Transformation to Upper Hessenberg form

Theorem 3 Given any matrix $A \in \mathbb{R}^{n \times n}$, there exists an orthogonal matrix Q and an upper Hessenberg matrix H such that $Q^T AQ = H$. If $A^T = A$, then, H is a symmetric tridiagonal matrix.

If $A \in \mathbb{C}^{n \times n}$, then there exists a unitary matrix Q such that $Q^* AQ = H$. In such a case if $A^* = A$, then H is a Hermitian tridiagonal matrix.

Transformation to Upper Hessenberg form: General Matrices

Step 1:

Partition $A \in \mathbb{R}^{n \times n}$ as $A = \begin{bmatrix} a_{11} & c^T \\ b & \hat{A} \end{bmatrix}$.

Let $\hat{Q}_1$ be a real $n-1 \times n-1$ reflector such that $\hat{Q}_1 b = [\pm\|b\|_2\, 0 \cdots 0]^T$ and

$$Q_1 = \begin{bmatrix} 1 & 0^T \\ 0 & \hat{Q}_1 \end{bmatrix}.$$

Let $A_{\frac{1}{2}} := Q_1 A = \left[\begin{array}{c|c} a_{11} & c^T \\ \hline \pm\|b\|_2 & \\ 0 & \\ \vdots & \hat{Q}_1 \hat{A} \\ 0 & \end{array}\right]$ (costs $4(n-1)^2$ flops.)

Transformation to Upper Hessenberg form: General Matrices

Recalling that $Q_1^{-1} = Q_1^* = Q_1$, let

$$A_1 := A_{\frac{1}{2}} Q_1 = \left[\begin{array}{c|c} a_{11} & c^T \hat{Q}_1 \\ \hline \pm\|b\|_2 & \\ 0 & \\ \vdots & \hat{Q}_1 \hat{A} \hat{Q}_1 \\ 0 & \end{array}\right] \quad \text{(costs } 4n(n-1) \text{ flops)}$$

$$= \left[\begin{array}{c|ccc} a_{11} & * & \cdots & * \\ \pm\|b\|_2 & & & \\ 0 & & & \\ \vdots & & \hat{A}_1 & \\ 0 & & & \end{array}\right].$$

Transformation to Upper Hessenberg form: General Matrices

Step 2: Let $Q_2 = \left[\begin{array}{cc|ccc} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \hline 0 & 0 & & & \\ \vdots & \vdots & & \hat{Q}_2 & \\ 0 & 0 & & & \end{array}\right]$, where $\hat{Q}_2$ is an $n-2 \times n-2$ reflector such that $\hat{Q}_2 \hat{b} = [\pm\|\hat{b}\|_2 \, 0 \cdots 0]^T$ where $\hat{b} = \hat{A}_1(2:n, 1)$. Then,

$$A_{\frac{3}{2}} := Q_2 A_1 = \left[\begin{array}{c|c|ccc} a_{11} & * & * & \cdots & * \\ \hline \pm\|b\|_2 & * & * & \cdots & * \\ \hline 0 & \pm\|\hat{b}\|_2 & & & \\ \vdots & \vdots & & \hat{Q}_2 \hat{A}_2 & \\ 0 & 0 & & & \end{array}\right].$$

(costs $4(n-2)^2$ flops)

Transformation to Upper Hessenberg form: General Matrices

and

$$A_2 := A_{\frac{3}{2}} Q_2 = \left[\begin{array}{c|c|ccc} a_{11} & * & * & \cdots & * \\ \hline \pm\|b\|_2 & * & * & \cdots & * \\ \hline 0 & \pm\|\hat{b}\|_2 & & & \\ \vdots & \vdots & & \hat{Q}_2 \hat{A}_2 \hat{Q}_2 & \\ 0 & 0 & & & \end{array}\right].$$

(costs $4n(n-2)$ flops)

After $n-2$ steps the process is complete and $Q^* A Q = H$ where H is upper Hessenberg and $Q = Q_1 Q_2 \cdots Q_{n-2}$ is an orthogonal matrix.

