

3.2 QR Factorization

Topics: 1. Reduced QR factorization

3. Gram-Schmidt Orthogonalization

2. Full QR factorization

4. Solving $A\vec{x} = \vec{b}$ by QR factorization

1. Reduced QR factorization:

Suppose $A \in \mathbb{C}^{m \times n}$ ($m \geq n$), $A = [\vec{a}_1 | \dots | \vec{a}_n]$

successive spaces spanned by columns of A : $\langle \vec{a}_1 \rangle \subseteq \langle \vec{a}_1, \vec{a}_2 \rangle \subseteq \dots \subseteq \langle \vec{a}_1, \dots, \vec{a}_n \rangle$.

We want to find orthonormal vectors $\vec{q}_1, \dots, \vec{q}_n$ such that

$$\langle \vec{q}_1, \dots, \vec{q}_j \rangle = \langle \vec{a}_1, \dots, \vec{a}_j \rangle, \quad j=1, \dots, n$$

$$\text{i.e. } \underbrace{\begin{bmatrix} \vec{a}_1 & \dots & \vec{a}_n \end{bmatrix}}_A = \underbrace{\begin{bmatrix} \vec{q}_1 & \dots & \vec{q}_n \end{bmatrix}}_{\hat{Q}} \cdot \underbrace{\begin{bmatrix} r_{11} & \dots & r_{1n} \\ & \ddots & \\ & & r_{nn} \end{bmatrix}}_{\hat{R}}$$

$A = \hat{Q} \cdot \hat{R}$, where $\hat{Q} \in \mathbb{C}^{m \times n}$ has orthonormal columns } reduced QR factorization of A
 $\hat{R} \in \mathbb{C}^{n \times n}$ is upper triangular

2. Full QR factorization:

If we add $(m-n)$ orthonormal columns to \hat{Q} and $(m-n)$ zero rows to \hat{R} , then

$$\begin{matrix} \boxed{A}_{m \times n} = \boxed{\hat{Q}}_{m \times n} \boxed{\hat{R}}_{n \times n} \\ \text{(reduced QR factorization)} \end{matrix} \Rightarrow \begin{matrix} \boxed{A}_{m \times n} = \boxed{Q}_{m \times m} \boxed{R}_{m \times n} \\ \text{(full QR factorization)} \end{matrix}$$

$A = QR$, where $Q \in \mathbb{C}^{m \times m}$ unitary } full QR factorization
 $R \in \mathbb{C}^{m \times n}$ upper triangular

Remark: For $j = n+1, \dots, m$, $q_j \perp \text{range}(A)$

3. Gram-Schmidt Orthogonalization:

Goal: Find unit vector $\vec{q}_j \in \langle \vec{a}_1, \dots, \vec{a}_j \rangle$ that is orthogonal to $\langle \vec{q}_1, \dots, \vec{q}_{j-1} \rangle$.

$$\text{Let } \vec{v}_j = \vec{a}_j - \underbrace{(\vec{q}_1^* \vec{a}_j)}_{r_{1j}} \vec{q}_1 - \underbrace{(\vec{q}_2^* \vec{a}_j)}_{r_{2j}} \vec{q}_2 - \dots - \underbrace{(\vec{q}_{j-1}^* \vec{a}_j)}_{r_{j-1,j}} \vec{q}_{j-1}$$

then $(\vec{q}_k, \vec{v}_j) = 0$ for $k=1, \dots, j-1$, i.e. $\vec{v}_j \perp \langle \vec{q}_1, \dots, \vec{q}_{j-1} \rangle$ (verify).

Let $\vec{q}_j = \vec{v}_j / \|\vec{v}_j\|$, then $\{\vec{q}_1, \dots, \vec{q}_j\}$ orthonormal and $\langle \vec{q}_1, \dots, \vec{q}_j \rangle = \langle \vec{a}_1, \dots, \vec{a}_j \rangle$.

So the process is: $\vec{q}_1 = \vec{a}_1 / r_{11}$

$$\vec{q}_2 = (\vec{a}_2 - r_{12} \vec{q}_1) / r_{22}$$

$$\vec{q}_3 = (\vec{a}_3 - r_{13} \vec{q}_1 - r_{23} \vec{q}_2) / r_{33}$$

\vdots

$$\vec{q}_n = (\vec{a}_n - r_{1n} \vec{q}_1 - \dots - r_{n-1,n} \vec{q}_{n-1}) / r_{nn} = (\vec{a}_n - \sum_{i=1}^{n-1} r_{in} \vec{q}_i) / r_{nn}$$

where $r_{ij} = (\vec{q}_i^* \vec{a}_j)$ for $i=1, \dots, j-1$,

$$r_{jj} = \|\vec{a}_j - \sum_{i=1}^{j-1} r_{ij} \vec{q}_i\|_2.$$

Algorithm (Classical Gram-Schmidt Orthogonalization (unstable)):

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for j=1:n
    v_j = a_j
    for i=1:(j-1)
        [
            r_ij = q_i^* a_j
            v_j = v_j - r_ij q_i
        ]
    r_jj = ||v_j||_2
    q_j = v_j / r_jj

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Theorem (Existence and Uniqueness of QR factorization):

Every $A \in \mathbb{C}^{m \times n}$ ($m \geq n$) has a reduced QR factorization and a full QR factorization.

If A has full rank, then it has a unique reduced QR factorization with $r_{jj} > 0$.

4. Solving $A\vec{x} = \vec{b}$ by QR factorization:

$$A\vec{x} = \vec{b} \Rightarrow QR\vec{x} = \vec{b} \Rightarrow R\vec{x} = Q^* \vec{b}, \quad \text{upper triangular system}$$

step 1: Compute QR factorization: $A = QR$

step 2: compute $\vec{y} = Q^* \vec{b}$

step 3: Use backward substitution to solve $R\vec{x} = \vec{y}$

Remark: Gaussian Elimination (or LU) is generally used in practice, requiring only half # of flops.