

Module – 4.2

MATRIX DECOMPOSITION METHODS

AN OVERVIEW

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MATRIX METHODS FOR SOLVING $Ax = b$

Two classes

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- ```
graph TD; A[Two classes] --> B["• Direct method"]; A --> C["• Iterative method"]
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- Direct method
  - Multiplicative decomposition of A
  - Complexity –  $O(n^3)$
  - Gives exact answer if there is no round – off
  - Three decompositions: LU, QR, SVD
  - Iterative method
  - Additive decomposition of A
  - Convergence proof
  - Rate of convergence
  - Complexity depends on the cost per iteration and the desired accuracy
  - Jacobi, Gauss-Seidel, SOR, etc

# DIRECT METHOD – LU – DECOMPOSITION OF A

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- LU decomposition derived from the classical Gaussian elimination method
- Given  $A$  – nonsingular, there exists  $L$ , a lower triangular and a  $U$  – upper triangular matrices:

$$A = LU$$

# LU DECOMPOSITION OF A

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$$\bullet \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ l_{21} & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & \cdots & \cdots & 1 \end{bmatrix} \begin{bmatrix} u_{11} & a_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

- L has  $\frac{n(n-1)}{2}$  unknowns and U has  $\frac{n(n+1)}{2}$  unknowns – a total of  $n^2$  unknowns
- Multiplying L and U and equating the elements we can easily solve the system of  $n^2$  equations in  $n^2$  unknowns

# EXAMPLE

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- $A = \begin{bmatrix} 1 & 3/2 \\ 3/2 & 1/2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ l_{21} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} \\ 0 & u_{22} \end{bmatrix} = LU$   
 $= \begin{bmatrix} u_{11} & u_{12} \\ l_{21}u_{11} & l_{21}u_{12} + u_{22} \end{bmatrix}$
- Verify:  $L = \begin{bmatrix} 1 & 0 \\ 3/2 & 1 \end{bmatrix}, U = \begin{bmatrix} 1 & 3/2 \\ 0 & 5/4 \end{bmatrix}$
- By exploiting the patterns in the  $n^2$  nonlinear equations in  $n^2$  unknowns we get the following algorithm for L and U

# LU DECOMPOSITION – PSEUDO CODE

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- Given  $A \in R^{n \times n}$ , non singular

For  $r = 1$  to  $n$

    For  $i = r$  to  $n$

$$u_{ri} = a_{ri} - \sum_{j=1}^{r-1} l_{rj} u_{ji} \text{ - Rows of U}$$

    End For

    For  $i = r + 1$  to  $n$

$$l_{ir} = \frac{1}{u_{rr}} [a_{ir} - \sum_{j=1}^{r-1} l_{rj} u_{ji}] \text{ - Columns of L}$$

    End For

End For

- Verify that the total number of operation is  $O(n^3)$

# LU DECOMPOSITION – A FRAME WORK FOR SOLUTION

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- Given L, U:  $A = LU$ , then
- $Ax = (LU)x = L(Ux) = Lg = b$  and  $Ux = g$
- Summary – a three step procedure
  - Decompose  $A = LU$
  - Solve  $Lg = b$  – lower triangular system
  - Solve  $Ux = g$  – upper triangular system

# SOLUTION LOWER TRIANGULAR SYSTEM: $Lg = b$

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- Let 
$$\begin{bmatrix} l_{11} & 0 & 0 & \cdots & 0 \\ l_{21} & l_{22} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & l_{nn} \end{bmatrix} \begin{bmatrix} g_1 \\ g_2 \\ \vdots \\ g_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

- Forward elimination method:

$$g_1 = \frac{b_{11}}{l_{11}}$$

For  $i = 2$  to  $n$

$$g_i = \frac{1}{l_{ii}} [b_i - \sum_{j=1}^{i-1} l_{ij}g_j]$$

End For

- Verify that it takes  $O(n^2)$  operations to compute  $g$

# SOLUTION UPPER TRIANGULAR SYSTEM: $Ux = g$

- Let  $\begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \\ \vdots \\ g_n \end{bmatrix}$

