

# CENG 216 – NUMERICAL COMPUTATION

## LEAST SQUARES - PART II

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May 25, 2022

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Slides are based on material from the main textbook:

“Numerical Analysis”, The new international edition, 2ed,  
by Timothy Sauer

PREVIOUSLY ON CENG 216

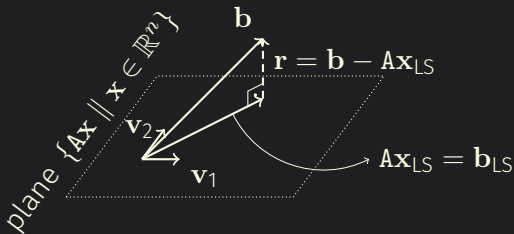
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## INCONSISTENT SYSTEMS AND THE NORMAL EQUATIONS

$A\mathbf{x} = \mathbf{b}$  with no solutions  $\rightarrow$  Equations are inconsistent.

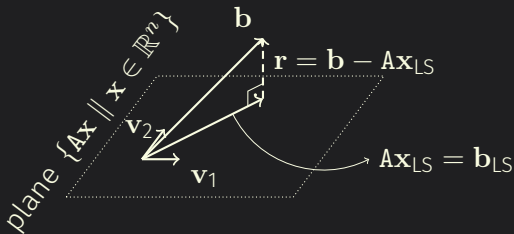
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$$(\mathbf{b} - A\mathbf{x}_{LS}) \perp \{A\mathbf{x} \mid \mathbf{x} \in \mathbb{R}^n\} \implies A^T A\mathbf{x}_{LS} = A^T \mathbf{b} \quad (\text{Normal Equations})$$

# SUMMARY OF REDUCED QR FACTORIZATION WITH GRAM-SCHMIDT

Input:  $\mathbf{A}_{m \times n} = [\mathbf{a}_1 \ \mathbf{a}_2 \ \cdots \ \mathbf{a}_n]$  with linearly independent columns.

```
for  $j \leftarrow 1$  to  $n$  do
   $\mathbf{y} = \mathbf{a}_j$ 
  for  $i \leftarrow 1$  to  $j - 1$ 
    do
       $r_{ij} = \mathbf{q}_i^\top \mathbf{a}_j$ 
       $\mathbf{y} = \mathbf{y} - r_{ij} \mathbf{q}_i$ 
    end
   $r_{jj} = \|\mathbf{y}\|$ 
   $\mathbf{q}_j = \frac{\mathbf{y}}{r_{jj}}$ 
end
```

Output:  $\mathbf{Q}_{m \times n}$  and  $\mathbf{R}_{n \times n}$  such that

$$\mathbf{A}_{m \times n} = [\mathbf{q}_1 \ \mathbf{q}_2 \ \cdots \ \mathbf{q}_n] \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix}$$
$$= \mathbf{Q}_{m \times n} \mathbf{R}_{n \times n}$$

# MODIFIED GRAM-SCHMIDT

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# MODIFIED GRAM-SCHMIDT ALGORITHM

Input:  $A_{m \times n} = [\mathbf{a}_1 \ \mathbf{a}_2 \ \cdots \ \mathbf{a}_n]$  with linearly independent columns.

Classical Gram-Schmidt:

```
for  $j \leftarrow 1$  to  $n$  do
     $\mathbf{y} = \mathbf{a}_j$ 
    for  $i \leftarrow 1$  to  $j - 1$  do
         $r_{ij} = \mathbf{q}_i^\top \mathbf{a}_j$ 
         $\mathbf{y} = \mathbf{y} - r_{ij} \mathbf{q}_i$ 
    end
     $r_{jj} = \|\mathbf{y}\|$ 
     $\mathbf{q}_j = \frac{\mathbf{y}}{r_{jj}}$ 
end
```

Modified Gram-Schmidt:

```
for  $j \leftarrow 1$  to  $n$  do
     $\mathbf{y} = \mathbf{a}_j$ 
    for  $i \leftarrow 1$  to  $j - 1$  do
         $r_{ij} = \mathbf{q}_i^\top \mathbf{y}$ 
         $\mathbf{y} = \mathbf{y} - r_{ij} \mathbf{q}_i$ 
    end
     $r_{jj} = \|\mathbf{y}\|$ 
     $\mathbf{q}_j = \frac{\mathbf{y}}{r_{jj}}$ 
end
```

## EXAMPLE: ALMOST PARALLEL VECTORS

Apply **classical** Gram-Schmidt to  $\begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix}$  with  $\delta = 10^{-10}$ .

