QR Factorization by Householder Reflectors

November 13, 2018

Full QR Factorization

Given $A \in \mathbb{R}^{n \times p}$ with $n \geq p$,

$$A = QR$$

- $Q \in \mathbb{R}^{n \times n}$ is orthogonal,
- $R \in \mathbb{R}^{n \times p}$ is upper triangular

Approach

$$Q_n \dots Q_2 Q_1 A \quad = \quad R$$

- $Q_j \in \mathbb{R}^{n \times n}$ - (orthogonal and symmetric)
  Householder reflector to introduce 0 on the jth column below (j, j) entry.

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This will yield

$$A = \underbrace{Q_1 Q_2 \dots Q_n}_{Q} R.$$

Householder reflector Q achieving

$$v \quad \mapsto \quad \begin{bmatrix} x \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = -\textbf{sign}(v_1)\|v\|_2 e_1 = Qv$$

$$Q \quad = \quad I_n - 2qq^T, \qquad q \quad = \quad \frac{v + \textbf{sign}(v_1)\|v\|_2 e_1}{\|\, v + \textbf{sign}(v_1)\|v\|_2 e_1 \,\|_2}$$

kth step of the algorithm

$$A^{(k)} = \begin{bmatrix} x & & & x & \dots & x \\ & \ddots & & & & \\ & & x & x & & x \\ 0 & & 0 & \color{red}{x} & & \color{blue}{x} \\ 0 & & 0 & \color{blue}{x} & & \color{blue}{x} \\ & & \vdots & \color{blue}{\vdots} & & \color{blue}{\vdots} \\ 0 & & 0 & \color{blue}{x} & & \color{blue}{x} \end{bmatrix} \mapsto A^{(k+1)} = \underbrace{\begin{bmatrix} x & & & x & \dots & x \\ & \ddots & & & & \\ & & x & x & & x \\ 0 & & 0 & \color{red}{x} & & \color{blue}{x} \\ 0 & & 0 & \color{blue}{0} & & \color{blue}{x} \\ & & \vdots & \color{blue}{\vdots} & & \color{blue}{\vdots} \\ 0 & & 0 & \color{blue}{0} & & \color{blue}{x} \end{bmatrix}}_{Q_k A^{(k)}}$$

x - (k, k) entry

kth step of the algorithm

$$A^{(k)} = \begin{bmatrix} x & & & x & \dots & x \\ & \ddots & & & & \\ & & x & x & & x \\ 0 & & 0 & \color{red}{x} & & \color{blue}{x} \\ 0 & & 0 & \color{blue}{x} & & \color{blue}{x} \\ & & \vdots & \color{blue}{\vdots} & & \color{blue}{\vdots} \\ 0 & & 0 & \color{blue}{x} & & \color{blue}{x} \end{bmatrix} \mapsto A^{(k+1)} = \underbrace{\begin{bmatrix} x & & & x & \dots & x \\ & \ddots & & & & \\ & & x & x & & x \\ 0 & & 0 & \color{red}{x} & & \color{blue}{x} \\ 0 & & 0 & \color{blue}{0} & & \color{blue}{x} \\ & & \vdots & \color{blue}{\vdots} & & \color{blue}{\vdots} \\ 0 & & 0 & \color{blue}{0} & & \color{blue}{x} \end{bmatrix}}_{Q_k A^{(k)}}$$

$\color{red}{x}$ - $\color{red}{(k, k)}$ entry

Letting $v^{(k)} := A^{(k)}(k : n, k)$,

$$Q_k := \begin{bmatrix} I_{k-1} & 0 \\ 0 & I - 2q_k q_k^T \end{bmatrix}, \qquad q_k := \frac{v^{(k)} + \text{sign}(v_1^{(k)})\|v^{(k)}\|_2 e_1}{\left\| v^{(k)} + \text{sign}(v_1^{(k)})\|v^{(k)}\|_2 e_1 \right\|_2}$$

QR Factorization by Householder Reflectors

for $k = 1, \ldots, p$ **do**

  $v^{(k)} \leftarrow A(k : n, k)$

  $q_k \leftarrow \left\{ v^{(k)} + \text{sign}(v_1^{(k)}) \|v^{(k)}\|_2 e_1 \right\} / \left\{ \left\| v^{(k)} + \text{sign}(v_1^{(k)}) \|v^{(k)}\|_2 e_1 \right\|_2 \right\}$

  $A(k : n, k : p) \leftarrow A(k : n, k : p) - 2q_k(q_k^T A(k : n, k : p))$

end for

$R \leftarrow A$

QR Factorization by Householder Reflectors

for $k = 1, \ldots, p$ **do**

$\quad v^{(k)} \leftarrow A(k:n,k)$

$\quad q_k \leftarrow \left\{ v^{(k)} + \text{sign}(v_1^{(k)}) \|v^{(k)}\|_2 e_1 \right\} / \left\{ \left\| v^{(k)} + \text{sign}(v_1^{(k)}) \|v^{(k)}\|_2 e_1 \right\|_2 \right\}$

