbf{v}_1}_{\text{Projection of } \mathbf{x}_3 \text{ onto } \mathbf{v}_1} + \underbrace{\frac{\mathbf{x}_3 \cdot \mathbf{v}'_2}{\mathbf{v}'_2 \cdot \mathbf{v}'_2} \mathbf{v}'_2}_{\text{Projection of } \mathbf{x}_3 \text{ onto } \mathbf{v}'_2} = \frac{2}{4} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} + \frac{2}{12} \begin{bmatrix} -3 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 2/3 \\ 2/3 \\ 2/3 \end{bmatrix}$$

### The Basis Theorem

Let  $V$  be a  $p$ -dimensional vector space,  $p \geq 1$ . Any linearly independent set of exactly  $p$  elements in  $V$  is automatically a basis for  $V$ . Any set of exactly  $p$  elements that spans  $V$  is automatically a basis for  $V$ .



# Orthogonal basis vs Orthonormal basis

The columns of  $Q$   
are orthogonal,  
as well as orthonormal!

$$Q^T Q = I$$

Orthonormal == orthogonal +  
(length of vector ==1)

## Orthonormal Bases

An orthonormal basis is constructed easily from an orthogonal basis  $\{\mathbf{v}_1, \dots, \mathbf{v}_p\}$ : simply normalize (i.e., “scale”) all the  $\mathbf{v}_k$ . When working problems by hand, this is easier than normalizing each  $\mathbf{v}_k$  as soon as it is found (because it avoids unnecessary writing of square roots).

**EXAMPLE 3** Example 1 constructed the orthogonal basis

$$\mathbf{v}_1 = \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix}$$

An orthonormal basis is

$$\mathbf{u}_1 = \frac{1}{\|\mathbf{v}_1\|} \mathbf{v}_1 = \frac{1}{\sqrt{45}} \begin{bmatrix} 3 \\ 6 \\ 0 \end{bmatrix} = \begin{bmatrix} 1/\sqrt{5} \\ 2/\sqrt{5} \\ 0 \end{bmatrix}$$

$$\mathbf{u}_2 = \frac{1}{\|\mathbf{v}_2\|} \mathbf{v}_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$





# The entries of R matrix during GS

Consider A has independent col (mxn matrix)

$$A = [x_1, x_2, x_3, \dots, x_n]$$

Gram-Schmidt Process

$$\text{Proj}_v x = \frac{v \cdot x}{v \cdot v} v$$

$$v_1 = x_1$$

$$v_2 = x_2 - \text{Proj}_{v_1} x_2$$

$$v_3 = x_3 - \text{Proj}_{v_1} x_3 - \text{Proj}_{v_2} x_3$$

$$v_i = x_i - \sum_{j=1}^{i-1} \text{Proj}_{v_j} x_i$$

Ortho-  
normalization

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

$$u_2 = \frac{v_2}{||v_2||}$$

$$u_i = \frac{v_i}{||v_i||}$$

We can now express the  $x_i$  over our newly computed orthonormal basis:

$$x_1 = u_1 \cdot x_1 u_1$$

$$x_2 = u_1 \cdot x_2 u_1 + u_2 \cdot x_2 u_2$$

$$x_3 = u_1 \cdot x_3 u_1 + u_2 \cdot x_3 u_2 + u_3 \cdot x_3 u_3$$

$\vdots$

$$x_n = \sum_{j=1}^n u_j \cdot x_n u_j$$

$e_j$

This can be written in matrix form:

$$A = QR$$

where:

$$Q = [u_1, u_2, u_3, \dots, u_n]$$

and

$$R = \begin{pmatrix} u_1 \cdot x_1 & u_1 \cdot x_2 & u_1 \cdot x_3 & \dots \\ 0 & u_2 \cdot x_2 & u_2 \cdot x_3 & \dots \\ 0 & 0 & u_3 \cdot x_3 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

# Example: Gram–Schmidt on a 3x3 matrix

**Example** [ [edit](#) ]

Consider the decomposition of

$$A = \begin{pmatrix} 12 & -51 & 4 \\ 6 & 167 & -68 \\ -4 & 24 & -41 \end{pmatrix}.$$