## EXAMPLE: ALMOST PARALLEL VECTORS

Apply **classical** Gram-Schmidt to  $\begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix}$  with  $\delta = 10^{-10}$ .

$$\mathbf{y}_1 = \mathbf{a}_1 = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix}$$

## EXAMPLE: ALMOST PARALLEL VECTORS

Apply **classical** Gram-Schmidt to  $\begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix}$  with  $\delta = 10^{-10}$ .

$$\mathbf{y}_1 = \mathbf{a}_1 = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix} \Rightarrow \mathbf{q}_1 = \frac{1}{\underbrace{\sqrt{1 + \delta^2}}_{\approx 1 \text{ since } \delta^2 = 10^{-20}}} \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix}$$

## EXAMPLE: ALMOST PARALLEL VECTORS

Apply **classical** Gram-Schmidt to  $\begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix}$  with  $\delta = 10^{-10}$ .

$$\mathbf{q}_1 = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix},$$

$$\mathbf{y}_2 = \begin{bmatrix} 1 \\ 0 \\ \delta \\ 0 \end{bmatrix} - \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix} \underbrace{\mathbf{q}_1^\top \mathbf{a}_2}_1 = \begin{bmatrix} 0 \\ -\delta \\ \delta \\ 0 \end{bmatrix}$$

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$$\mathbf{q}_1 = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix},$$

$$\mathbf{y}_2 = \begin{bmatrix} 1 \\ 0 \\ \delta \\ 0 \end{bmatrix} - \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix} \underbrace{\mathbf{q}_1^\top \mathbf{a}_2}_1 = \begin{bmatrix} 0 \\ -\delta \\ \delta \\ 0 \end{bmatrix} \implies \mathbf{q}_2 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}$$

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Apply **classical** Gram-Schmidt to  $\begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix}$  with  $\delta = 10^{-10}$ .

$$\mathbf{q}_1 = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix}, \mathbf{q}_2 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix},$$

$$\mathbf{y}_3 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \delta \end{bmatrix} - \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix} \underbrace{\mathbf{q}_1^\top \mathbf{a}_3}_1 - \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} \underbrace{\mathbf{q}_2^\top \mathbf{a}_3}_0 = \begin{bmatrix} 0 \\ -\delta \\ 0 \\ \delta \end{bmatrix}$$

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Apply **classical** Gram-Schmidt to  $\begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix}$  with  $\delta = 10^{-10}$ .

$$\mathbf{q}_1 = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix}, \mathbf{q}_2 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix},$$

$$\mathbf{y}_3 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \delta \end{bmatrix} - \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix} \underbrace{\mathbf{q}_1^\top \mathbf{a}_3}_1 - \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} \underbrace{\mathbf{q}_2^\top \mathbf{a}_3}_0 = \begin{bmatrix} 0 \\ -\delta \\ 0 \\ \delta \end{bmatrix} \implies \mathbf{q}_3 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$



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$$\Rightarrow \mathbf{q}_2^T \mathbf{q}_3 = \begin{bmatrix} 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{2} \quad (\text{Not orthogonal!})$$

## EXAMPLE: ALMOST PARALLEL VECTORS

Apply **modified** Gram-Schmidt to  $\begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix}$  with  $\delta = 10^{-10}$ .

## EXAMPLE: ALMOST PARALLEL VECTORS

Apply **modified** Gram-Schmidt to  $\begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix}$  with  $\delta = 10^{-10}$ .

$$\mathbf{q}_1 = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix}, \mathbf{q}_2 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} \text{ (Same as before),}$$

$$\mathbf{y} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \delta \end{bmatrix} - \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix} \underbrace{\mathbf{q}_1^\top \mathbf{a}_3}_1 = \begin{bmatrix} 0 \\ -\delta \\ 0 \\ \delta \end{bmatrix},$$

## EXAMPLE: ALMOST PARALLEL VECTORS

Apply **modified** Gram-Schmidt to  $\begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix}$  with  $\delta = 10^{-10}$ .