- Back substitution method:

$$x_n = \frac{g_n}{u_{nn}}$$

For  $i = n - 1$  to  $n$

$$x_i = \frac{1}{u_{ii}} [g_i - \sum_{j=i+1}^{i-1} u_{ij} x_j]$$

End For

- Verify that it takes  $O(n^2)$  operations to compute  $x$

# TOTAL CASE OF SOLVING $Ax = b$

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- LU decomposition step –  $O(n^3)$
- Lower triangular system –  $O(n^2)$
- Upper triangular system –  $O(n^2)$
- Total cost is  $O(n^3)$

# COMPLEXITY OF LARGE PROBLEM

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- Let  $n = 10^6$  and  $n^3 = 10^{18}$  – operations
- Consider a machine that takes  $10^{-12}$  second per operation. It's a TERA FLOP MACHINE
- TIME needed =  $10^{18} \times 10^{-12} = 10^6$  seconds
- There are only  $60 \times 60 \times 24 \times 365 = 32,536,000 = 31.5 \times 10^6$  seconds in one year
- It takes =  $\frac{10^6}{60 \times 60 \times 24} = \frac{10^6}{86,400} = 11.575$  days to solve  $Ax = b$

# WHEN A IS SYMMETRIC

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- Let  $D = \text{diag}(u_{11}, u_{22}, \dots u_{nn})$  a diagonal matrix with the diagonal elements of  $U$
- Then  $U = DM$  where the diagonal of  $M$  are all 1
- Then  $A = LDM$
- If  $A$  is symmetric, then  $M = L^T$  and  $A = LDL^T$

# EXAMPLE

- Recall

$$A = \begin{bmatrix} 1 & 3/2 \\ 3/2 & 1/2 \end{bmatrix} = LU = \begin{bmatrix} 1 & 0 \\ 3/2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 3/2 \\ 0 & 5/4 \end{bmatrix}$$

$$U = \begin{bmatrix} 1 & 3/2 \\ 0 & 5/4 \end{bmatrix} = DM = \begin{bmatrix} 1 & 0 \\ 0 & 5/4 \end{bmatrix} \begin{bmatrix} 1 & 3/2 \\ 0 & 1 \end{bmatrix}$$

$$M = \begin{bmatrix} 1 & 3/2 \\ 0 & 1 \end{bmatrix} = L^T \text{ since } A \text{ is symmetric}$$

$$D^{1/2} = \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{5}/2 \end{bmatrix}$$

$$\begin{aligned} A &= \begin{bmatrix} 1 & 0 \\ 3/2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{5}/2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \sqrt{5}/2 \end{bmatrix} \begin{bmatrix} 1 & 3/2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 3/2 & \sqrt{5}/2 \end{bmatrix} \begin{bmatrix} 1 & 3/2 \\ 0 & \sqrt{5}/2 \end{bmatrix} \\ &= GG^T \end{aligned}$$

# WHEN A – SPD – CHOLESKY DECOMPOSITION

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- When A is PD => diagonal elements of D are positive
- $A = LDL^T = LD^{\frac{1}{2}}D^{\frac{1}{2}}L^T$   
 $= (LD^{\frac{1}{2}})(LD^{\frac{1}{2}})^T$   
 $= GG^T - \underline{\text{Choleskey decomposition}}$
- $G = LD^{\frac{1}{2}}$  is called the Choleskey factor
- $D^{\frac{1}{2}} = \text{diag}(u_{11}^{\frac{1}{2}}, u_{22}^{\frac{1}{2}}, \dots u_{nn}^{\frac{1}{2}})$  is the square root of the diagonal matrix D
- G is also known as the square root of A

# COMPUTATION OF G GIVEN A

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For  $j = 1$  to  $n$

$$g_{jj} = [a_{jj} - \sum_{k=1}^{j-1} g_{jk}^2]^{1/2} \text{ - diagonal of } G$$

For  $i = j + 1$  to  $n$

$$g_{ij} = \frac{1}{g_{jj}} [a_{ij} - \sum_{k=1}^{j-1} g_{ik} g_{kj}] \text{ - column of } G$$

End For

End For

- Verify that it still takes  $O(n^3)$  operations but the leading coefficient is one-half of that required for LU - decomposition

# CHOLESKY FRAME WORK: $Ax = b$

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- $A$  SPD and  $A = GG^T$
- $Ax = (GG^T)x = G(G^Tx) = Gy = b$
- Compute  $G$ :  $A = GG^T - O(n^3)$  operations
- Solve  $Gg = b$  – Lower triangular –  $O(n^2)$  operations
- Solve  $G^Tx = g$  – upper triangular –  $O(n^2)$  operations
- Total cost still is  $O(n^3)$  with a smaller coefficient in the leading term

