$\vec{u}$ is stored over x.

$\beta \leftarrow \max_{1 \le i \le n} |x_i|$
if $\beta = 0$
  then $\gamma \leftarrow 0$
else
  $x \leftarrow x/\beta$ (vector divided by β)
  $\tau \leftarrow \sqrt{x_1^2 + x_2^2 + \dots x_n^2}$
  if $(x_1 < 0)$ $\tau \leftarrow -\tau$
    $x_1 \leftarrow \tau + x_1$
    $\gamma \leftarrow x_1/\tau$
    $x(1 \text{ to } n-1) \leftarrow \frac{x(1 \text{ to } n-1)}{x_1}$
    $x_1 \leftarrow 1$
    $\tau \leftarrow \tau\beta$

Cancellation cannot occur

$x_1^2 + x_2^2 + \dots x_n^2$ involves only positive numbers.

Cancellation does not occur sum $\tau + x_1$.

Therefore, τ, γ, and u are accurate.

Many algorithms, that use QR decomposition, do not calculate Q explicitly.

It suffices to save γ and u.

When reflectors are used to compute the QR-decomposition we need to multiply each reflector Q by a matrix that is a submatrix of the matrix going under the transformation.

Suppose $Q \in \mathbb{R}^{n \times n}$
and $B \in \mathbb{R}^{n \times m}$

then $QB = (I - \gamma u u^T) B = B - \gamma u u^T B$.

So our main focus $\gamma u u^T B$.

There are "good" ways and "bad" ways to do this.

The first good thing we can do is absorb the scalar γ into one of the vectors.

- Let $v^T = \gamma u^T$

so that $QB = B - u v^T B$

* Let $v' = \gamma u'$
so that $QB = B - uv^T B$

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* See exercise online (Exercise 3.2.37)

$B - u(v^T B)$

Algorithm to calculate QB and store it over B, where $B \in \mathbb{R}^{n \times m}$ and $Q = I - \gamma u u^T$. An auxillary $v \in \mathbb{R}^n$

$$v^T \leftarrow \gamma u^T$$
$$v^T \leftarrow v^T B$$
$$B \leftarrow B - u v^T$$

The total flop count is about $4nm$. which should significantly less than multiplying QB with "normal" matrix multiplication.

This saving of flop count, because Q is rank-one update of the identity.

Theorem (QR-decomposition with reflectors)

(Proof by induction on n)

Let $n = 1$ take $Q = [1]$ and $R = [a_{11}]$

then $A = QR$.

Now take an arbitrary $n \geq 2$

Show theorem holds for an n by n matrix if it holds for $(n-1)$ by $(n-1)$ matrices.

Let $Q_1 \in \mathbb{R}^{n \times n}$ be a reflector that creates zeros in the first column of A.

Creates zeros in the first column of A.

$$Q_1 \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{bmatrix} = \begin{bmatrix} -\tau_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Recall Q_1 is symmetric

$$Q_1^T A = Q_1 A = \left[\begin{array}{c|ccc} -\tau_1 & \hat{a}_{12} & \cdots & \hat{a}_{1n} \\ \hline 0 & & & \\ \vdots & & \hat{A}_2 & \\ 0 & & & \end{array}\right]$$

By the induction hypothesis $\hat{A}_2$ has a QR-decomposition $\hat{A}_2 = \hat{Q}_2 \hat{R}_2$ where $\hat{Q}_2$ is orthogonal and $\hat{R}_2$ is upper triangular.

$\tilde{Q}_2 \in \mathbb{R}^{n \times n}$

Define
$$\tilde{Q}_2 = \left[\begin{array}{c|ccc} 1 & 0 & \cdots & 0 \\ \hline 0 & & & \\ \vdots & & \hat{Q}_2 & \\ 0 & & & \end{array}\right]$$

$\tilde{Q}_2$ is orthogonal

and
$$R = \tilde{Q}_2^T Q_1^T A = \left[\begin{array}{c|ccc} 1 & 0 & \cdots & 0 \\ \hline 0 & & & \\ \vdots & & \hat{Q}_2^T & \\ 0 & & & \end{array}\right] \left[\begin{array}{c|ccc} -\tau_1 & \hat{a}_{12} & \cdots & \hat{a}_{1n} \\ \hline 0 & & & \\ \vdots & & \hat{A}_2 & \\ 0 & & & \end{array}\right]$$

$$= \left[\begin{array}{c|ccc} -\tau_1 & \hat{a}_{12} & \cdots & \hat{a}_{1n} \\ \hline 0 & & & \\ \vdots & & \hat{R}_2 & \\ 0 & & & \end{array}\right]$$