$$\mathbf{q}_1 = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix}, \mathbf{q}_2 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} \quad (\text{Same as before}),$$

$$\mathbf{y} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \delta \end{bmatrix} - \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix} \underbrace{\mathbf{q}_1^\top \mathbf{a}_3}_1 = \begin{bmatrix} 0 \\ -\delta \\ 0 \\ \delta \end{bmatrix}, \mathbf{y}_3 = \mathbf{y} - \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix} \underbrace{\mathbf{q}_2^\top \mathbf{y}}_{\frac{\delta}{\sqrt{2}}} = \begin{bmatrix} 0 \\ -\frac{\delta}{2} \\ -\frac{\delta}{2} \\ \delta \end{bmatrix} \Rightarrow \mathbf{q}_3 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \end{bmatrix}$$

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Apply **modified** Gram-Schmidt to  $\begin{bmatrix} 1 & 1 & 1 \\ \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix}$  with  $\delta = 10^{-10}$ .

$$\mathbf{q}_1 = \begin{bmatrix} 1 \\ \delta \\ 0 \\ 0 \end{bmatrix}, \mathbf{q}_2 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}, \mathbf{q}_3 = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \end{bmatrix},$$

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$$\implies \mathbf{q}_2^\top \mathbf{q}_3 = \begin{bmatrix} 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \end{bmatrix} = 0 \quad (\text{Orthogonal})$$

# THE FULL QR FACTORIZATION

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# THE FULL QR FACTORIZATION

Given the  $n < m$  columns of an  $m \times n$  matrix  $\mathbf{A}$ , add  $m - n$  extra independent vectors to  $\{\mathbf{a}_j\}$  and compute  $\mathbf{q}_1$  to  $\mathbf{q}_m$ .

$$\underbrace{\begin{bmatrix} \mathbf{a}_1 & \cdots & \mathbf{a}_n \end{bmatrix}}_{\mathbf{A}_{m \times n}} = \underbrace{\begin{bmatrix} \mathbf{q}_1 & \cdots & \mathbf{q}_n & \mathbf{q}_{n+1} & \cdots & \mathbf{q}_m \end{bmatrix}}_{\mathbf{Q}_{m \times m}} \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}}_{\mathbf{R}_{m \times n}}$$

## EXAMPLE

Find the full QR factorization of  $\mathbf{A} = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}$ .

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Previously, we computed  $\mathbf{q}_1 = \begin{bmatrix} \frac{1}{3} \\ \frac{2}{3} \\ \frac{2}{3} \end{bmatrix}$  and  $\mathbf{q}_2 = \begin{bmatrix} -\frac{14}{15} \\ \frac{1}{3} \\ \frac{2}{15} \end{bmatrix}$  from  $\mathbf{a}_1$

and  $\mathbf{a}_2$ . Add  $\mathbf{a}_3 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ .

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and  $\mathbf{a}_2$ . Add  $\mathbf{a}_3 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ .

$$\mathbf{y}_3 = \mathbf{a}_3 - \mathbf{q}_1 \underbrace{\mathbf{q}_1^\top \mathbf{a}_3}_{\frac{1}{3}} - \mathbf{q}_2 \underbrace{\mathbf{q}_2^\top \mathbf{a}_3}_{-\frac{14}{15}} = \frac{2}{225} \begin{bmatrix} 2 \\ 10 \\ -11 \end{bmatrix}, \quad \mathbf{q}_3 = \begin{bmatrix} \frac{2}{15} \\ \frac{10}{15} \\ -\frac{11}{15} \end{bmatrix}$$

## EXAMPLE

Find the full QR factorization of  $\mathbf{A} = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}$ .

$$\begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix} = \frac{1}{15} \begin{bmatrix} 5 & -14 & 2 \\ 10 & 5 & 10 \\ 10 & 2 & -11 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 0 & 5 \\ 0 & 0 \end{bmatrix} \quad (\text{Full QR})$$

## EXAMPLE

Find the full QR factorization of  $\mathbf{A} = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}$ .

$$\begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix} = \frac{1}{15} \begin{bmatrix} 5 & -14 & 2 \\ 10 & 5 & 10 \\ 10 & 2 & -11 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 0 & 5 \\ 0 & 0 \end{bmatrix} \quad (\text{Full QR})$$

$$= \frac{1}{15} \begin{bmatrix} 5 & -14 \\ 10 & 5 \\ 10 & 2 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 0 & 5 \end{bmatrix} \quad (\text{Reduced QR})$$

