Numerical Analysis Hilary Term 2024
Lecture 3: QR Factorization

Definition: a square real matrix Q is **orthogonal** if $Q^{\mathrm{T}} = Q^{-1}$. This is true if, and only if, $Q^{\mathrm{T}}Q = I = QQ^{\mathrm{T}}$.

Example: the permutation matrices P in LU factorization with partial pivoting are orthogonal.

Proposition. The product of orthogonal matrices is an orthogonal matrix.

Proof. If S and T are orthogonal, $(ST)^{\mathrm{T}} = T^{\mathrm{T}}S^{\mathrm{T}}$ so

$$(ST)^{\mathrm{T}}(ST) = T^{\mathrm{T}}S^{\mathrm{T}}ST = T^{\mathrm{T}}(S^{\mathrm{T}}S)T = T^{\mathrm{T}}T = I.$$

Definition: The **scalar (dot)(inner) product** of two vectors

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad \text{and} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

in $\mathbb{R}^n$ is

$$x^{\mathrm{T}}y = y^{\mathrm{T}}x = \sum_{i=1}^{n} x_i y_i \in \mathbb{R}$$

Definition: Two vectors $x,\ y \in \mathbb{R}^n$ are **orthogonal** if $x^{\mathrm{T}}y = 0$. A set of vectors $\{u_1, u_2, \ldots, u_r\}$ is an **orthogonal set** if $u_i^{\mathrm{T}}u_j = 0$ for all $i, j \in \{1, 2, \ldots, r\}$ such that $i \neq j$.

Lemma. The columns of an orthogonal matrix Q form an orthogonal set, which is moreover an orthonormal basis for $\mathbb{R}^n$.

Proof. Suppose that $Q = [q_1 \;\; q_2 \;\; \cdots \;\; q_n]$, i.e., q_j is the jth column of Q. Then

$$Q^{\mathrm{T}}Q = I = \begin{bmatrix} q_1^{\mathrm{T}} \\ q_2^{\mathrm{T}} \\ \vdots \\ q_n^{\mathrm{T}} \end{bmatrix} [q_1 \;\; q_2 \;\; \cdots \;\; q_n] = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}.$$

Comparing the (i, j)th entries yields

$$q_i^{\mathrm{T}}q_j = \begin{cases} 0 & i \neq j \\ 1 & i = j. \end{cases}$$

Note that the columns of an orthogonal matrix are of length 1 as $q_i^{\mathrm{T}}q_i = 1$, so they form an orthonormal.

To see that it forms a basis, let $x \in \mathbb{R}^n$ be any vector. One has $x = QQ^T x = Qc$ where $c = Q^T x$, so $x = \sum_{i=1}^n c_i q_i$.

Lemma. If $u \in \mathbb{R}^n$, P is n-by-n orthogonal and $v = Pu$, then $u^{\mathrm{T}}u = v^{\mathrm{T}}v$.

Proof. $v^{\mathrm{T}}v = (Pu)^{\mathrm{T}}(Pu) = (u^{\mathrm{T}}P^{\mathrm{T}})(Pu) = u^{\mathrm{T}}(P^{\mathrm{T}}P)u = u^{\mathrm{T}}u$.

Definition: The **outer product** of two vectors x and $y \in \mathbb{R}^n$ is

$$xy^{\mathrm{T}} = \begin{bmatrix} x_1y_1 & x_1y_2 & \cdots & x_1y_n \\ x_2y_1 & x_2y_2 & \cdots & x_2y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_ny_1 & x_ny_2 & \cdots & x_ny_n \end{bmatrix},$$

an n-by-n matrix (notation: $xy^{\mathrm{T}} \in \mathbb{R}^{n\times n}$). More usefully, if $z \in \mathbb{R}^n$, then

$$(xy^{\mathrm{T}})z = xy^{\mathrm{T}}z = x(y^{\mathrm{T}}z) = \left(\sum_{i=1}^n y_i z_i\right) x.$$

Definition: For $w \in \mathbb{R}^n$, $w \neq 0$, the **Householder** reflector $H(w) \in \mathbb{R}^{n\times n}$ is the matrix

$$H(w) = I - \frac{2}{w^{\mathrm{T}}w} ww^{\mathrm{T}}.$$

Proposition. $H(w)$ is a symmetric orthogonal matrix.

Proof.

Symmetry is straightforward to verify. For orthogonality,

$$\begin{aligned} H(w)H(w)^{\mathrm{T}} &= \left(I - \frac{2}{w^{\mathrm{T}}w} ww^{\mathrm{T}}\right)\left(I - \frac{2}{w^{\mathrm{T}}w} ww^{\mathrm{T}}\right) \\ &= I - \frac{4}{w^{\mathrm{T}}w} ww^{\mathrm{T}} + \frac{4}{(w^{\mathrm{T}}w)^2} w(w^{\mathrm{T}}w)w^{\mathrm{T}} \\ &= I. \end{aligned}$$

□

Lemma. Given $u \in \mathbb{R}^n$, there exists a $w \in \mathbb{R}^n$ such that

$$H(w)u = \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix} \equiv v,$$

say, where $\alpha = \pm\sqrt{u^{\mathrm{T}}u}$.