This matrix is upper triangular

Let $Q = Q_1 \tilde{Q}_2$ then Q is orthogonal and $Q^T A = R$. Therefore

$$A = QR.$$

Step 1 $\quad Q_1 = I - \gamma_1 u^{(1)} u^{(1)T}$

Step 1 $\quad Q_1 = I - \gamma_1 u^{(1)} u^{(1)T}$

then $Q_1 \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{bmatrix} = \begin{bmatrix} \tau_1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$

as noted it suffices to only store $\gamma_1, -\tau_1, u_i^{(1)}$

$$A \to R_1 = \left[\begin{array}{c|ccc} \tau_1 & \hat{a}_{21} & \cdots & \hat{a}_{n1} \\ \hline 0 & & & \\ \vdots & & \hat{A}_2 & \\ 0 & & & \end{array}\right]$$

we could store $-\tau_1$ in the first position

$u^{(1)}$ stored in first column because $u_1^{(1)}$

the rest of $u^{(1)}$ is first column of A divided by $\tau_1 + a_{11}$.

The rest of A can be transformed as indicated above since $m = n-1$ columns are involved

the total flop count of step 1 is about $4n^2$.

need $\hat{A}_2$ upper triangular.

follow outline of step 1

$$\left[\begin{array}{c|ccc} -\tau_2 & \hat{a}_{23} & -- & \hat{a}_{2n} \\ \hline 0 & & & \\ \vdots & & \hat{A}_3 & \end{array}\right]$$

once again store $u^{(2)}$ in first column.

cost for this step is $4(n-1)^2$ flops

(process identical to step 1 except it performed on $(n-1)\times(n-1)$ matrix)

Step 3 $\quad 4(n-2)^2$ flops

After $n-1$ steps

A has been transformed to upper triangular

$u^{(1)}, \dots u^{(n-1)}$

The array that held A now holds R.

Another array holds $\gamma_1, \dots \gamma_{n-1}$

$R = Q_{n-1} Q_{n-2} \cdots Q_1 A$ where $Q_1 = I - \gamma u^{(1)} u^{(1)T}$

$$Q_2 = \left[\begin{array}{c|c} 1 & 0 \cdots 0 \\ \hline 0 & \\ \vdots & I - \gamma_2 u^{(2)} u^{(2)T} \\ 0 & \end{array}\right]$$

in general

$$Q_i = \left[\begin{array}{c|c} I_{i-1} & 0 \\ \hline 0 & I - \gamma_i u^{(i)} u^{(i)T} \end{array}\right]$$

$$Q = Q_1 Q_2 Q_3 \cdots Q_{n-1}.$$

$$Q^T = Q_{n-1}^T Q_{n-2}^T \cdots Q_1^T$$

$$R = Q^T A$$

and thus $A = QR$

Algorithm to calculate QR decomposition of $A \in \mathbb{R}^{n \times n}$ using reflectors

for $k = 1 \dots n-1$

Determine a reflector $Q_k = I - \gamma_k u^{(k)} u^{(k)T}$ such that

$$Q_k \begin{bmatrix} a_{kk} \\ \vdots \\ a_{nk} \end{bmatrix} = \begin{bmatrix} -\tau_k \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

store $u^{(k)}$ over $a_{k:n,k}$

$a_{k:n,k+1:n} \leftarrow Q_k a_{k:n,k+1:n}$ (transforming values of A to get R)

$a_{kk} \leftarrow \tau_k$

$a_{k:n,k+1:n} \leftarrow Q_k a_{k:n,k+1:n}$ (transforming values of A to get R)

$a_{kk} \leftarrow \tau_k$

$r_n \leftarrow a_{nn}$

Uniqueness of the QR-decomposition

Theorem Let $A \in \mathbb{R}^{n \times n}$ be non singular, then there exists unique $Q, R \in \mathbb{R}^{n \times n}$ such that Q is orthogonal, R is upper triangular with positive main diagonal entries, and $A = QR$

By previous theorems $A = \hat{Q}\hat{R}$ where $\hat{Q}$ is ortogonal and $\hat{R}$ is upper triangular but does not necessarily have positive main diagonal entries

Since A is nonsingular, $\hat{R}$ must also be nonsingular

So the main-diagonal entries are non-zero

Let D be the diagonal matrix given by

$$d_{ii} = \begin{cases} 1 & \text{if } \hat{r}_{ii} > 0 \\ -1 & \text{if } \hat{r}_{ii} < 0 \end{cases}$$

Then $D = D^T = D^{-1}$ is orthogonal.