# SUMMARY OF FULL QR FACTORIZATION WITH MODIFIED GRAM-SCHMIDT

Input:  $\mathbf{A}_{m \times n} = [\mathbf{a}_1 \ \mathbf{a}_2 \ \cdots \ \mathbf{a}_n]$  with linearly independent columns and  $m - n$  extra linearly independent vectors.

```
for  $j \leftarrow 1$  to  $m$  do
   $\mathbf{y} = \mathbf{a}_j$ 
  for  $i \leftarrow 1$  to  $j - 1$ 
    do
       $r_{ij} = \mathbf{q}_i^\top \mathbf{y}$ 
       $\mathbf{y} = \mathbf{y} - r_{ij} \mathbf{q}_i$ 
    end
   $r_{jj} = \|\mathbf{y}\|$ 
   $\mathbf{q}_j = \frac{\mathbf{y}}{r_{jj}}$ 
end
```

Output:  $\mathbf{Q}_{m \times m}$  and  $\mathbf{R}_{m \times n}$  such that

$$\mathbf{A}_{m \times n} = \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$
$$= \mathbf{Q}_{m \times m} \mathbf{R}_{m \times n}$$

# LEAST SQUARES BY QR FACTORIZATION

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# ORTHOGONAL MATRICES

**Def:** A square matrix  $Q$  is **orthogonal** if  $Q^{-1} = Q^T$ .

$$Q^T Q = I \implies \begin{bmatrix} \mathbf{q}_1^T \\ \mathbf{q}_2^T \\ \vdots \\ \mathbf{q}_m^T \end{bmatrix} \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_m \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1^T \mathbf{q}_1 & \mathbf{q}_1^T \mathbf{q}_2 & \cdots & \mathbf{q}_1^T \mathbf{q}_m \\ \mathbf{q}_2^T \mathbf{q}_1 & \mathbf{q}_2^T \mathbf{q}_2 & \cdots & \mathbf{q}_2^T \mathbf{q}_m \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{q}_n^T \mathbf{q}_1 & \mathbf{q}_n^T \mathbf{q}_2 & \cdots & \mathbf{q}_n^T \mathbf{q}_m \end{bmatrix}$$

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$$\implies \mathbf{q}_j^T \mathbf{q}_j = 1 \text{ and } \mathbf{q}_i^T \mathbf{q}_j = 0 \quad \forall i \neq j.$$

# ORTHOGONAL MATRICES

**Def:** A square matrix  $Q$  is **orthogonal** if  $Q^{-1} = Q^T$ .

$$\begin{aligned} Q^T Q = I &\implies \begin{bmatrix} \mathbf{q}_1^T \\ \mathbf{q}_2^T \\ \vdots \\ \mathbf{q}_m^T \end{bmatrix} \begin{bmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \cdots & \mathbf{q}_m \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1^T \mathbf{q}_1 & \mathbf{q}_1^T \mathbf{q}_2 & \cdots & \mathbf{q}_1^T \mathbf{q}_m \\ \mathbf{q}_2^T \mathbf{q}_1 & \mathbf{q}_2^T \mathbf{q}_2 & \cdots & \mathbf{q}_2^T \mathbf{q}_m \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{q}_n^T \mathbf{q}_1 & \mathbf{q}_n^T \mathbf{q}_2 & \cdots & \mathbf{q}_n^T \mathbf{q}_m \end{bmatrix} \\ &\implies \mathbf{q}_j^T \mathbf{q}_j = 1 \text{ and } \mathbf{q}_i^T \mathbf{q}_j = 0 \quad \forall i \neq j. \end{aligned}$$

A set of vectors satisfying the above conditions is called an **orthonormal** set of vectors.

**Lemma:** If  $Q$  is an orthogonal  $m \times m$  matrix and  $\mathbf{x}$  is an  $m$  dimensional vector,

$$\|Q\mathbf{x}\|^2$$

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**Lemma:** If  $Q$  is an orthogonal  $m \times m$  matrix and  $\mathbf{x}$  is an  $m$  dimensional vector,

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# ORTHOGONAL MATRICES

**Lemma:** If  $Q$  is an orthogonal  $m \times m$  matrix and  $\mathbf{x}$  is an  $m$  dimensional vector,

$$\|Q\mathbf{x}\|^2 = (Q\mathbf{x})^T Q\mathbf{x} = \mathbf{x}^T Q^T Q\mathbf{x} = \mathbf{x}^T \mathbf{x} = \|\mathbf{x}\|^2.$$

**Lemma:** If  $Q_1$  and  $Q_2$  are orthogonal then the result of the matrix multiplications  $Q_1 Q_2$  and  $Q_2 Q_1$  are also orthogonal.



## LEAST SQUARES BY QR FACTORIZATION

Given  $m \times n$  inconsistent system  $\mathbf{Ax} = \mathbf{b}$ , find  $\mathbf{A} = \mathbf{QR}$ , the full QR factorization of  $\mathbf{A}$ .

