

# ECSE 343 Numerical Methods in Engineering

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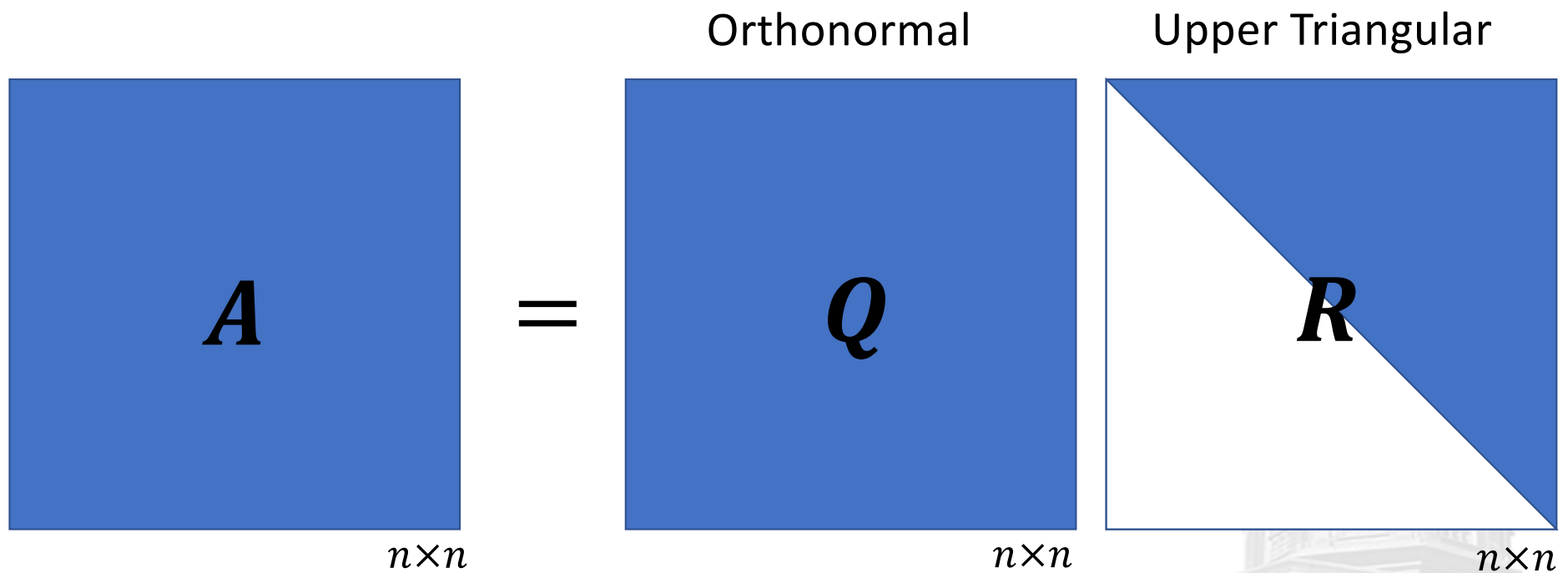
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# QR Decomposition





# QR Decomposition

Orthonormal      Upper Triangular

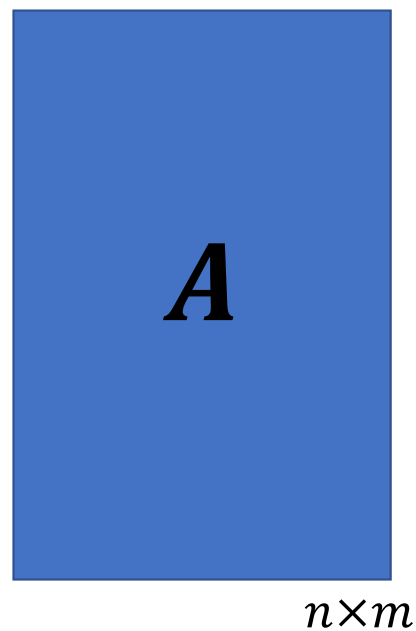
$$\begin{matrix} \text{Blue square} & = & \text{Blue square} & \begin{matrix} \text{White square with blue upper triangle} \\ \text{Blue square} \end{matrix} \\ \mathbf{A} & & \mathbf{Q} & \mathbf{R} \\ n \times m & & n \times m & m \times m \end{matrix}$$