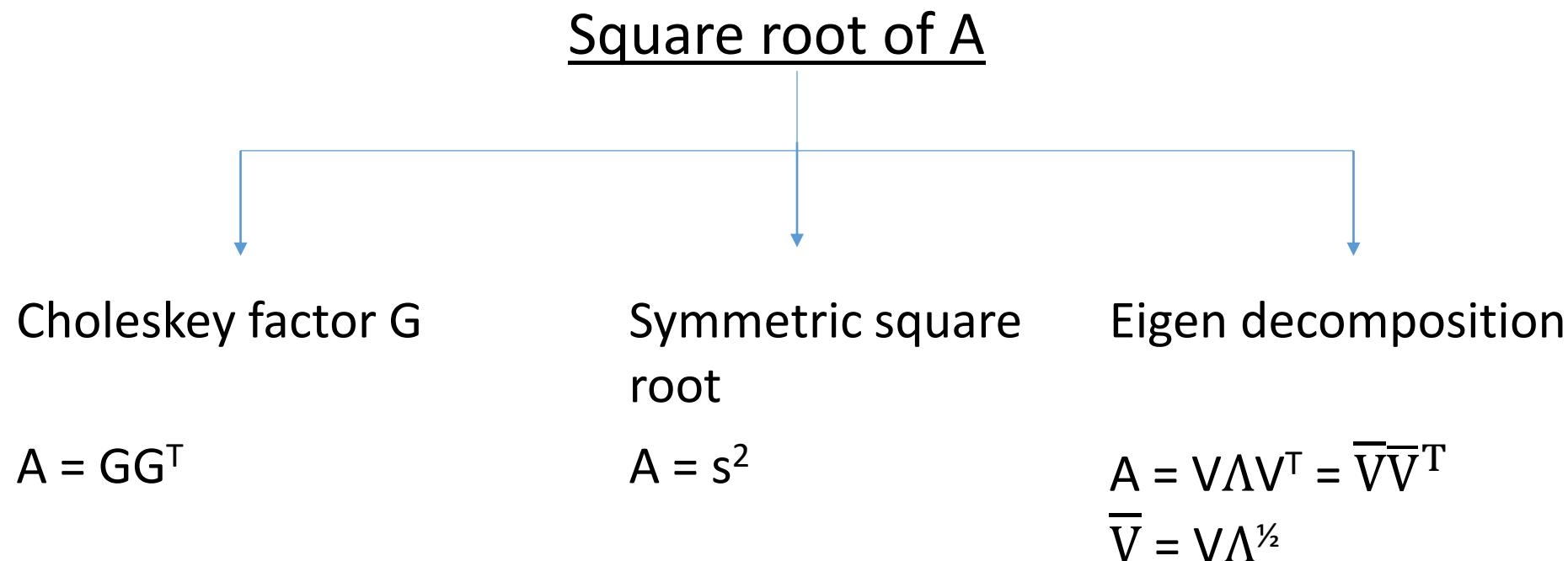
# SOLUTION OF NORMAL EQUATION: $(H^T H)x = H^T Z$

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- Given  $H \in \mathbb{R}^{m \times n}$  of full rank,  $Z \in \mathbb{R}^m$
- Step 1: Compute  $H^T H - O(nm^2)$  operations
- Step 2: Compute  $H^T Z - O(nm)$  operations
- Step 3: Compute the cholesky factor  $G$ :  
$$(H^T H) = GG^T - O(n^3)$$
 operations
- Step 4: Solve lower triangular system  
$$Gg = H^T Z - O(n^2)$$
 operations
- Step 5: Solve upper triangular system  
$$G^T x = g - O(n^2)$$
 operations
- Similarly for  $(HH^T)y = Z$  and  $x = H^T y$

