

Module – 4.2

MATRIX DECOMPOSITION METHODS

AN OVERVIEW

S. Lakshmivarahan

School of Computer Science

University of Oklahoma

Norman, Ok – 73069, USA

varahan@ou.edu

MATRIX METHODS FOR SOLVING $Ax = b$

Two classes



- 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

- 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

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

- 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

- $A = \begin{bmatrix} 1 & 3/2 \\ 3/2 & 1/2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ l_{21} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} \\ 0 & u_{22} \end{bmatrix} = LU$
 $= \begin{bmatrix} u_{11} & u_{12} \\ l_{21}u_{11} & l_{21}u_{12} + u_{22} \end{bmatrix}$
- 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

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

- 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: $Lg = b$

- 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 $Ax = b$

- 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

- 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

- 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

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

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

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

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

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

$= GG^T$

WHEN A – SPD – CHOLESKY DECOMPOSITION

- When A is PD => diagonal elements of D are positive
- $$\begin{aligned} A &= LDL^T = LD^{\frac{1}{2}}D^{\frac{1}{2}}L^T \\ &= (LD^{\frac{1}{2}})(LD^{\frac{1}{2}})^T \\ &= GG^T - \text{Choleskey decomposition} \end{aligned}$$
- $G = LD^{\frac{1}{2}}$ 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

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: $Ax = b$

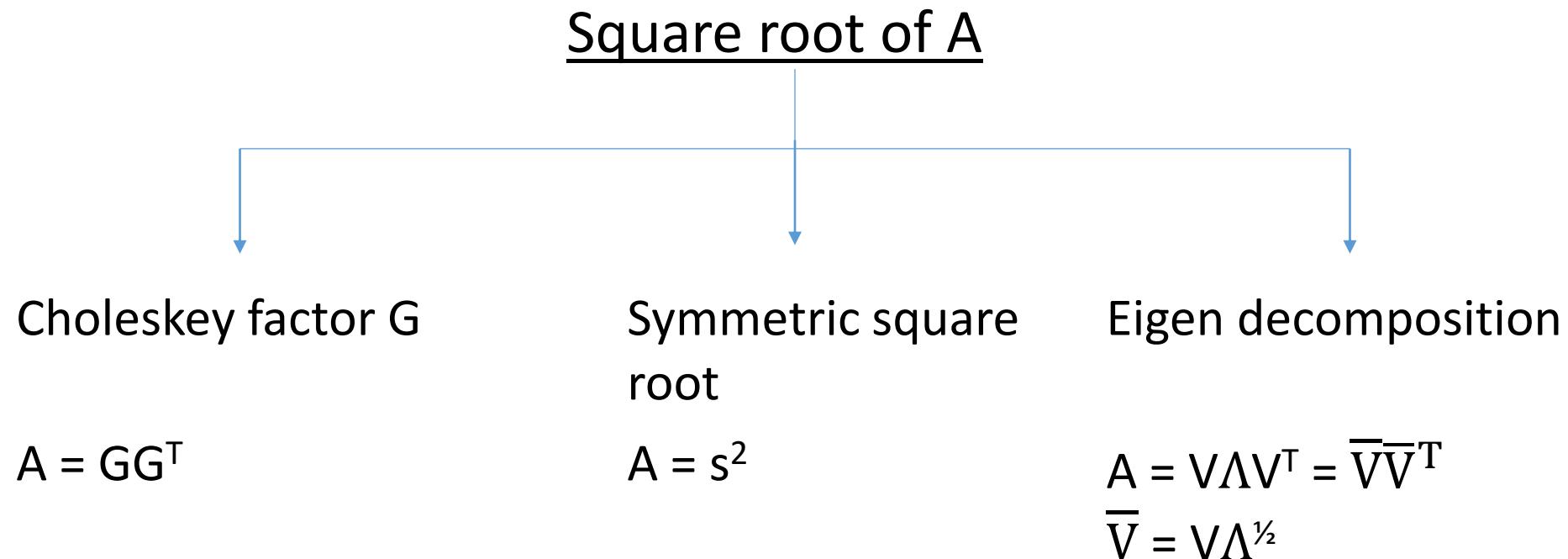
- A SPD and $A = GG^T$
- $Ax = (GG^T)x = G(G^Tx) = Gy = b$
- Compute G : $A = GG^T - O(n^3)$ operations
- Solve $Gg = b$ – Lower triangular – $O(n^2)$ operations
- Solve $G^Tx = g$ – upper triangular – $O(n^2)$ operations
- Total cost still is $O(n^3)$ with a smaller coefficient in the leading term

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

- 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

- FACT: A matrix $A \in \mathbb{R}^{n \times n}$ 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 ($m > n$)

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

$Q_1 \in \mathbb{R}^{m \times n}$ with first n columns of Q

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

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

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

$R_2 \in \mathbb{R}^{m-n \times n}$ 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: $Z = Hx$

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

LEAST SQUARE SOLUTION – QR METHOD

- $f(x) = \|Q_1^T Z - R_1 x\|_2^2 + \|Q_2 Z\|_2^2$
- 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: $m < n$

- $Z = Hx, H \in \mathbb{R}^{m \times n}, m < n$
- 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)

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

FORM OF THE LEAST SQUARE SOLUTION

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

THE LEAST SQUARE SOLUTION: $m < n$

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

SUMMARY: QR ALGORITHM

- 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

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

- 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}

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

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

- 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

- Given $\{h_1, h_2, h_3, \dots, h_n\}$, $h_i \in \mathbb{R}^m$, $m > n$ linearly independent
- Find $\{q_1, q_2, q_3, \dots, q_n\}$, $h_i \in \mathbb{R}^m$, 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 : $r_{ij} = \|v_j\|$

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

- Let (λ_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, $V^T V = V V^T = I$
- $(H^T H)V = V \Lambda$ or $(H^T H) = V \Lambda V^T$

EIGENVALUES AND VECTORS OF HH^T

- Define $u_i = \frac{1}{\sqrt{\lambda_i}} Hv_i$, $u_i \in \mathbb{R}^m$, $1 \leq i \leq n$
- $$\begin{aligned}(HH^T)u_i &= (HH^T)\frac{1}{\sqrt{\lambda_i}}Hv_i \\ &= \frac{1}{\sqrt{\lambda_i}}H(H^TH)v_i \\ &= \frac{1}{\sqrt{\lambda_i}}H\lambda_i v_i = \sqrt{\lambda_i}Hv_i = \lambda_i u_i\end{aligned}$$
- Thus, (λ_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 HH^T

- Set $U = [u_1, u_2, \dots, u_n] \in \mathbb{R}^{m \times n}$
- $u_i = \frac{1}{\sqrt{\lambda_i}} Hv_i \Rightarrow U\Lambda^{1/2} = HV$
- $U^T U = (HV\Lambda^{-1/2})^T (HV\Lambda^{-1/2})$
 $= \Lambda^{-1/2} V^T (H^T H) V \Lambda^{-1/2}$
 $= \Lambda^{-1/2} V^T V \Lambda \Lambda^{-1/2}$
 $= I \text{ (because } V^T V = I\text{)}$
- Columns of U are orthonormal

SVD OF H

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

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

- $H = \sum_{i=1}^n \sqrt{\lambda_i} u_i v_i^T$
- λ_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

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

ALGORITHM - SVD

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

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

STEP 2: Compute $U^T Z$ – (rotation)

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

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

EXERCISES

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

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

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

- 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*