$[Q \ R] = \text{qr}(A, 1)$   
Economy-Size

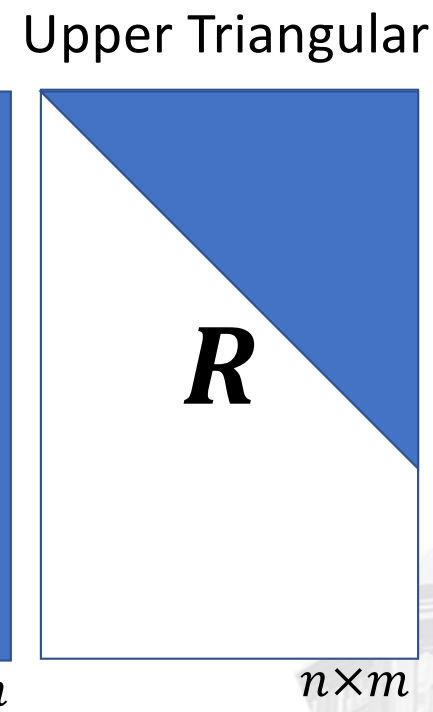
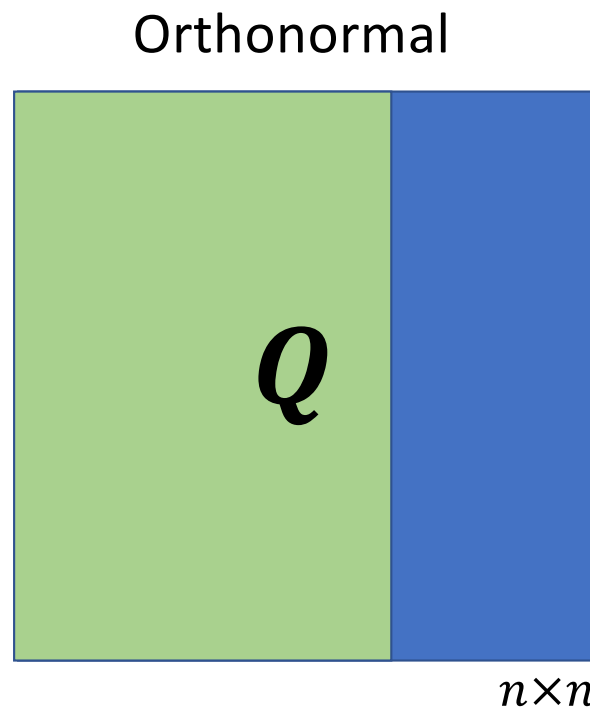


# QR Decomposition

$$[Q \ R] = \text{qr}(A)$$



=



# QR Decomposition



Orthonormal

$$\begin{bmatrix} \begin{bmatrix} a_1 \end{bmatrix} & \begin{bmatrix} a_2 \end{bmatrix} & \cdots & \begin{bmatrix} a_m \end{bmatrix} \end{bmatrix} = \begin{bmatrix} \begin{bmatrix} q_1 \end{bmatrix} & \begin{bmatrix} q_2 \end{bmatrix} & \cdots & \begin{bmatrix} q_m \end{bmatrix} \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ r_{22} & r_{23} & & \cdots & r_{2m} \\ & r_{33} & & \cdots & r_{3m} \\ & & \ddots & & \vdots \\ & & & r_{mm} \end{bmatrix}$$

$$q_i^T q_j = \begin{cases} 1 ; i = j \\ 0 ; i \neq j \end{cases}$$



# Gram-Schmidt Algorithm

Orthonormal

$$\begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_m \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ & r_{22} & r_{23} & \cdots & r_{2m} \\ & & r_{33} & \cdots & r_{3m} \\ & & & \ddots & \vdots \\ & & & & r_{mm} \end{bmatrix}$$

$$\mathbf{a}_1 = r_{11} \mathbf{q}_1$$

$$\mathbf{a}_2 = r_{12} \mathbf{q}_1 + r_{22} \mathbf{q}_2$$

$$\mathbf{a}_3 = r_{13} \mathbf{q}_1 + r_{23} \mathbf{q}_2 + r_{33} \mathbf{q}_3$$