# SQUARE ROOT OF A - SPD

- Three possible definitions of square root of A – SPD



# ORTHOGONAL MATRIX

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- FACT: A matrix  $A \in R^{n \times n}$  is orthogonal if  $A^{-1} = A^T$ , that is,  $A^T A = A A^T = I$
- Let  $y = Ax$  and  $A$  be orthogonal. Then

$$\|y\|_2^2 = \|Ax\|_2^2 = (Ax)^T(Ax) = x^T A^T A x = x^T x = \|x\|_2^2$$

Thus, 2 –norm is invariant under orthogonal transformation

# QR – DECOMPOSITION ( $m > n$ )

- FACT: Let  $H \in \mathbb{R}^{mxn}$ . Then exists an orthogonal matrix  $Q \in \mathbb{R}^{mxm}$  and an upper triangular matrix  $R \in \mathbb{R}^{mxn}$  such that

$$H = QR, QQ^T = Q^TQ = I_m$$

$$\begin{bmatrix} h_{11} & h_{12} & \cdots & h_{1n} \\ h_{21} & h_{22} & \cdots & h_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ h_{m1} & h_{m2} & \cdots & h_{mn} \end{bmatrix} = \begin{bmatrix} q_{11} & q_{12} & \cdots & q_{1m} \\ q_{21} & q_{22} & \cdots & q_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ q_{m1} & q_{m2} & \cdots & q_{mm} \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & r_{nn} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

called the full QR decomposition

- Columns of  $Q$  are orthonormal vectors

# REDUCED QR – DECOMPOSITION ( $m > n$ )

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- Let  $Q = [Q_1, Q_2]$ ,

$Q_1 \in R^{mxn}$  with first  $n$  columns of  $Q$

$Q_2 \in R^{mx(m-n)}$  with the last  $(m - n)$  columns of  $Q$

- $R = \begin{bmatrix} R_1 \\ R_2 \end{bmatrix}$

$R_1 \in R^{nxn}$  with first  $n$  columns of  $R$

$R_2 \in R^{(m-n)xn}$  is a zero matrix

- Then  $H = QR = [Q_1, Q_2] \begin{bmatrix} R_1 \\ R_2 \end{bmatrix} = Q_1 R_1$  called reduced QR decomposition
- $Q_1^T Q_1 = I_n$

# LINEAR LEAST SQUARE PROBLEM: $Z = Hx$

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- $r(x) = Z - Hx$  – residual
- $f(x) = \|r(x)\|_2^2 = \|Q^T r(x)\|_2^2 = \|Q^T(Z - Hx)\|_2^2$  – ( $Q$  – orthogonal)  
 $= \|Q^T Z - Q^T Hx\|_2^2$
- $Q^T Z = \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix} Z = \begin{bmatrix} Q_1^T Z \\ Q_2^T Z \end{bmatrix}$
- $Q^T Hx = Q^T QRx = Rx = \begin{bmatrix} R_1 \\ R_2 \end{bmatrix} x = \begin{bmatrix} R_1 x \\ 0 \end{bmatrix}$
- $f(x) = \|Q_1^T Z - R_1 x\|_2^2 + \|Q_2^T Z\|_2^2$

# LEAST SQUARE SOLUTION – QR METHOD

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- $f(x) = \|Q_1^T Z - R_1 x\|_2^2 + \|Q_2 Z\|_2^2$
- Only the first term depends on  $x$
- $f(x)$  is a minimum when  $R_1 x = Q_1^T Z$
- $x_{LS} = R_1^{-1}(Q_1^T Z)$  is obtained by solving an upper triangular system

# QR DECOMPOSITION: $m < n$

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- $Z = Hx, H \in \mathbb{R}^{m \times n}, m < n$
- Then  $H^T = QR$  as above, since  $n > m$   
with  $Q = [Q_1, Q_2]$ ,  $R = \begin{bmatrix} R_1 \\ R_2 \end{bmatrix}$ ,  $Q_1 \in \mathbb{R}^{n \times m}$ ,  $Q_2 \in \mathbb{R}^{n \times (n-m)}$   
 $R_1 \in \mathbb{R}^{m \times m}$  and  $R_2 \in \mathbb{R}^{n-m \times m}$  is a zero matrix
- $Q_1^T Q_1 = I_m$  and  $H = R^T Q^T$

# LEAST SQUARE SOLUTION – QR METHOD (m < n)

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- $f(x) = \|r(x)\|_2^2 = (Z - R^T Q^T x)^T (Z - R^T Q^T x)$   
 $= Z^T Z - 2Z^T R^T Q^T x + x^T (Q R R^T Q^T) x$
- $\nabla_x f(x) = -2QRZ + 2(QRR^TQ^T)x = 0$
- $\nabla_x^2 f(x) = 2QRR^TQ^T$
- $x_{LS}$  is the solution of:  $RR^TQ^TQ = RZ$