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

## LEAST SQUARES BY QR FACTORIZATION

Given  $m \times n$  inconsistent system  $\mathbf{Ax} = \mathbf{b}$ , find  $\mathbf{A} = \mathbf{QR}$ , the full QR factorization of  $\mathbf{A}$ .

$$\|\mathbf{r}\| = \|\mathbf{Ax} - \mathbf{b}\| = \|\mathbf{QRx} - \mathbf{b}\| = \|\mathbf{Q}^\top \mathbf{QRx} - \mathbf{Q}^\top \mathbf{b}\|$$

## LEAST SQUARES BY QR FACTORIZATION

Given  $m \times n$  inconsistent system  $\mathbf{Ax} = \mathbf{b}$ , find  $\mathbf{A} = \mathbf{QR}$ , the full QR factorization of  $\mathbf{A}$ .

$$\|\mathbf{r}\| = \|\mathbf{Ax} - \mathbf{b}\| = \|\mathbf{QRx} - \mathbf{b}\| = \|\mathbf{Q}^\top \mathbf{QRx} - \mathbf{Q}^\top \mathbf{b}\| = \left\| \mathbf{Rx} - \underbrace{\mathbf{Q}^\top \mathbf{b}}_{\mathbf{d}} \right\|$$

# LEAST SQUARES BY QR FACTORIZATION

Given  $m \times n$  inconsistent system  $\mathbf{Ax} = \mathbf{b}$ , find  $\mathbf{A} = \mathbf{QR}$ , the full QR factorization of  $\mathbf{A}$ .

$$\|\mathbf{r}\| = \|\mathbf{Ax} - \mathbf{b}\| = \|\mathbf{QRx} - \mathbf{b}\| = \|\mathbf{Q}^\top \mathbf{QRx} - \mathbf{Q}^\top \mathbf{b}\| = \left\| \mathbf{Rx} - \underbrace{\mathbf{Q}^\top \mathbf{b}}_{\mathbf{d}} \right\|$$

$$\|\mathbf{Ax} - \mathbf{b}\| = \underbrace{\begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \\ e_{n+1} \\ \vdots \\ e_m \end{bmatrix}}_{\begin{bmatrix} \hat{\mathbf{e}} \\ \mathbf{e}' \end{bmatrix}}$$

# LEAST SQUARES BY QR FACTORIZATION

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$$\|\mathbf{Ax} - \mathbf{b}\| = \underbrace{\begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \\ e_{n+1} \\ \vdots \\ e_m \end{bmatrix}}_{\begin{bmatrix} \hat{\mathbf{e}} \\ \mathbf{e}' \end{bmatrix}} = \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}}_{\begin{bmatrix} \hat{\mathbf{R}} \\ 0 \end{bmatrix}} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} - \underbrace{\begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \\ d_{n+1} \\ \vdots \\ d_m \end{bmatrix}}_{\begin{bmatrix} \hat{\mathbf{d}} \\ \mathbf{d}' \end{bmatrix}}$$

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# HOUSEHOLDER REFLECTORS

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- We will cover Householder reflections, see the book for Givens rotations in case you are curious.

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**Def:** Let  $P = \frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T \mathbf{v}}$  then

$$P^2 = \frac{\mathbf{v}\mathbf{v}^T \mathbf{v}\mathbf{v}^T}{(\mathbf{v}^T \mathbf{v})^2} = \frac{\mathbf{v}^T \mathbf{v}}{\mathbf{v}^T \mathbf{v}} \frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T \mathbf{v}} = P = P^T.$$

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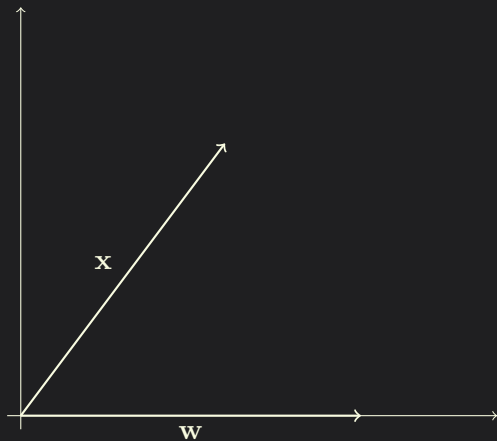
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$\mathbf{P}$  is a symmetric projection matrix with  $\mathbf{P}\mathbf{v} = \mathbf{v}$  and  $\mathbf{P}\mathbf{u}$  is the projection of  $\mathbf{u}$  onto  $\mathbf{v}$ .