$$\text{colspan}\{\mathbf{A}\} = \text{colspan}\{\mathbf{Q}\}$$

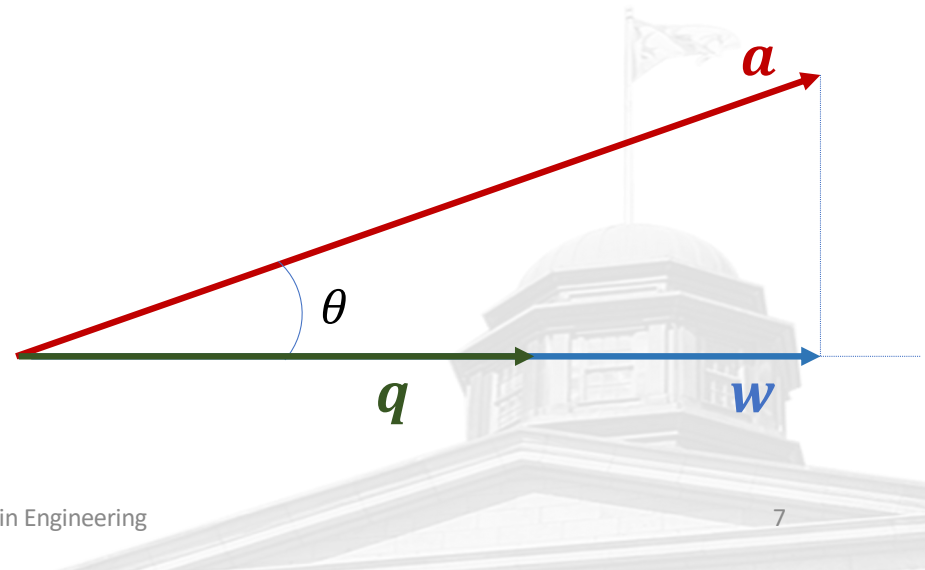


# Projectors Review

$$\|q\|_2 = 1$$

$$\langle a, q \rangle = q^T a = \|q\|_2 \|a\|_2 \cos(\theta) = \|a\|_2 \cos(\theta)$$

$$w = q \langle a, q \rangle = q q^T a$$



# Gram-Schmidt Algorithm



$$\begin{bmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \vdots \\ \mathbf{a}_m \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ r_{22} & r_{23} & & & r_{2m} \\ & r_{33} & & & r_{3m} \\ & & \ddots & & \vdots \\ & & & r_{mm} \end{bmatrix}$$

$$\left. \begin{aligned} \mathbf{a}_1 &= \mathbf{q}_1 r_{11} \\ \|\mathbf{q}_1\| &= 1 \end{aligned} \right\} \begin{aligned} r_{11} &= \|\mathbf{a}_1\| \\ \mathbf{q}_1 &= \frac{\mathbf{a}_1}{r_{11}} \end{aligned}$$







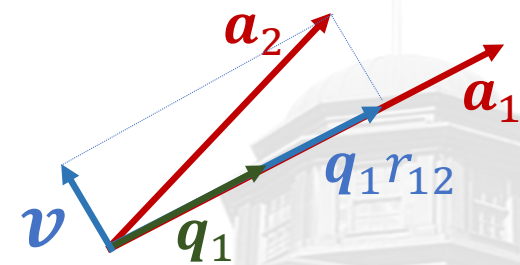
# Gram-Schmidt Algorithm

$$\begin{bmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \vdots \\ \mathbf{a}_m \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ & r_{22} & r_{23} & \cdots & r_{2m} \\ & & r_{33} & \cdots & r_{3m} \\ & & & \ddots & \vdots \\ & & & & r_{mm} \end{bmatrix}$$

$$\mathbf{a}_2 = \mathbf{q}_1 r_{12} + \mathbf{q}_2 r_{22}$$

$$\mathbf{q}_1^T \mathbf{a}_2 = \mathbf{q}_1^T \mathbf{q}_1 r_{12} + \mathbf{q}_1^T \mathbf{q}_2 r_{22} = r_{12}$$

$$\mathbf{v} = \mathbf{a}_2 - \underbrace{\mathbf{q}_1 r_{12}} = \mathbf{q}_2 r_{22}$$

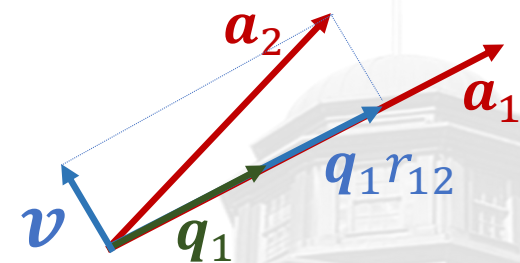




# Gram-Schmidt Algorithm

$$\begin{bmatrix} \mathbf{a}_1 \end{bmatrix} \begin{bmatrix} \mathbf{a}_2 \end{bmatrix} \cdots \begin{bmatrix} \mathbf{a}_m \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1 \end{bmatrix} \begin{bmatrix} \mathbf{q}_2 \end{bmatrix} \cdots \begin{bmatrix} \mathbf{q}_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ & r_{22} & r_{23} & \cdots & r_{2m} \\ & & r_{33} & \cdots & r_{3m} \\ & & & \ddots & \vdots \\ & & & & r_{mm} \end{bmatrix}$$

$$\left. \begin{array}{l} \mathbf{v} = \mathbf{q}_2 r_{22} \\ \|\mathbf{q}_2\| = 1 \end{array} \right\} \begin{array}{l} r_{22} = \|\mathbf{v}\| \\ \mathbf{q}_2 = \frac{\mathbf{v}}{r_{22}} \end{array}$$