# FORM OF THE LEAST SQUARE SOLUTION

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- $y = Q^T x = \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix} x = \begin{bmatrix} Q_1^T x \\ Q_2^T x \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \quad y_1 \in \mathbb{R}^m, y_2 \in \mathbb{R}^{n-m}$
- $RR^{T+} = \begin{bmatrix} R_1 \\ 0 \end{bmatrix} [R_1^T : 0] = \begin{bmatrix} R_1 R_1^T & 0 \\ 0 & 0 \end{bmatrix}$
- $\begin{bmatrix} R_1 R_1^T & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} R_1 Z \\ 0 \end{bmatrix} \Rightarrow R_1 R_1^T y_1 = R_1 Z, y_2 \text{ is arbitrary}$
- $Y_1$  is obtained by solving a lower triangular system  $R_1^T y_1 = Z$

# THE LEAST SQUARE SOLUTION: $m < n$

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- $X = Qy = Q \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = [Q_1 \ Q_2] \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = Q_1 y_1 + Q_2 y_2$
- Since  $y_2$  is arbitrary, there are infinitely many solutions
- Clearly,  $x_{LS} = Q_1 y_1 = Q_1 (R_1^{-T} Z)$
- $\|x\|_2^2 = \|Q_1 y_1\|_2^2 + \|Q_2 y_2\|_2^2$       ( $Q_1^T Q_1 = I_m$ ,  $Q_1^T Q_2 = I_{n-m}$ )  
 $= \|y_1\|_2^2 + \|y_2\|_2^2$   
 $\geq \|y_1\|_2^2 = \|x_{LS}\|_2^2$

# SUMMARY: QR ALGORITHM

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- Over determined case  $H \in \mathbb{R}^{m \times n}$ ,  $m > n$
- Step 1: Compute  $Q_1 \in \mathbb{R}^{m \times n}$  and  $R_1 \in \mathbb{R}^{n \times n}$  such that  $H = Q_1 R_1$  using Gramm-Schmidt orthogonalization method – See below
- Step 2: Compute  $Q_1^T Z$
- Step 3: Solve upper triangular system  $R_1 x = Q_1^T Z$  and  $x_{LS} = R_1^{-T} (Q_1^T Z)$

# SUMMARY: QR ALGORITHM

---

- Under determined case  $H \in \mathbb{R}^{m \times n}$ ,  $m < n$
- Step 1: Compute  $H^T = Q_1 R_1$ ,  $Q_1 \in \mathbb{R}^{n \times m}$  and  $R_1 \in \mathbb{R}^{m \times m}$
- Step 2: Solve the lower triangular system  $R_1^T y_1 = Z$
- Step 3:  $x_{LS} = Q_1 y_1 = Q_1 (R_1^{-T} Z)$

# GRAMM- SCHMIDT ORTHOGONALIZATION

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- Let  $H = [h_1, h_2, \dots, h_n]$ ,  $h_i \in R^m$ ,  $1 \leq i \leq n$ ,  $m > n$
- Let the columns of  $H$  are linearly independent
- Find  $Q = [q_1, q_2, \dots, q_n]$ ,  $q_i \in R^m$ ,  $1 \leq i \leq n$  and  $\{q_i\}_{i=1}^n$  is an orthogonal system:

$$\begin{aligned} q_i^T q_j &= 0 \text{ if } i \neq j \\ &= 1 \text{ if } i = j \end{aligned}$$

- Problem: Given  $\{h_i\}_{i=1}^n$ , find  $\{q_i\}_{i=1}^n$  with the above properties