(costs $10n^3/3 + O(n^2)$ flops)

Transformation to Upper Hessenberg form: Symmetric Matrices

Suppose that A is an $n \times n$ real symmetric matrix. Then it may be partitioned as

$$A = \begin{bmatrix} a_{11} & b^T \\ b & \hat{A} \end{bmatrix}.$$

In **Step 1** A is transformed to $A_1 = Q_1 A Q_1$ where $Q_1 = \begin{bmatrix} 1 & 0 \\ 0 & \hat{Q}_1 \end{bmatrix}$ and

$$\begin{aligned} A_1 &= \left[\begin{array}{c|c} a_{11} & b^T \hat{Q}_1 \\ \hline \hat{Q}_1 b & \hat{Q}_1 \hat{A} \hat{Q}_1 \end{array}\right] \\ &= \left[\begin{array}{c|cccc} a_{11} & \pm\|b\|_2 & 0 & \cdots & 0 \\ \pm\|b\|_2 & & & & \\ 0 & & & & \\ \vdots & & & \hat{A}_1 & \\ 0 & & & & \end{array}\right]. \end{aligned}$$

Transformation to Upper Hessenberg form: Symmetric Matrices

Since $\hat{Q}_1$ is a reflector, it is of the form $\hat{Q}_1 = I - \gamma u u^T$. Thus,

$$
\begin{aligned}
\hat{A}_1 &= (I - \gamma u u^T)\hat{A}(I - \gamma u u^T) \\
&= \hat{A} - \gamma \hat{A} u u^T - \gamma u u^T \hat{A} + \gamma^2 u u^T \hat{A} u u^T \\
&= \hat{A} + v u^T + u v^T + 2\alpha u u^T \\
& \left(\text{where} \quad \underbrace{v := -\gamma \hat{A} u}_{\text{costs } 2(n-1)^2+n-1 \text{ flops}} \quad \& \ \underbrace{\alpha := -(\gamma(u^T v))/2}_{\text{costs } 3(n-1)+1 \text{ flops}} \right) \\
&= \hat{A} + w u^T + u w^T, \quad \text{where } w := v + \alpha u \text{ (costs } 2(n-1) \text{ flops)}
\end{aligned}
$$

Therefore, $\hat{A}_1(i,j) \leftarrow \underbrace{\hat{A}(i,j) + w_i u_j + u_i w_j}_{\text{costs 4 flops}}, \ 2 \le j \le n, j \le i \le n,$

and the total cost of finding $\hat{A}_1$ and hence A_1 is $4n^2 + O(n)$ flops.

Transformation to Upper Hessenberg form: Symmetric Matrices

Since $\hat{Q}_1$ is a reflector, it is of the form $\hat{Q}_1 = I - \gamma uu^T$. Thus,

$$\begin{aligned}
\hat{A}_1 &= (I - \gamma uu^T)\hat{A}(I - \gamma uu^T) \\
&= \hat{A} - \gamma \hat{A}uu^T - \gamma uu^T\hat{A} + \gamma^2 uu^T\hat{A}uu^T \\
&= \hat{A} + vu^T + uv^T + 2\alpha uu^T \\
& \left(\text{where} \quad \underbrace{v := -\gamma\hat{A}u}_{\text{costs } 2(n-1)^2+n-1 \text{ flops}} \quad \& \quad \underbrace{\alpha := -(\gamma(u^Tv))/2}_{\text{costs } 3(n-1)+1 \text{ flops}} \right) \\
&= \hat{A} + wu^T + uw^T, \quad \text{where } w := v + \alpha u \text{ (costs } 2(n-1) \text{ flops)}
\end{aligned}$$

Therefore, $\hat{A}_1(i,j) \leftarrow \underbrace{\hat{A}(i,j) + w_iu_j + u_iw_j}_{\text{costs 4 flops}}$, $2 \le j \le n, j \le i \le n$,

and the total cost of finding $\hat{A}_1$ and hence A_1 is $4n^2 + O(n)$ flops.

Thus the total flop count of the orthogonal similarity transformation of A to upper Hessenberg (and hence symmetric tridiagonal) form is

$$4\sum_{k=1}^{n-1}(n-k+1)^2 + O(n) = 4n^3/3 + O(n^2) \text{ flops} .$$