# Gram-Schmidt Algorithm

$$\begin{bmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \vdots \\ \mathbf{a}_m \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ r_{22} & r_{23} & & & r_{2m} \\ & r_{33} & & & r_{3m} \\ & & \ddots & & \vdots \\ & & & r_{mm} \end{bmatrix}$$

$$\mathbf{a}_3 = \mathbf{q}_1 r_{13} + \mathbf{q}_2 r_{23} + \mathbf{q}_3 r_{33}$$

$$\mathbf{q}_1^T \mathbf{a}_3 = r_{13}$$

$$\mathbf{q}_2^T \mathbf{a}_3 = r_{23}$$

$$\mathbf{v} = \mathbf{a}_3 - \mathbf{q}_1 r_{13} - \mathbf{q}_2 r_{23} = \mathbf{q}_3 r_{33}$$

# Gram-Schmidt Algorithm



$$\begin{bmatrix} \mathbf{a}_1 \end{bmatrix} \begin{bmatrix} \mathbf{a}_2 \end{bmatrix} \cdots \begin{bmatrix} \mathbf{a}_m \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1 \end{bmatrix} \begin{bmatrix} \mathbf{q}_2 \end{bmatrix} \cdots \begin{bmatrix} \mathbf{q}_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ r_{22} & r_{23} & & \cdots & r_{2m} \\ & r_{33} & & \cdots & r_{3m} \\ & & \ddots & & \vdots \\ & & & & r_{mm} \end{bmatrix}$$

$$\left. \begin{array}{l} \mathbf{v} = \mathbf{q}_3 r_{34} \\ \|\mathbf{q}_3\| = 1 \end{array} \right\} \begin{array}{l} r_{33} = \|\mathbf{v}\| \\ \mathbf{q}_3 = \frac{\mathbf{v}}{r_{33}} \end{array}$$





# Gram-Schmidt Algorithm

$$r_{11} = \|\mathbf{a}_1\| \quad \mathbf{q}_1 = \frac{\mathbf{a}_1}{r_{11}}$$

---

$$r_{12} = \mathbf{q}_1^T \mathbf{a}_2 \quad \mathbf{v} = \mathbf{a}_2 - \underbrace{\mathbf{q}_1 r_{12}}_p \quad r_{22} = \|\mathbf{v}\| \quad \mathbf{q}_2 = \frac{\mathbf{v}}{r_{22}}$$

---

$$\begin{aligned} r_{13} &= \mathbf{q}_1^T \mathbf{a}_3 & \mathbf{v} &= \mathbf{a}_3 - \underbrace{\mathbf{q}_1 r_{13} - \mathbf{q}_2 r_{23}}_p & r_{33} &= \|\mathbf{v}\| \\ r_{23} &= \mathbf{q}_2^T \mathbf{a}_3 & & & \mathbf{q}_3 &= \frac{\mathbf{v}}{r_{33}} \end{aligned}$$



# Gram-Schmidt Pseudocode

```
r11 ← ||a1||  
q1 ← a1/r11  
for j ← 2, 3, ..., m  
    p ← 0  
    for i ← 1, 2, ..., j - 1  
        rij ← qiT aj  
        p ← p + rij qi  
    endfor  
    v ← aj - p  
    rjj ← ||v||  
    qj ← v/rjj  
endfor
```





# Gram-Schmidt

- For each vector in  $A$  starting from the left, remove its projection on all previously computed vectors in  $Q$ , then normalize to length 1.
- The entries of  $R$  are computed column by column.





# Modified Gram-Schmidt Pseudocode

```
for i ← 1, 2, ..., m
    rii ← ||ai||
    qi ← ai/rii
    for j ← i + 1, ..., m
        rij ← qiT aj
        aj ← aj − rijqi
    endfor
endfor
```