# ALGORITHM – AN IDEA

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- Set  $q_1 = \frac{h_1}{r_{11}}$  with  $r_{11} = \|h_1\|_2$  and  $\|q_1\| = 1$
- Set  $q_2 = \frac{1}{r_{22}}[h_2 - r_{12}q_1]$  – 2 unknowns:  $r_{12}, r_{22}$

$$\text{Thus, } 0 = q_1^T q_2 = \frac{1}{r_{22}}[q_1^T h_2 - r_{12}]$$

Therefore,  $r_{12} = q_1^T h_2$  and  $r_{22} = \|h_2 - r_{12}q_1\|$

- In general: j – unknowns ( $1 \leq j \leq n$ )

$$q_j = \frac{1}{r_{jj}}[h_j - \sum_{i=1}^{j-1} r_{ij}q_i]$$

$$\Rightarrow r_{ij} = q_i^T h_j \quad 1 \leq i \leq j-1$$

$$r_{ji} = \left\| h_j - \sum_{i=1}^{j-1} r_{ij}q_i \right\|$$

# QR – ALGORITHM – PSEUDO CODE

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- Given  $\{h_1, h_2, h_3, \dots, h_n\}$ ,  $h_i \in R^m$ ,  $m > n$  linearly independent
- Find  $\{q_1, q_2, q_3, \dots, q_n\}$ ,  $h_i \in R^m$ , orthonormal

Step 1: Repeat the following steps 2 to 5 for  $j = 1$  to  $n$

Step 2:  $v_j = h_j$

Step 3: For  $i = 1$  to  $j - 1$

    Compute:  $r_{ij} = q_i^T h_j$

    Update:  $v_j = v_j - r_{ij} q_i$

Step 4: Compute norm of  $v_j$ :  $r_{jj} = \|v_j\|$

Step 5:  $q_j = \frac{v_j}{r_{jj}}$

# SINGULAR VALUE DECOMPOSITION - SVD

- Let  $H \in \mathbb{R}^{m \times n}$  be of full rank

Grammians ( $m > n$ )

- 
- $H^T H \in \mathbb{R}^{n \times n}$
  - $\text{Rank}(H^T H) = n$
  - Symmetric
  - Positive definite
  - $HH^T \in \mathbb{R}^{m \times m}$
  - $\text{Rank}(HH^T) = m$
  - Symmetric
  - Positive semi-definite

- Let  $(\lambda_i, v_i)$  be the  $n$ -eigenvalue eigenvector pair for  $H^T H$  with  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n > 0$
- $(H^T H)v_i = \lambda_i v_i \quad 1 \leq i \leq n$
- $V = [v_1, v_2, \dots, v_n], \Lambda = \text{Diag}[\lambda_1, \lambda_2, \dots, \lambda_n]$
- $V$  is orthogonal matrix,  $V^T V = VV^T = I$
- $(H^T H)V = V\Lambda$  or  $(H^T H) = V\Lambda V^T$

# EIGENVALUES AND VECTORS OF $HH^T$

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- Define  $u_i = \frac{1}{\sqrt{\lambda_i}} Hv_i$ ,  $u_i \in \mathbb{R}^m$ ,  $1 \leq i \leq n$
- $(HH^T)u_i = (HH^T)\frac{1}{\sqrt{\lambda_i}}Hv_i$   
 $= \frac{1}{\sqrt{\lambda_i}}H(H^TH)v_i$   
 $= \frac{1}{\sqrt{\lambda_i}}H\lambda_i v_i = \sqrt{\lambda_i}Hv_i = \lambda_i u_i$
- Thus,  $(\lambda_i, u_i)$ ,  $1 \leq i \leq n$  are the eigenvectors of  $HH^T$
- The rest of  $(m-n)$  eigenvalues of  $(HH^T)$  are zeros

# EIGENDECOMPOSITION OF $\mathbf{H}\mathbf{H}^T$

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- Set  $\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n] \in \mathbb{R}^{m \times n}$
- $\mathbf{u}_i = \frac{1}{\sqrt{\lambda_i}} \mathbf{H}\mathbf{v}_i \Rightarrow \mathbf{U}\Lambda^{1/2} = \mathbf{H}\mathbf{V}$
- $$\begin{aligned}\mathbf{U}^T\mathbf{U} &= (\mathbf{H}\mathbf{V}\Lambda^{-1/2})^T(\mathbf{H}\mathbf{V}\Lambda^{-1/2}) \\ &= \Lambda^{-1/2}\mathbf{V}^T(\mathbf{H}^T\mathbf{H})\mathbf{V}\Lambda^{-1/2} \\ &= \Lambda^{-1/2}\mathbf{V}^T\mathbf{V}\Lambda\Lambda^{-1/2} \\ &= \mathbf{I} \text{ (because } \mathbf{V}^T\mathbf{V} = \mathbf{I})\end{aligned}$$
- Columns of  $\mathbf{U}$  are orthonormal

