QR Decomposition by Householder Reflectors

Householder Reflectors

Let $u \in \mathbb{R}^n \setminus \{0\}$ and $H = \{u\}^\perp$. Then

$$\mathbb{R}^n = \mathrm{span}\{u\} \oplus H.$$

For each $x \in \mathbb{R}^n$ there exists unique $a \in \mathbb{R}$ and $v \in H$ (satisfying $v^T u = 0$) such that

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Suppose $Q \in \mathbb{R}^{n \times n}$ such that $Qu = -u$ and $Qw = w$ for all $w \in H$. Then

$$Qx = -au + v$$

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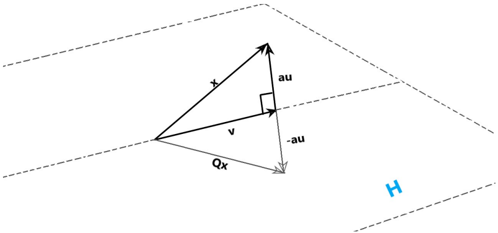

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Theorem Let $x, y \in \mathbb{R}^n$ such that $x \neq y$ and $\|x\|_2 = \|y\|_2$. Then there exists a unique Householder reflector $Q \in \mathbb{R}^{n \times n}$ such that $Qx = y$.

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Theorem Let $x, y \in \mathbb{R}^n$ such that $x \neq y$ and $\|x\|_2 = \|y\|_2$. Then there exists a unique Householder reflector $Q \in \mathbb{R}^{n\times n}$ such that $Qx = y$.

Proof: Since $\|x\|_2 = \|y\|_2$, $(x-y)^T(x+y) = 0$. Let $u = \frac{1}{2}(x-y)$. Then $u \neq 0$ as $x \neq y$ and $v := \frac{1}{2}(x+y) \in \{u\}^\perp$. Now $x = u + v$ and the reflector $Q = I - \frac{2}{\|u\|_2^2} uu^T$ is such that $Qx = -u + v = y$. $\square$

Creating zeroes in vectors by using Householder Reflectors

Corollary Let $x \in \mathbb{R}^n \setminus \{0\}$. There exists a Householder reflector $Q = I_n - \gamma u u^T \in \mathbb{R}^{n \times n}$ such that $Qx = [-\tau \, 0 \, \cdots \, 0]^T$ where $\tau = \|x\|_2$ or $-\|x\|_2$. Also γ, u and τ can be computed in $O(n)$ flops.

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Corollary Let $x \in \mathbb{R}^n \setminus \{0\}$. There exists a Householder reflector $Q = I_n - \gamma uu^T \in \mathbb{R}^{n \times n}$ such that $Qx = [-\tau \; 0 \; \cdots \; 0]^T$ where $\tau = \|x\|_2$ or $-\|x\|_2$. Also γ, u and τ can be computed in $O(n)$ flops.

Proof: Suppose $x = [x_1 \; \cdots \; x_n]^T$ and assume without loss of generality that $x_j \neq 0$ for some $j = 2, \ldots, n$. Let $y = [-\tau \; 0 \; \cdots \; 0]^T$ where $\tau = \mathrm{sign}(x_1)\|x\|_2$. The choice of the sign of τ avoids catastrophic cancellation in computing the first entry of $x - y$ wich is $x_1 + \tau$. As $x \neq y$ and $\|x\|_2 = \|y\|_2$, the Householder reflector $Q = I - \frac{2}{\|x-y\|_2^2}(x-y)(x-y)^T$ is such that $Qx = y$.

Suppose $u = \frac{1}{x_1+\tau}(x - y)$. Then $Q = I - \gamma uu^T$ where $\gamma = \frac{2}{\|u\|_2^2} = \frac{\tau + x_1}{\tau}$. Clearly, γ, u and τ can all be computed in $O(n)$ flops. $\square$

QR decomposition via Householder Reflectors

Let $A \in \mathbb{R}^{n \times m}$, $n \geq m$. Let Q_1 be a reflector such that

$$Q_1 A(:,1) = \begin{bmatrix} \pm\|A(:,1)\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Then,

$$Q_1 A = \underbrace{\begin{bmatrix} \pm\|A(:,1)\|_2 & a_{12}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & a_{22}^{(1)} & \cdots & a_{2m}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2}^{(1)} & \cdots & a_{nm}^{(1)} \end{bmatrix}}_{=:A_1}$$

QR Decomposition by Reflectors

Let $Q_2 = \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \underbrace{I_{n-1} - \frac{2}{\|u^{(2)}\|_2^2} u^{(2)} u^{(2)T}}_{:=\tilde{Q}_2} \end{array}\right]$ where

$Q_2 e_1 = e_1$

$Q_2(\alpha e_1) \quad \alpha e_1$

$$\tilde{Q}_2 A_1(2:n,2) = [\pm\|A_1(2:n,2)\|_2, 0, \cdots, 0]^T,$$

Then,

$$Q_2 A_1(:,2) = \begin{bmatrix} a_{12}^{(1)} \\ \pm\|A_1(2:n,2)\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

and

$$Q_2 A_1 = \underbrace{\begin{bmatrix} \pm\|A(:,1)\|_2 & a_{12}^{(1)} & a_{13}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & \pm\|A_1(2:n,2)\|_2 & a_{23}^{(2)} & \cdots & a_{2m}^{(2)} \\ 0 & 0 & a_{33}^{(2)} & \cdots & a_{3m}^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a_{n3}^{(2)} & \cdots & a_{nm}^{(2)} \end{bmatrix}}_{=:A_2}$$

QR Decomposition by Reflectors

$Q_i e_j = e_j \quad \forall j = 1, \dots, i-1$

Thus there exist reflectors

$$Q_i = \left[\begin{array}{c|c} I_{i-1} & 0 \\ \hline 0 & I_{n-i+1} - \frac{2}{\|u^{(i)}\|_2^2} u^{(i)} u^{(i)T} \end{array}\right], i = 1, 2, \dots, p,$$

(where $p = m$ if $n > m$ and $p = n - 1$ otherwise) such that

$$Q_p^T \cdots Q_2^T Q_1^T A = R \text{ is upper triangular}$$

Hence, $A = QR$ where $Q = Q_1 Q_2 \cdots Q_p$.