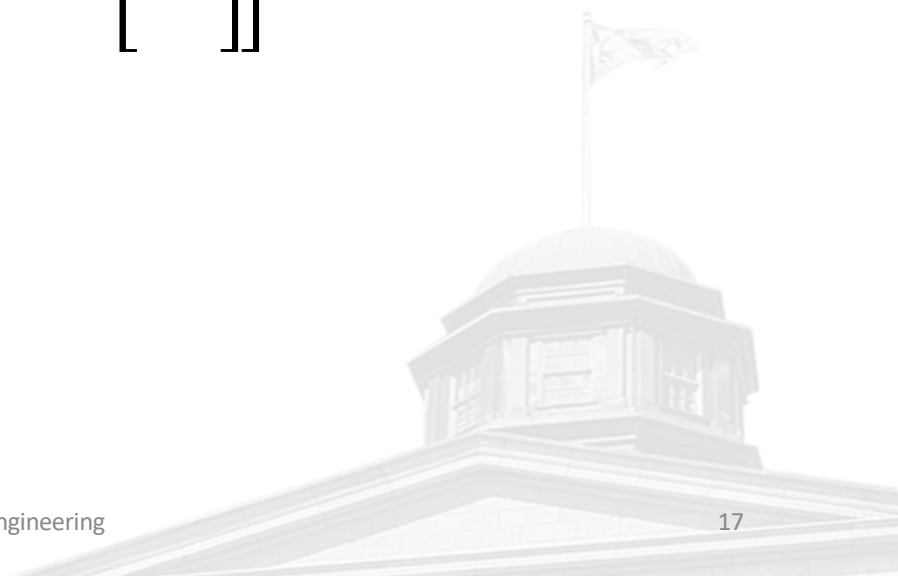




# Modified Gram-Schmidt



$$\left[ \begin{array}{c} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \\ \vdots \\ \mathbf{a}_m \end{array} \right]$$





# Modified Gram-Schmidt

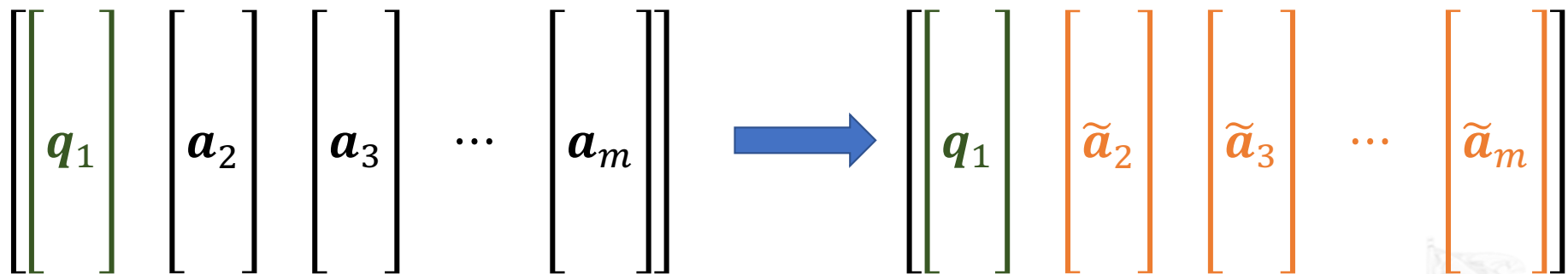
$$\left[ \begin{array}{c} \mathbf{q}_1 \\ \mathbf{a}_2 \\ \mathbf{a}_3 \\ \vdots \\ \mathbf{a}_m \end{array} \right]$$

$$r_{11} \leftarrow \|\mathbf{a}_1\|$$

$$\mathbf{q}_1 \leftarrow \mathbf{a}_1 / r_{11}$$



# Modified Gram-Schmidt



```
for j ← 2, ..., m
    r1j ← q1Taj
    aj ← aj − r1jq1
endfor
```



# Modified Gram-Schmidt



$$\left[ \begin{array}{c} \left[ q_1 \right] \\ \left[ \tilde{a}_2 \right] \\ \left[ \tilde{a}_3 \right] \\ \dots \\ \left[ \tilde{a}_m \right] \end{array} \right]$$





# Modified Gram-Schmidt

$$\left[ \begin{array}{c|c|c|c|c} \left[ \begin{array}{c} q_1 \end{array} \right] & \left[ \begin{array}{c} q_2 \end{array} \right] & \left[ \begin{array}{c} \tilde{a}_3 \end{array} \right] & \cdots & \left[ \begin{array}{c} \tilde{a}_m \end{array} \right] \end{array} \right]$$

$$r_{22} \leftarrow \|a_2\|$$

$$q_2 \leftarrow a_2 / r_{22}$$



# Modified Gram-Schmidt



$$\left[ \begin{array}{c} \left[ \begin{array}{c} q_1 \end{array} \right] \quad \left[ \begin{array}{c} q_2 \end{array} \right] \quad \left[ \begin{array}{c} \tilde{a}_3 \end{array} \right] \quad \cdots \quad \left[ \begin{array}{c} \tilde{a}_m \end{array} \right] \end{array} \right] \rightarrow \left[ \begin{array}{c} \left[ \begin{array}{c} q_1 \end{array} \right] \quad \left[ \begin{array}{c} q_2 \end{array} \right] \quad \left[ \begin{array}{c} \hat{a}_3 \end{array} \right] \quad \cdots \quad \left[ \begin{array}{c} \hat{a}_m \end{array} \right] \end{array} \right]$$

```
for j ← 3, ..., m
    r2j ← q2Taj
    aj ← aj − r2jq2
endfor
```