# SVD OF H

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- $u_i = \frac{1}{\sqrt{\lambda_i}} Hv_i \Rightarrow Hv_i = u_i \sqrt{\lambda_i}$
- $HV = U\Lambda^{1/2}$  or  $H = U\Lambda^{1/2}V^T$  is called the SVD of H

$$\bullet H = [u_1, u_2, \dots, u_n] \begin{bmatrix} \lambda_1^{1/2} & 0 & \cdots & 0 \\ 0 & \lambda_2^{1/2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n^{1/2} \end{bmatrix} \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_n^T \end{bmatrix}$$

- $H = \sum_{i=1}^n \sqrt{\lambda_i} u_i v_i^T$
- $\lambda_i$  are eigenvalues of  $H^T$  and  $\lambda_i^{1/2}$  are the singular values of H by definition

# SVD BASED SOLUTION OF LEAST SQUARES

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- $Z = Hx$ ,  $H \in \mathbb{R}^{m \times n}$  – full rank
- $H = U\Lambda^{\frac{1}{2}}V^T$ ,  $VV^T = V^TV = I_n$ ,  $U^TU = I_n$
- $f(x) = (Z - Hx)^T(Z - Hx)$ 
$$= (Z - U\Lambda^{\frac{1}{2}}V^T x)^T(Z - U\Lambda^{\frac{1}{2}}V^T x)$$
$$= Z^TZ - 2Z^TU\Lambda^{\frac{1}{2}}V^Tx + x^T(V\Lambda V^T)x$$
- $0 = \nabla_x f(x) = -2V\Lambda^{\frac{1}{2}}U^TZ - 2(V\Lambda V^T)x$
- $x_{LS}$  is the solution of:  $(V\Lambda V^T)x = V\Lambda^{\frac{1}{2}}U^TZ$
- $x_{LS} = V\Lambda^{-\frac{1}{2}}U^TZ$

# ALGORITHM - SVD

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- Given  $H \in \mathbb{R}^{m \times n}$

STEP 1: Compute  $H = U\Lambda^{\frac{1}{2}}V^T$

STEP 2: Compute  $U^T Z$  – (rotation)

STEP 3: Compute  $y = \Lambda^{-\frac{1}{2}}U^T Z$  – (Scaling)

STEP 4: Compute  $x^* = Vy$  – (rotation)

# EXERCISES

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- 13.1) Consider the matrix  $H \in \mathbb{R}^{4 \times 16}$  built using the 2-D bilinear interpolation in Module 3.6
- (a) Pick for pairs  $(a_i, b_i)$ ,  $1 \leq i \leq 4$  of uniformly distributed random numbers in range  $[0, 1]$
  - (b) Compute the elements of the rows of  $H$  and verify that they add up to 1
  - (c) Compute  $HH^T$
  - (d) Generate observation  $Z_i = 75 + V_i$ ,  $V_i \sim N(0, \sigma^2)$  for  $1 \leq i \leq 4$

# EXERCISES

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13.2) Develop your own MATLAB program to do the following

- (a) LU - decomposition
- (b) Solving lower and upper triangular system
- (c) Cholesy decomposition
- (d) Gramm–Schmidt orthogonalization
- (e) SVD

# EXERCISES

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13.3)

(a) Apply Cholesky decomposition to solve  $(HH^T)y = Z$  and compute  
 $x_{LS} = H^T y$

(b) Compute  $\hat{Z} = Z - Hx_{LS}$  and  $r(x_{LS}) = Z - \hat{Z}$ . Compute  $\|r(x_{LS})\|_2$

13.4) Apply QR Decomposition to  $H$  using Gramm-Schmidt and solve the resulting linear least square problem

13.5) Apply SVD to  $H$  and solve the resulting least square problem

13.6) Compare the norm of the residual  $r(x) = Z - \hat{Z}$  computed using the three methods

# REFERENCES

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- This module follows closely the developments in chapter 9 of LLD (2006)
- Basic iterative methods for solving  $Ax = b$  are covered in the following books:
  - G. H. Golub and C. F. Van Loan (1989) Matrix Computation, Johns Hopkins University Press (Second Edition)
  - Hageman, L. A. and D. Young (1981) Applied Iterative Methods, Academic Press