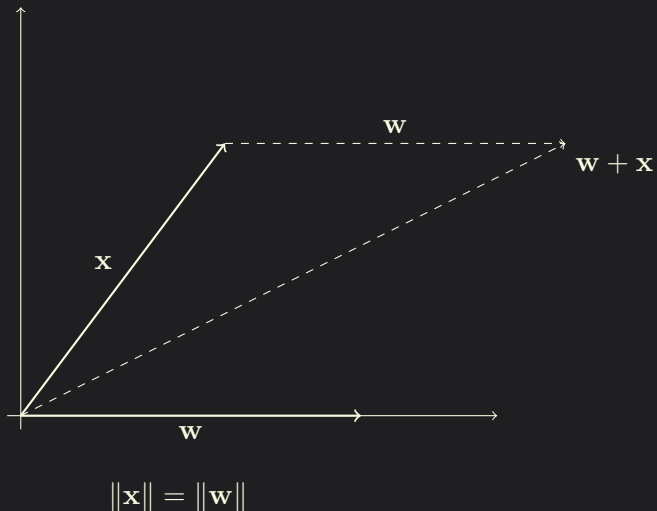


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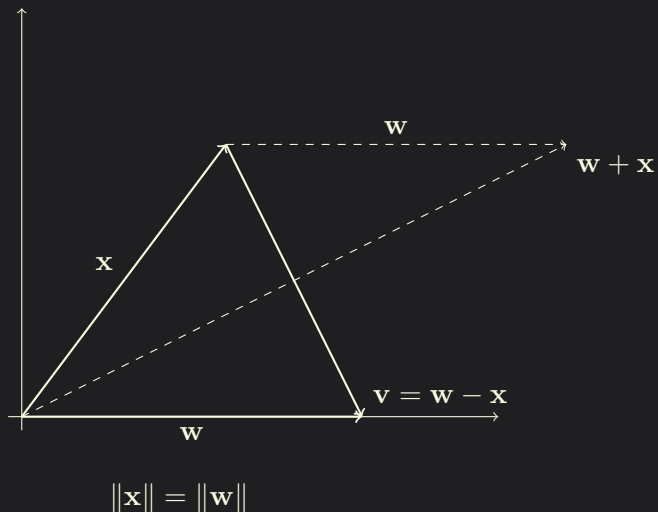


$$\|x\| = \|w\|$$

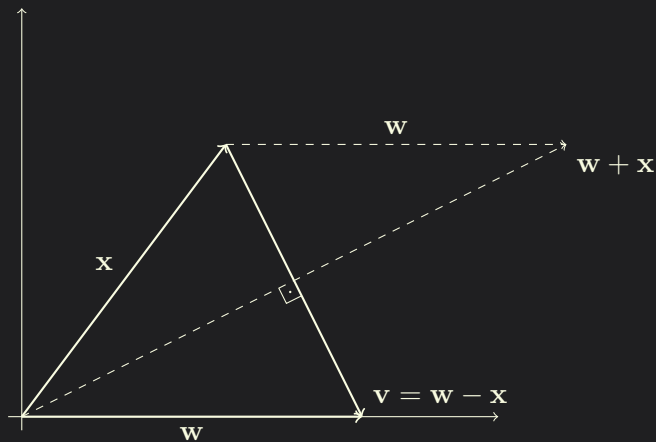
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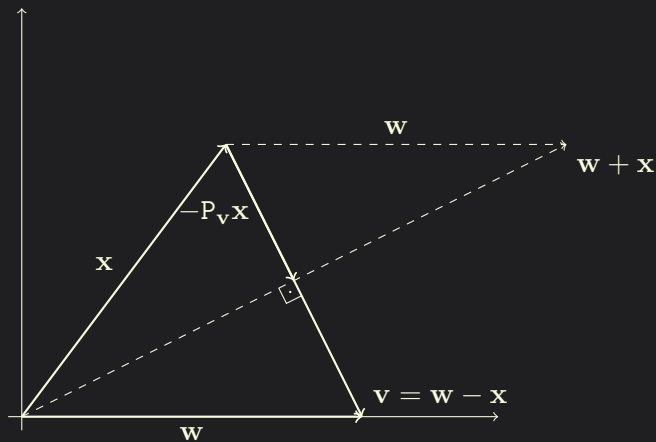