# Modified Gram-Schmidt



$$\left[ \begin{array}{c} \left[ \begin{array}{c} q_1 \end{array} \right] \quad \left[ \begin{array}{c} q_2 \end{array} \right] \quad \left[ \begin{array}{c} \hat{a}_3 \end{array} \right] \quad \cdots \quad \left[ \begin{array}{c} \hat{a}_m \end{array} \right] \end{array} \right]$$





# Modified Gram-Schmidt

$$\left[ \begin{array}{c} \left[ \begin{array}{c} q_1 \end{array} \right] \quad \left[ \begin{array}{c} q_2 \end{array} \right] \quad \left[ \begin{array}{c} q_3 \end{array} \right] \quad \cdots \quad \left[ \begin{array}{c} \hat{a}_m \end{array} \right] \end{array} \right]$$

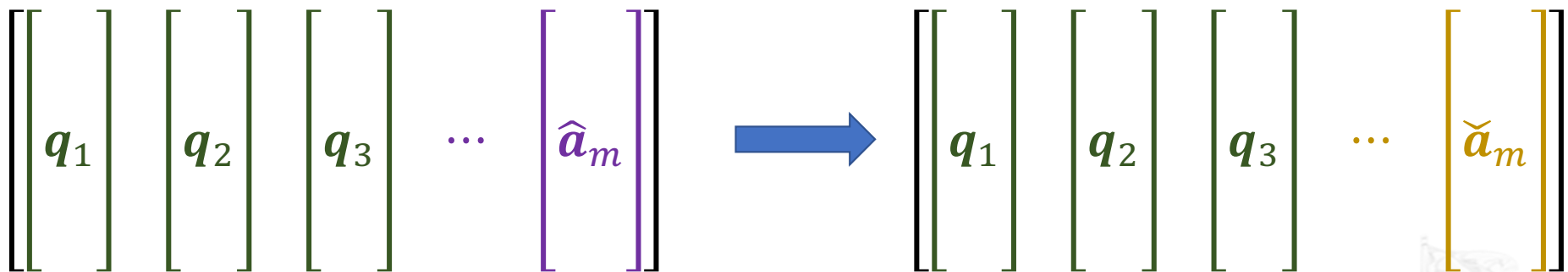
$$r_{33} \leftarrow \|a_3\|$$
$$q_3 \leftarrow a_3 / r_{33}$$







# Modified Gram-Schmidt



```
for j ← 4, ..., m
    r3j ← q3Taj
    aj ← aj − r3jq3
endfor
```





# Modified Gram-Schmidt

$$\begin{bmatrix} \begin{bmatrix} a_1 \end{bmatrix} & \begin{bmatrix} a_2 \end{bmatrix} & \cdots & \begin{bmatrix} a_m \end{bmatrix} \end{bmatrix} \begin{matrix} R_1 \\ \left[ \begin{array}{ccccc} 1 & -\frac{r_{12}}{r_{11}} & -\frac{r_{13}}{r_{11}} & \cdots & -\frac{r_{1m}}{r_{11}} \\ r_{11} & 1 & 0 & \cdots & 0 \\ & & 1 & \cdots & 0 \\ & & & \ddots & \vdots \\ & & & & 1 \end{array} \right] \end{matrix} = \begin{bmatrix} \begin{bmatrix} q_1 \end{bmatrix} & \begin{bmatrix} \tilde{a}_2 \end{bmatrix} & \begin{bmatrix} \tilde{a}_3 \end{bmatrix} & \cdots & \begin{bmatrix} \tilde{a}_m \end{bmatrix} \end{bmatrix}$$

$$\begin{aligned} q_1 &\leftarrow a_1 / r_{11} \\ a_2 &\leftarrow a_2 - \frac{r_{12}}{r_{11}} a_1 = a_2 - r_{12} q_1 \\ a_3 &\leftarrow a_3 - \frac{r_{13}}{r_{11}} a_1 = a_3 - r_{13} q_1 \end{aligned}$$



# Modified Gram-Schmidt

$$\begin{bmatrix} \begin{bmatrix} q_1 \end{bmatrix} & \begin{bmatrix} \tilde{a}_2 \end{bmatrix} & \begin{bmatrix} \tilde{a}_3 \end{bmatrix} & \dots & \begin{bmatrix} \tilde{a}_m \end{bmatrix} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ \frac{1}{r_{22}} & -\frac{r_{23}}{r_{22}} & \dots & -\frac{r_{2m}}{r_{22}} \\ 1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 1 \end{bmatrix} =$$

$$\begin{aligned} q_2 &\leftarrow a_2 / r_{22} \\ a_3 &\leftarrow a_3 - \frac{r_{23}}{r_{22}} a_2 = a_3 - r_{23} q_2 \\ a_4 &\leftarrow a_4 - \frac{r_{24}}{r_{22}} a_2 = a_4 - r_{24} q_2 \end{aligned}$$

$$= \begin{bmatrix} \begin{bmatrix} q_1 \end{bmatrix} & \begin{bmatrix} q_2 \end{bmatrix} & \begin{bmatrix} \hat{a}_3 \end{bmatrix} & \dots & \begin{bmatrix} \hat{a}_m \end{bmatrix} \end{bmatrix}$$