Remark: Since $H(w)$ is an orthogonal matrix for any $w \in \mathbb{R}$, $w \neq 0$, it is necessary for the validity of the equality $H(w)u = v$ that $v^{\mathrm{T}}v = u^{\mathrm{T}}u$, i.e., $\alpha^2 = u^{\mathrm{T}}u$; hence our choice of $\alpha = \pm\sqrt{u^{\mathrm{T}}u}$.

Proof. Take $w = \gamma(u - v)$, where $\gamma \neq 0$. Recall that $u^{\mathrm{T}}u = v^{\mathrm{T}}v$. Thus,

$$\begin{aligned} w^{\mathrm{T}}w &= \gamma^2(u-v)^{\mathrm{T}}(u-v) = \gamma^2(u^{\mathrm{T}}u - 2u^{\mathrm{T}}v + v^{\mathrm{T}}v) \\ &= \gamma^2(u^{\mathrm{T}}u - 2u^{\mathrm{T}}v + u^{\mathrm{T}}u) = 2\gamma u^{\mathrm{T}}(\gamma(u-v)) \\ &= 2\gamma w^{\mathrm{T}}u. \end{aligned}$$

So

$$H(w)u = \left(I - \frac{2}{w^{\mathrm{T}}w}ww^{\mathrm{T}}\right)u = u - \frac{2w^{\mathrm{T}}u}{w^{\mathrm{T}}w}w = u - \frac{1}{\gamma}w = u - (u - v) = v.$$

□

Now if u is the first column of the n-by-n matrix A,

$$H(w)A = \left[\begin{array}{c|ccc} \alpha & \times & \cdots & \times \\ \hline 0 & & & \\ \vdots & & B & \\ 0 & & & \end{array}\right], \quad \text{where } \times = \text{general entry.}$$

Similarly for B, we can find $\hat{w} \in \mathbb{R}^{n-1}$ such that

$$H(\hat{w})B = \left[\begin{array}{c|ccc} \beta & \times & \cdots & \times \\ \hline 0 & & & \\ \vdots & & C & \\ 0 & & & \end{array}\right]$$

and then

$$\left[\begin{array}{c|ccc} 1 & 0 & \cdots & 0 \\ \hline 0 & & & \\ \vdots & & H(\hat{w}) & \\ 0 & & & \end{array}\right] H(w)A = \left[\begin{array}{cc|ccc} \alpha & \times & \times & \cdots & \times \\ 0 & \beta & \times & \cdots & \times \\ \hline 0 & 0 & & & \\ 0 & 0 & & & \\ \vdots & \vdots & & C & \\ 0 & 0 & & & \end{array}\right].$$

Note

$$\begin{bmatrix} 1 & 0 \\ 0 & H(\hat{w}) \end{bmatrix} = H(w_2), \quad \text{where } w_2 = \begin{bmatrix} 0 \\ \hat{w} \end{bmatrix}.$$

Thus if we continue in this manner for the $n-1$ steps, we obtain

$$\underbrace{H(w_{n-1})\cdots H(w_3)H(w_2)H(w)}_{Q^{\mathrm{T}}}A = \begin{bmatrix} \alpha & \times & \cdots & \times \\ 0 & \beta & \cdots & \times \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \gamma \end{bmatrix} = (\,\urcorner\,).$$

The matrix Q^{T} is orthogonal as it is the product of orthogonal (Householder) matrices, so we have constructively proved that

Theorem. Given any square matrix A, there exists an orthogonal matrix Q and an upper triangular matrix R such that

$$A = QR$$

Notes: 1. This could also be established using the Gram–Schmidt Process.
2. If u is already of the form $(\alpha,\ 0,\ \cdots,\ 0)^{\mathrm{T}}$, we just take $H = I$.
3. Householder reflectors can be applied to a vector in $O(n^2)$ flops; $4n^2$ to be precise. To

see this, note that $Hv = (I - 2ww^T)v = v - 2w(w^Tv)$. Using this, the QR factorisation can be computed in $O(n^3)$ flops. 4. It is not necessary that A is square: if $A \in \mathbb{R}^{m\times n}$, then we need the product of (a) $m - 1$ Householder matrices if $m \le n \Longrightarrow$

$$(\square) = A = QR = (\square)(\urcorner)$$

or (b) n Householder matrices if $m > n \Longrightarrow$

$$\left(\square\right) = A = QR = \left(\square\right)\left(\urcorner\right). \tag{1}$$

This $m > n$ case is particular important, and we note that one can also write

$$\left(\square\right) = A = QR = \left(\square\right)(\urcorner).$$

This is called the *thin* QR factorization, wherein $Q \in \mathbb{R}^{m\times n}$ has orthonormal columns and has the same size as A; by contrast, in (1) Q is square orthogonal, and (1) is called the *full* QR.