Let $Q = \hat{Q} D^{-1}$ and $R = D\hat{R}$

Then Q is orthogonal, R is upper triangular with $r_{ii} = d_{ii}\hat{r}_{ii} > 0$ and $A = QR$.

This establishes existence,

with $r_{11} = \ldots > 0$ and ...

This establishes existence.

There are various to show uniqueness

suppose $A = Q_1 R_1 = Q_2 R_2$ where Q_1 Q_2 orthogonal

R_1, R_2 upper triangular with positive main diagonal entries

$A^T A$ is a positive definite matrix

and $A^T A = (Q_1R_1)^T Q_1 R_1 = R_1^T \underbrace{Q_1^T Q_1}_{} R_1 = R_1^T R_1$

(since $Q_1^T Q_1 = I$)

Thus R_1 is a cholesky factor of $A^T A$

Same applies to R_2

But we argued previously the uniqueness of Cholesky decomposition.

So $R_1 = R_2$ and $Q_1 = A R_1^{-1} = A R_2^{-1} = Q_2$.

The Complex Case

Inner product on $\mathbb{C}^n$ is defined by

$$\langle x, y \rangle = \sum_{i=1}^{n} x_i \overline{y_i} \qquad x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \text{ and } y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

Exercise Show that the inner product of $\mathbb{C}^n$ satisfies the following properties

(a) $\langle x, y \rangle = \overline{\langle y, x \rangle}$

(b) $\langle \alpha_1 x_1 + \alpha_2 x_2, y \rangle = \alpha_1 \langle x_1, y \rangle + \alpha_2 \langle x_2, y \rangle$

(c) $\langle x, \alpha_1 y_1 + \alpha_2 y_2 \rangle = \overline{\alpha_1} \langle x, y_1 \rangle + \overline{\alpha_2} \langle x, y_2 \rangle$

(d) $\langle x, x \rangle$ is real, $\langle x, x \rangle \geq 0$ and

(d) $\langle x, x\rangle$ is real, $\langle x, x\rangle \geq 0$ and

$\langle x, x\rangle = 0$ if and only if $x = 0$.

(e) $\sqrt{\langle x, x\rangle} = \|x\|_2$

Complex analogues of orthogonal matrices are unitary matrices.

> A matrix $U \in \mathbb{C}^{n\times n}$ is <u>unitary</u> if $UU^* = I$, where U^* is the conjugate transpose of U.

Equivalent statements to above are:

$$U^*U = I$$

$$U^* = U^{-1}$$

<u>Exercise</u> (complex rotators) $\begin{bmatrix} a \\ b \end{bmatrix} \in \mathbb{C}^2$

define $U \in \mathbb{C}^{2\times 2}$ by

$$U = \frac{1}{\gamma}\begin{bmatrix} a & -\bar{b} \\ b & \bar{a} \end{bmatrix} \quad \text{where } \gamma = \sqrt{|a|^2 + |b|^2}$$

verify that

(a) U is unitary

(b) $\det(U) = 1$

(c) $U^*\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \gamma \\ 0 \end{bmatrix}$.

Exercise (complex reflectors) Let $u \in \mathbb{C}^n$ with $\|u\|_2 = 1$ and define $Q \in \mathbb{C}^{n \times n}$ by $Q = I - 2uu^*$ verify that

(a) $Qu = -u$

(b) $Qv = v$ if $\langle u, v \rangle = 0$

(c) $Q = Q^*$ (Q is Hermitian)

(d) $Q^* = Q^{-1}$ (Q is unitary)

(e) $Q^{-1} = Q$ (Q is an involution)

Solution of least squares problem

Consider an overdetermined system

$$Ax = b, \quad A \in \mathbb{R}^{n \times m}, \quad b \in \mathbb{R}^n, \quad n > m$$