# Modified Gram-Schmidt

$$\underbrace{A R_1 R_2 R_3 \cdots R_m}_{R^{-1}} = Q$$

$$A = QR$$





## Another Approach

$$\underbrace{E_m \cdots E_4 E_3 E_2 E_1}_{\text{Elimination Matrices}} \mathbf{A} = \mathbf{U}$$

$\mathbf{L}^{-1}$

$$\underbrace{H_m \cdots H_4 H_3 H_2 H_1}_{\text{Orthonormal Matrices}} \mathbf{A} = \mathbf{R}$$

$\mathbf{Q}^T$





# LU Factorization

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -3 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{Elimination Matrices}} \underbrace{\begin{bmatrix} 2 & 1 & -2 \\ 4 & 5 & -3 \\ 6 & 9 & -2 \end{bmatrix}}_A = \underbrace{\begin{bmatrix} 2 & 1 & -2 \\ 0 & 3 & +1 \\ 0 & 0 & +2 \end{bmatrix}}_U$$



# QR Decomposition: Key Property

$$\begin{matrix} \text{Blue rectangle} \\ \mathbf{A} \\ n \times m \end{matrix} = \begin{matrix} \text{Blue rectangle} \\ \mathbf{Q} \\ n \times m \end{matrix} \begin{matrix} \text{Blue triangle} \\ \mathbf{R} \\ m \times m \end{matrix}$$

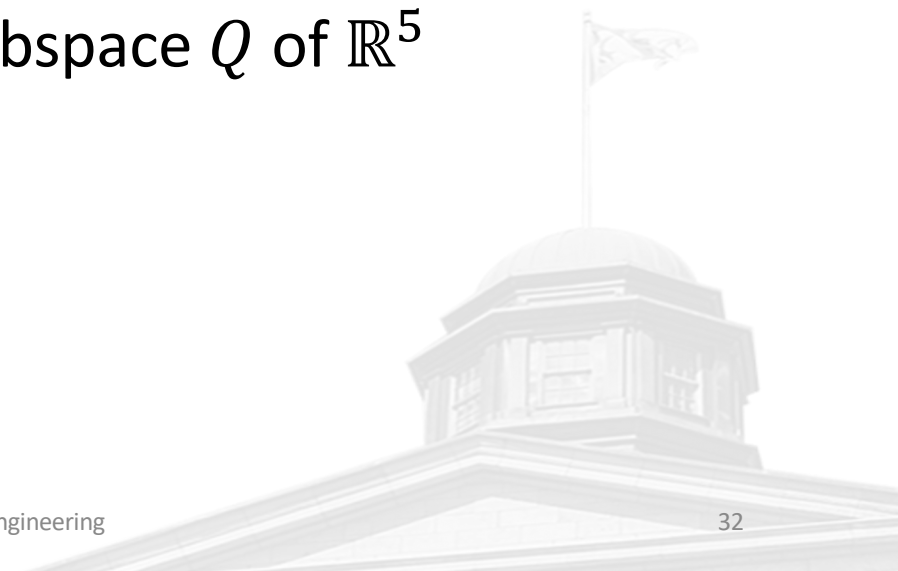
$$\text{colsp}\{\mathbf{A}\} = \text{colsp}\{\mathbf{Q}\}$$



# Overdetermined Systems

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \\ a_{51} & a_{52} & a_{53} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}$$

- Assume columns of  $A$  are linearly independent
- Columns of  $A$  form a 3D subspace  $Q$  of  $\mathbb{R}^5$