$\quad A(k:n, k:p) \leftarrow A(k:n, k:p) - 2q_k(q_k^T A(k:n, k:p))$

end for

$R \leftarrow A$

Now suppose $T \in \mathbb{R}^{n \times n}$ is tridiagonal.

$$Q_{n-1} \ldots Q_2 Q_1 T \quad = \quad R$$

- $Q_j \in \mathbb{R}^{n \times n}$ - (orthogonal)
  A plane rotator to make $(j+1, j)$ entry 0

Again this yields

$$T = \underbrace{Q_1^T Q_2^T \ldots Q_{n-1}^T}_{Q} R.$$

Illustration (3×3 case)

$$\underbrace{\begin{bmatrix} x & x & 0 \\ x & x & x \\ 0 & x & x \end{bmatrix}}_{T} \mapsto \underbrace{\begin{bmatrix} x & x & 0 \\ 0 & x & x \\ 0 & x & x \end{bmatrix}}_{R^{(12)}(\theta_1)T} \mapsto \underbrace{\begin{bmatrix} x & x & 0 \\ 0 & x & x \\ 0 & 0 & x \end{bmatrix}}_{R^{(23)}(\theta_2)R^{(12)}(\theta_1)T}$$

$$\begin{aligned} R^{(23)}(\theta_2)R^{(12)}(\theta_1)T &= R \\ T &= \underbrace{R^{(12)}(\theta_1)^T R^{(23)}(\theta_2)^T}_{Q} R \end{aligned}$$

kth step

$$A^{(k)} = \begin{bmatrix} x & x & & & \cdots & & \\ & \ddots & \ddots & & & & \\ & & x & x & & & \\ & & & x & x & & \\ & & & x & x & \ddots & \\ & & & & \ddots & \ddots & x \\ & & & & & x & x \end{bmatrix} \mapsto A^{(k+1)} = \underbrace{\begin{bmatrix} x & x & & & \cdots & & \\ & \ddots & \ddots & & & & \\ & & x & x & & & \\ & & & x & x & & \\ & & & 0 & x & \ddots & \\ & & & & \ddots & \ddots & x \\ & & & & & x & x \end{bmatrix}}_{R^{(k,k+1)}(\theta_k)A^{(k)}}$$

x - (k,k) entry

$$R^{(k,k+1)}(\theta_k) = \begin{bmatrix} I & & & \\ & c & s & \\ & -s & c & \\ & & & I \end{bmatrix}$$

Choose c, s so that

$$0 \;=\; a_{k+1,k}^{(k+1)} \;=\; -s a_{kk}^{(k)} + c a_{k+1,k}^{(k)},$$

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for instance, choose

$$s \;=\; \frac{a_{k+1,k}^{(k)}}{\rho}, \quad c \;=\; \frac{a_{kk}^{(k)}}{\rho} \quad \text{where} \quad \rho := \sqrt{\left[a_{kk}^{(k)}\right]^2 + \left[a_{k+1,k}^{(k)}\right]^2}$$

$$\begin{bmatrix} I & & & \\ & c & s & \\ & -s & c & \\ & & & I \end{bmatrix} A^{(k)} \quad = \quad A^{(k+1)}$$

$$\begin{aligned} a_{kk}^{(k+1)} &= c a_{kk}^{(k)} + s a_{k+1,k}^{(k)} \\ a_{k,k+1}^{(k+1)} &= c a_{k,k+1}^{(k)} + s a_{k+1,k+1}^{(k)} \\ a_{k+1,k+1}^{(k+1)} &= -s a_{k,k+1}^{(k)} + c a_{k+1,k+1}^{(k)} \end{aligned}$$

QR Factorization for a Tridiagonal Matrix by Rotators

for $k = 1, \ldots, n-1$ **do**

  $\rho \leftarrow \sqrt{a_{kk}^2 + a_{k+1,k}^2}, \quad s \leftarrow a_{k+1,k}/\rho, \quad c \leftarrow a_{kk}/\rho$

  $a_{kk} \leftarrow c a_{kk} + s a_{k+1,k}$

  $\widetilde{a}_{k,k+1} \leftarrow c a_{k,k+1} + s a_{k+1,k+1}$

  $a_{k+1,k+1} \leftarrow -s a_{k,k+1} + c a_{k+1,k+1}$

  $a_{k+1,k} \leftarrow 0$, $a_{k,k+1} \leftarrow \widetilde{a}_{k,k+1}$

end for

$R \leftarrow A$