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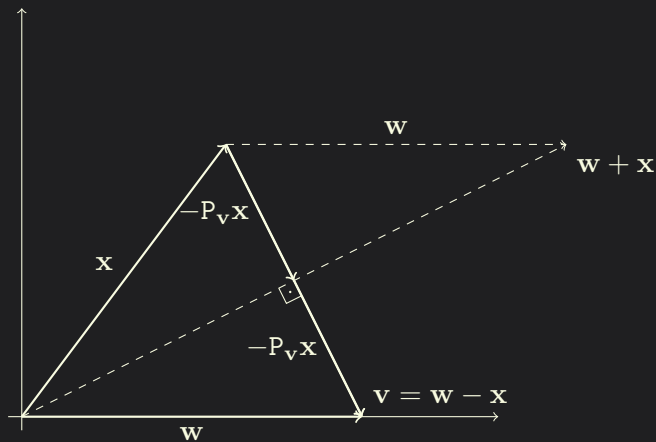
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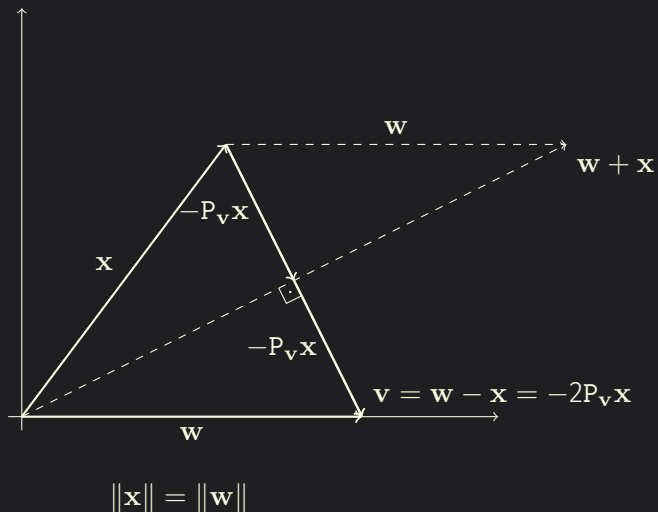
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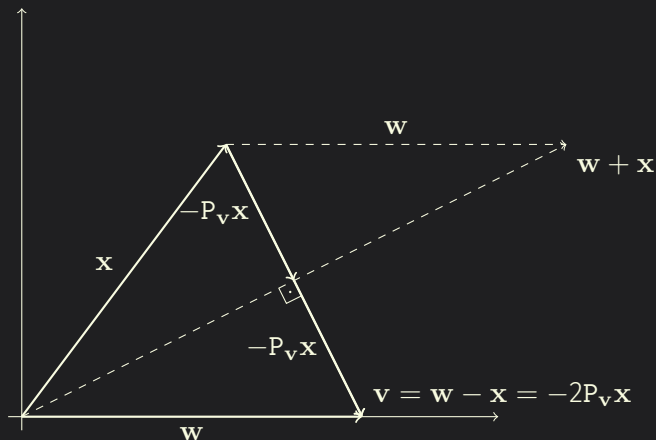


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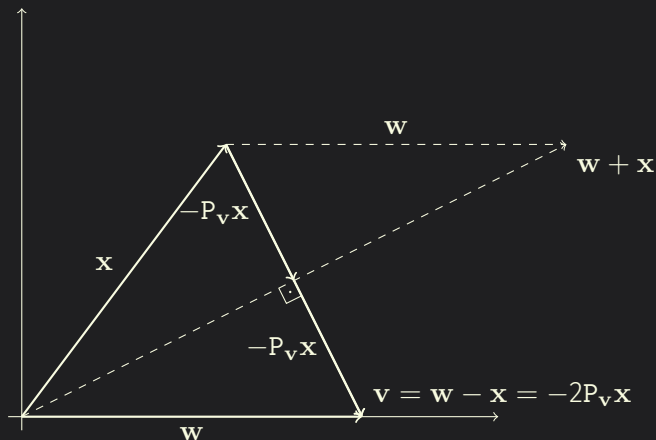
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$$\begin{aligned}\|x\| &= \|w\|, \quad w = x - 2P_v x = (I - 2P_v)x = Hx \\ H^T H &= (I - 2P_v)^T (I - 2P_v) = (I - 2P_v)(I - 2P_v) \\ &= I - 2P_v - 2P_v + 4P_v^2 = I.\end{aligned}$$

## EXAMPLE

Let  $\mathbf{x} = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$  and  $\mathbf{w} = \begin{bmatrix} 5 \\ 0 \end{bmatrix}$ , find  $\mathbf{H}$  s.t.  $\mathbf{H}\mathbf{x} = \mathbf{w}$ .