# Overdetermined Systems

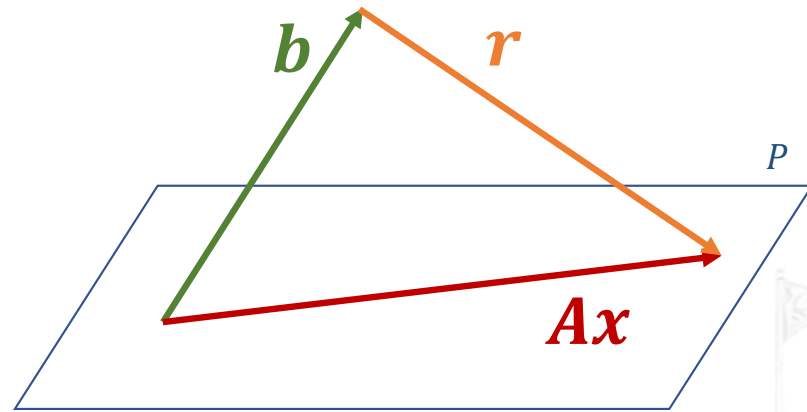
Find  $\mathbf{x}$  such that:  $\mathbf{Ax} = \mathbf{b}$

Impossible:

$$\mathbf{Ax} \in P \quad \mathbf{b} \notin P$$

Minimize  $\mathbf{r} = \mathbf{Ax} - \mathbf{b}$

i.e. minimize  $\|\mathbf{r}\| = \|\mathbf{Ax} - \mathbf{b}\|$





# Overdetermined Systems

Minimize  $\|\mathbf{r}\| = \|\mathbf{Ax} - \mathbf{b}\|$

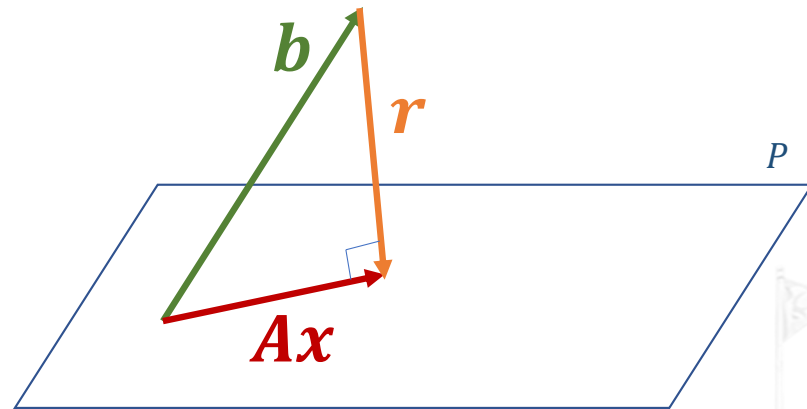
$$\Rightarrow \mathbf{r} \perp P$$

$$\Rightarrow \mathbf{A}^T \mathbf{r} = \mathbf{0}$$

$$\Rightarrow \mathbf{A}^T (\mathbf{Ax} - \mathbf{b}) = \mathbf{0}$$

$$\Rightarrow \mathbf{A}^T \mathbf{Ax} = \mathbf{A}^T \mathbf{b}$$

$$\Rightarrow \mathbf{x} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{b}$$



Avoid  $\mathbf{A}^T \mathbf{A}$  due to possible ill-conditioning



# Overdetermined Systems

Minimize  $\|\mathbf{r}\| = \|\mathbf{Ax} - \mathbf{b}\|$

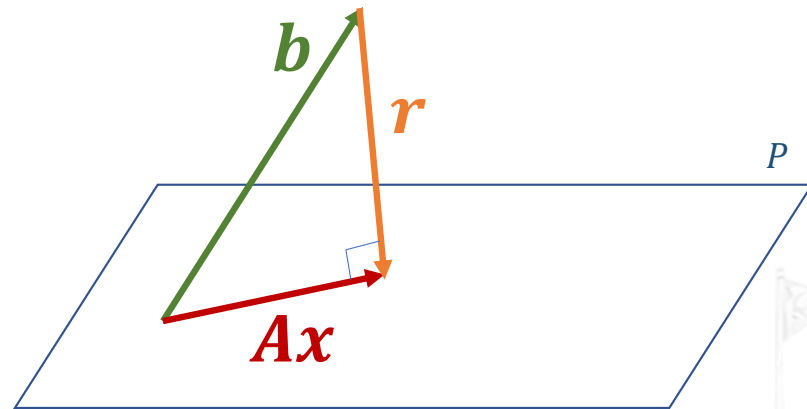
$$\Rightarrow \mathbf{r} \perp P$$

$$\Rightarrow \mathbf{Q}^T \mathbf{r} = \mathbf{0}$$

$$\Rightarrow \mathbf{Q}^T (\mathbf{Ax} - \mathbf{b}) = \mathbf{0}$$

$$\Rightarrow \boxed{\mathbf{Q}^T \mathbf{Ax} = \mathbf{Q}^T \mathbf{b}}$$

$$\Rightarrow \mathbf{Rx} = \mathbf{Q}^T \mathbf{b}$$



$$\mathbf{A} = \mathbf{QR}$$

$$\text{colsp}\{\mathbf{A}\} = \text{colsp}\{\mathbf{Q}\}$$