Recall that an orthonormal matrix  $Q$  has the property

$$Q^T Q = I.$$

Then, we can calculate  $Q$  by means of Gram–Schmidt as follows:

$$U = (\mathbf{u}_1 \quad \mathbf{u}_2 \quad \mathbf{u}_3) = \begin{pmatrix} 12 & -69 & -58/5 \\ 6 & 158 & 6/5 \\ -4 & 30 & -33 \end{pmatrix};$$
$$Q = \left( \frac{\mathbf{u}_1}{\|\mathbf{u}_1\|} \quad \frac{\mathbf{u}_2}{\|\mathbf{u}_2\|} \quad \frac{\mathbf{u}_3}{\|\mathbf{u}_3\|} \right) = \begin{pmatrix} 6/7 & -69/175 & -58/175 \\ 3/7 & 158/175 & 6/175 \\ -2/7 & 6/35 & -33/35 \end{pmatrix}$$

Thus, we have

$$Q^T A = Q^T Q R = R;$$
$$R = Q^T A = \begin{pmatrix} 14 & 21 & -14 \\ 0 & 175 & -70 \\ 0 & 0 & 35 \end{pmatrix}$$

Hence,

$$A = \begin{pmatrix} 12 & -51 & 4 \\ 6 & 167 & -68 \\ -4 & 24 & -41 \end{pmatrix} =$$
$$\begin{pmatrix} 6/7 & -69/175 & -58/175 \\ 3/7 & 158/175 & 6/175 \\ -2/7 & 6/35 & -33/35 \end{pmatrix} \times \begin{pmatrix} 14 & 21 & -14 \\ 0 & 175 & -70 \\ 0 & 0 & 35 \end{pmatrix}$$

$Q$ : Orthogonal Matrix

$R$ : Upper Triangular Matrix

# Warning: modify QR when A has dependent column!

## QR decomposition

From: pg 4-6 <http://ee263.stanford.edu/lectures/qr.pdf>

Note: here the columns of Q are denoted as  $q_i$

written in matrix form:  $A = QR$ , where  $A \in \mathbb{R}^{m \times n}$ ,  $Q \in \mathbb{R}^{m \times n}$ ,  $R \in \mathbb{R}^{n \times n}$ :

$$\underbrace{\begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}}_A = \underbrace{\begin{bmatrix} q_1 & q_2 & \cdots & q_n \end{bmatrix}}_Q \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix}}_R$$

- ▶ in basic G-S we assume  $a_1, \dots, a_n \in \mathbb{R}^m$  are independent
- ▶ if  $a_1, \dots, a_n$  are dependent, we find  $\tilde{q}_j = 0$  for some  $j$ , which means  $a_j$  is linearly dependent on  $a_1, \dots, a_{j-1}$
- ▶ modified algorithm: when we encounter  $\tilde{q}_j = 0$ , skip to next vector  $a_{j+1}$  and continue:

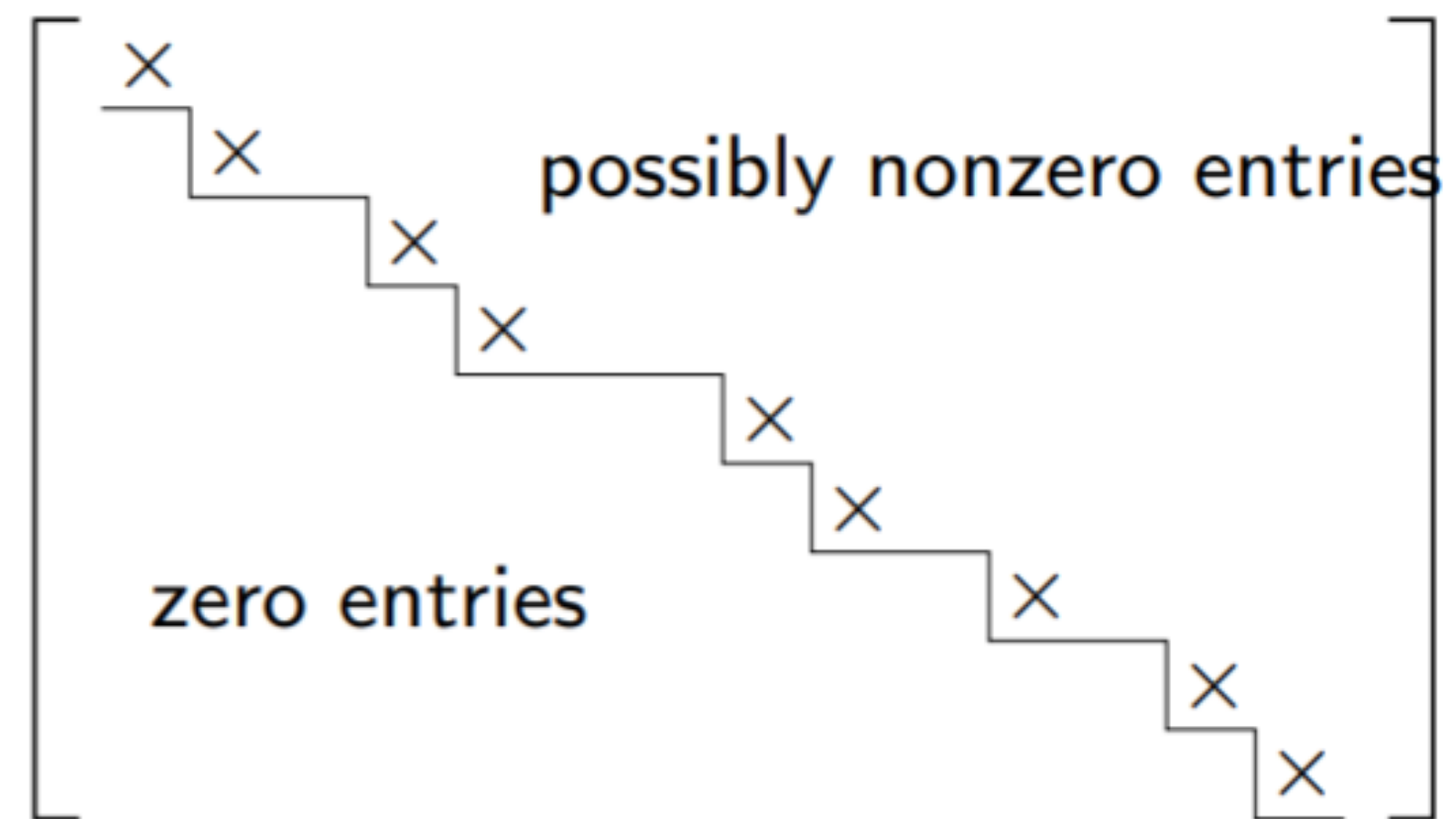
```
r = 0
for i = 1, ..., n
     $\tilde{a} = a_i - \sum_{j=1}^r q_j q_j^T a_i$ 
    if  $\tilde{a} \neq 0$ 
        r = r + 1
         $q_r = \tilde{a} / \|\tilde{a}\|$ 
```

# Warning: modify QR when A has dependent column!

on exit,

- ▶  $q_1, \dots, q_r$  is an orthonormal basis for **range**( $A$ ) (hence  $r = \mathbf{Rank}(A)$ )
- ▶ each  $a_i$  is linear combination of previously generated  $q_j$ 's

in matrix notation we have  $A = QR$  with  $Q^T Q = I$  and  $R \in \mathbb{R}^{r \times n}$  in *upper staircase form*



'corner' entries (shown as  $\times$ ) are nonzero



# How to get **full** QR decomposition when $A$ is tall and skinny?

## ‘Full’ $QR$ factorization

with  $A = Q_1 R_1$  the  $QR$  factorization as above, write

$$A = [Q_1 \quad Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$$

where  $[Q_1 \quad Q_2]$  is orthogonal, *i.e.*, columns of  $Q_2 \in \mathbb{R}^{m \times (m-r)}$  are orthonormal, orthogonal to  $Q_1$

to find  $Q_2$ :

- ▶ find any matrix  $\tilde{A}$  s.t.  $[A \quad \tilde{A}]$  has rank  $m$  (*e.g.*,  $\tilde{A} = I$ )
- ▶ apply general Gram-Schmidt to  $[A \quad \tilde{A}]$
- ▶  $Q_1$  are orthonormal vectors obtained from columns of  $A$
- ▶  $Q_2$  are orthonormal vectors obtained from extra columns ( $\tilde{A}$ )

*i.e.*, any set of orthonormal vectors can be **extended** to an orthonormal basis for  $\mathbb{R}^m$

# look ahead: $QQ^T$ relationship to Least Squares

Ref: relating  $QQ^T$  to least squares solution (see Sec 7.1.4)

and Boyd's lecture:

<https://see.stanford.edu/materials/Isoeldsee263/05-ls.pdf> Pg 5-8

## Least-squares via $QR$ factorization

- $A \in \mathbf{R}^{m \times n}$  skinny, full rank
- factor as  $A = QR$  with  $Q^T Q = I_n$ ,  $R \in \mathbf{R}^{n \times n}$  upper triangular, invertible
- pseudo-inverse is

$$(A^T A)^{-1} A^T = (R^T Q^T Q R)^{-1} R^T Q^T = R^{-1} Q^T$$

so  $x_{ls} = R^{-1} Q^T y$

- projection on  $\mathcal{R}(A)$  given by matrix

$$A(A^T A)^{-1} A^T = A R^{-1} Q^T = Q Q^T$$

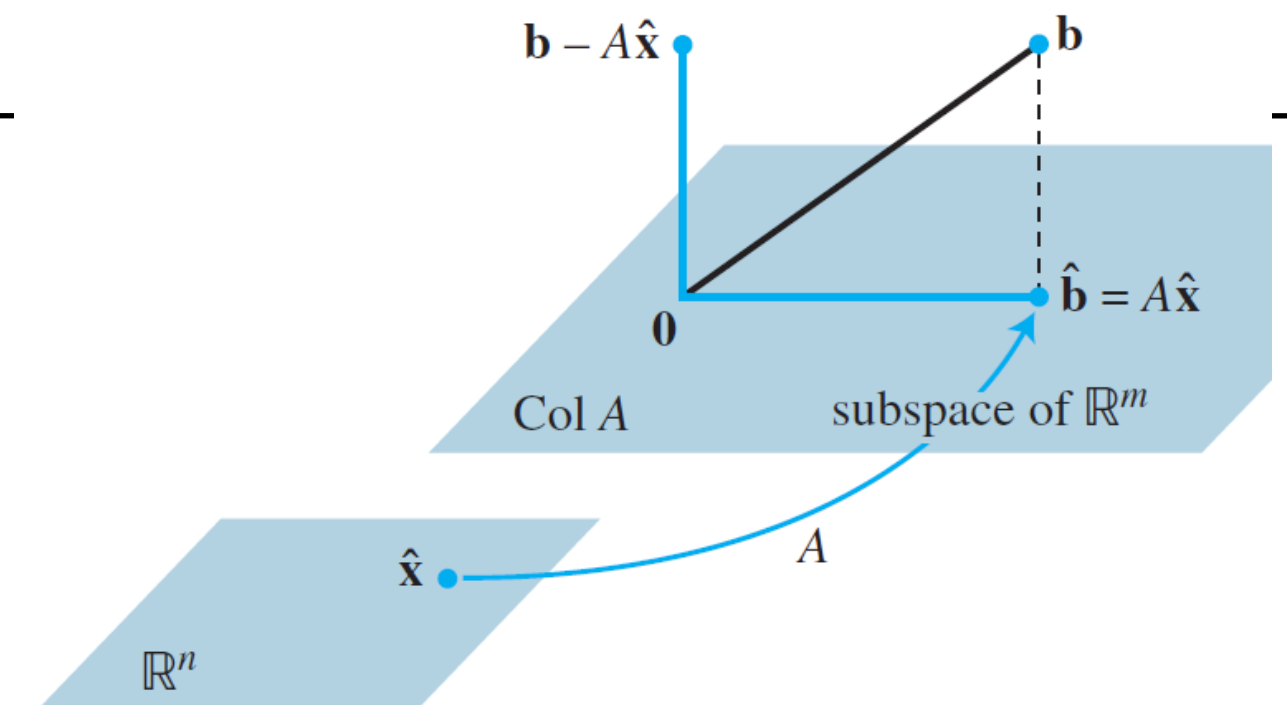


FIGURE 2 The least-squares solution  $\hat{\mathbf{x}}$  is in  $\mathbf{R}^n$ .

### THEOREM 14

Let  $A$  be an  $m \times n$  matrix. The following statements are logically equivalent:

- The equation  $A\mathbf{x} = \mathbf{b}$  has a unique least-squares solution for each  $\mathbf{b}$  in  $\mathbf{R}^m$ .
- The columns of  $A$  are linearly independent.
- The matrix  $A^T A$  is invertible.

When these statements are true, the least-squares solution  $\hat{\mathbf{x}}$  is given by

$$\hat{\mathbf{x}} = (A^T A)^{-1} A^T \mathbf{b} \quad (4)$$

Therefore if  $\hat{\mathbf{x}} = (A^T A)^{-1} A^T \mathbf{b}$ , then

$$\begin{aligned} \hat{\mathbf{b}} &= A\hat{\mathbf{x}}, \text{ means} \\ \hat{\mathbf{b}} &= A(A^T A)^{-1} A^T \mathbf{b} \end{aligned}$$

And this matrix  $A(A^T A)^{-1} A^T$  is a projection matrix, projecting  $\mathbf{b}$  into the column space of  $A$ .

See 7.1.3 (pg 4) : projection matrix of least squares