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$$\mathbf{H}\mathbf{x} = \begin{bmatrix} 1.8 + 3.2 \\ 2.4 - 2.4 \end{bmatrix} = \begin{bmatrix} 5 \\ 0 \end{bmatrix} = \mathbf{w}.$$

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Given  $A = [\mathbf{a}_1 \quad \mathbf{a}_2 \quad \cdots, \mathbf{a}_n]$ , take  $\mathbf{x}_1 = \mathbf{a}_1$  and  $\mathbf{w} = \pm \begin{bmatrix} \|\mathbf{x}_1\| \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ .

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$$A = H_1 H_2 R \quad (H_i^{-1} = H_i)$$

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$$\mathbf{H}_1 \mathbf{A} = \begin{bmatrix} 3 & 2 \\ 0 & -3 \\ 0 & -4 \end{bmatrix}, \hat{\mathbf{x}}_2 = \begin{bmatrix} -3 \\ -4 \end{bmatrix}, \hat{\mathbf{w}}_2 = \begin{bmatrix} 5 \\ 0 \end{bmatrix}, \mathbf{H}_2 = \begin{bmatrix} -0.6 & -0.8 \\ -0.8 & 0.6 \end{bmatrix}$$

## EXAMPLE

Find the QR factorization of  $\mathbf{A} = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}$ .

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 2 \\ 2 \end{bmatrix}, \mathbf{w}_1 = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix}, \mathbf{v} = \begin{bmatrix} 2 \\ -2 \\ -2 \end{bmatrix}, \mathbf{H}_1 = \begin{bmatrix} \frac{1}{3} & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & \frac{1}{3} & -\frac{2}{3} \\ \frac{2}{3} & -\frac{2}{3} & \frac{1}{3} \end{bmatrix}$$

$$\mathbf{H}_1\mathbf{A} = \begin{bmatrix} 3 & 2 \\ 0 & -3 \\ 0 & -4 \end{bmatrix}, \hat{\mathbf{x}}_2 = \begin{bmatrix} -3 \\ -4 \end{bmatrix}, \hat{\mathbf{w}}_2 = \begin{bmatrix} 5 \\ 0 \end{bmatrix}, \mathbf{H}_2 = \begin{bmatrix} -0.6 & -0.8 \\ -0.8 & 0.6 \end{bmatrix}$$

$$\mathbf{H}_2\mathbf{H}_1\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.6 & -0.8 \\ 0 & -0.8 & 0.6 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 0 & -3 \\ 0 & -4 \end{bmatrix} = \begin{bmatrix} 3 & 2 \\ 0 & 5 \\ 0 & 0 \end{bmatrix} = \mathbf{R},$$

## EXAMPLE

Find the QR factorization of  $\mathbf{A} = \begin{bmatrix} 1 & -4 \\ 2 & 3 \\ 2 & 2 \end{bmatrix}$ .

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$$\mathbf{H}_1\mathbf{A} = \begin{bmatrix} 3 & 2 \\ 0 & -3 \\ 0 & -4 \end{bmatrix}, \hat{\mathbf{x}}_2 = \begin{bmatrix} -3 \\ -4 \end{bmatrix}, \hat{\mathbf{w}}_2 = \begin{bmatrix} 5 \\ 0 \end{bmatrix}, \mathbf{H}_2 = \begin{bmatrix} -0.6 & -0.8 \\ -0.8 & 0.6 \end{bmatrix}$$

$$\mathbf{H}_2\mathbf{H}_1\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -0.6 & -0.8 \\ 0 & -0.8 & 0.6 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 0 & -3 \\ 0 & -4 \end{bmatrix} = \begin{bmatrix} 3 & 2 \\ 0 & 5 \\ 0 & 0 \end{bmatrix} = \mathbf{R},$$

$$\mathbf{Q} = \mathbf{H}_1\mathbf{H}_2 = \frac{1}{15} \begin{bmatrix} 5 & -14 & -2 \\ 10 & 5 & -10 \\ 10 & 2 & 11 \end{bmatrix}$$

# UNIQUENESS OF QR FACTORIZATION

QR factorization is not unique since if  $D = \text{diag}(d_1, \dots, d_m)$  with  $d_i = \pm 1$  then

$$A = QR = \underbrace{QD}_{Q'} \underbrace{DR}_{R'}$$

since

$$D^2 = I$$