Flop count of computing the R of a QR Decomposition by Reflectors

Let $Q = I_n - \gamma uu^T$ be an $n \times n$ reflector and B be an $n \times m$ matrix. $W := QB = B - \gamma uu^T B$ may be computed in a number of ways.

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Bad idea :

$$\left(B - \left(\left((\gamma u)u^T\right) B\right)\right)$$

Find $v := \gamma u$. (Costs n flops)
Find $W := vu^T$. (Costs n^2 flops)
Find $G := WB$. (Costs $2n^2m$ flops)
Find $B - G$. (Cost nm flops)

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Find $B - G$. (Cost nm flops)

Total cost is $n^2(2m+1) + nm + n$ flops.

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But $W = B - \gamma u u^T B$ may also be computed as follows:

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Find $v := \gamma u$. (Costs n flops)
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Find $W := B - C$. (Costs nm flops)

Total cost is $4nm + n \approx 4nm$ flops.

Flop count of finding R of a QR Decomposition by Reflectors

Let $A \in \mathbb{R}^{n\times m}$, $n \geq m$. Finding reflector Q_1 such that

$$Q_1 A(:,1) = \begin{bmatrix} \pm\|A(:,1)\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

costs $O(n)$ flops.
Computing

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costs 4n(m-1) flops.

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Finding $Q_2 = \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \underbrace{I_{n-1} - \frac{2}{\|u^{(2)}\|_2^2} u^{(2)} u^{(2)T}}_{:=\tilde{Q}_2} \end{array}\right]$ such that

$$\tilde{Q}_2 A(2:n,2) = [\pm\|A(2:n,2)\|_2, 0, \cdots, 0]^T,$$

costs $O(n-1)$ flops. Computing,

$$Q_2 A_1 = \underbrace{\begin{bmatrix} \pm\|A(:,1)\|_2 & a_{12}^{(1)} & a_{13}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & \pm\|A_1(2:n,2)\|_2 & a_{23}^{(2)} & \cdots & a_{2m}^{(2)} \\ 0 & 0 & a_{33}^{(2)} & \cdots & a_{3m}^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a_{n3}^{(2)} & \cdots & a_{nm}^{(2)} \end{bmatrix}}_{=:A_2}$$

costs 4(n-1)(m-2) flops.

Flop count of finding R of a QR Decomposition by Reflectors

Setting $p = n - 1$ if $n = m$ and $p = m$ if $n > m$, the total costs of finding the p reflectors is

$$\Sigma_{k=1}^{p} O(n - k + 1) = \begin{cases} O(n^2) & \text{if } n = m, \\ O(nm) + O(m^2) & \text{if } n > m. \end{cases}$$

The cost of applying the p reflectors is $4\Sigma_{k=1}^{p}(n - k + 1)(m - k)$.

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Exercise: Show that the flop count of finding the R of a QR decomposition of $A \in \mathbb{R}^{n \times m}$ by reflectors is $2nm^2 - \frac{2}{3}m^3 + O(nm) + O(m^2)$ flops if $n > m$ and $\frac{4}{3}n^3 + O(n^2)$ flops if $n = m$.

Computing the Q of a Condensed QR decomposition via reflectors

Given $A \in \mathbb{R}^{n \times m}$, $n > m$, the flop count for finding the isometry Q of a condensed QR decomposition is equal to that of finding R if it is done efficiently.

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Let $\hat{Q}$ be the orthogonal matrix in the full QR decomposition of A. Then $\hat{Q} = Q_1 Q_2 \cdots Q_m$ and $Q = \left[\hat{Q} e_1 \cdots \hat{Q} e_m\right]$.

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$$Q_i = \left[\begin{array}{c|c} I_{i-1} & 0 \\ \hline 0 & I_{n-i+1} - \frac{2}{\|u^{(i)}\|_2^2} u^{(i)} u^{(i)T} \end{array}\right], i = 1, 2, \ldots, p,$$

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which is equal to that of computing R.

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Exercise: Prove that finding a QR decomposition of $A \in \mathbb{R}^{n \times n}$ costs $(8n^3)/3 + O(n^2)$ flops.

Practice exercises

Exercise: Let A be a $n \times n$ nonsingular real or complex matrix. Prove the following.

1. A has a unique QR decomposition such the diagonal entries of R are positive.
2. If $A = Q_1 R_1$ and $A = Q_2 R_2$ be two QR decompositions of A, and $A_1 := Q_1^* A Q_1,$ and $A_2 := Q_2^* A Q_2$, then there exists a unitary diagonal matrix D, such that $A_2 = D^* A_1 D$.

Solve all problems on pages 206-210 and pages 236-239 of *Fundamentals of Matrix Computations,* by D. S. Watkins, (2nd edition).