Numerical Analysis – Lecture 8[1]

Theorem 2.22 *(The first column of A_{k+1}). Let the conditions of Property 2.21 be satisfied and suppose that the QR algorithm calculates the sequence $\{A_k\ :\ k=0,1,2,\ldots\}$. Then, as $k\to\infty$, the first column of A_{k+1} tends to $\lambda_l \boldsymbol{e}_1$, rendering A_{k+1} suitable for deflation.*

Proof In the notation of Lemma 2.20, the first column of A_{k+1} is $\bar{Q}_k^\top A\bar{Q}_k\boldsymbol{e}_1$. Further, using Property 2.21, we deduce that

$$A_{k+1}\boldsymbol{e}_1=\bar{Q}_k^\top A\bar{Q}_k\boldsymbol{e}_1=\bar{Q}_k^\top A\bar{\boldsymbol{q}}_{k+1}=\bar{Q}_k^\top A(\pm\boldsymbol{w}_l+\boldsymbol{h}_{k+1}).$$

Since $A\boldsymbol{w}_l=\lambda_l\boldsymbol{w}_l$, we conclude that

$$\begin{aligned}A_{k+1}\boldsymbol{e}_1&=\pm\lambda_l\bar{Q}_k^\top\boldsymbol{w}_l+\bar{Q}_k^\top A\boldsymbol{h}_{k+1}=\lambda_l\bar{Q}_k^\top(\bar{\boldsymbol{q}}_{k+1}-\boldsymbol{h}_{k+1})+\bar{Q}_k^\top A\boldsymbol{h}_{k+1}\\&=\lambda_l\boldsymbol{e}_1+\bar{Q}_k^\top(A-\lambda_l I)\boldsymbol{h}_{k+1},\end{aligned}$$

since $\bar{Q}_k^\top\bar{\boldsymbol{q}}_{k+1}=\boldsymbol{e}_1$ follows from orthogonality of $\bar{Q}_k^\top$. The theorem follows from $\boldsymbol{h}_{k+1}\to\boldsymbol{0}$. □

Remark 2.23 (Relation between QR and inverse iteration). In practice, the statement of Theorem 2.22 is hardly ever important, because usually, as $k\to\infty$, the off-diagonal elements in the bottom row of A_{k+1} tend to zero *much faster* than the off-diagonal elements in the first column. The reason is that, besides the connection with the power method in Property 2.21, the QR algorithm also enjoys a close relation with *inverse iteration* (Method 2.7). Indeed, assuming that A is nonsingular, we can write the equation $A^k=\bar{Q}_{k-1}\bar{R}_{k-1}$ in the form $A^{-k}=\bar{R}_{k-1}^{-1}\bar{Q}_{k-1}^\top$. Consider the bottom row of this equation: we obtain $\boldsymbol{e}_n^\top A^{-k}=(\boldsymbol{e}_n^\top\bar{R}_{k-1}^{-1})\bar{Q}_{k-1}^\top$. However, $\bar{R}_{k-1}$ is upper triangular $\Rightarrow\bar{R}_{k-1}^{-1}$ is upper triangular $\Rightarrow\boldsymbol{e}_n^\top\bar{R}_{k-1}^{-1}$ is a multiple of $\boldsymbol{e}_n^\top$. We deduce that the bottom row of $\bar{Q}_{k-1}^\top$, whick we denote by $\boldsymbol{p}_k^\top$, is a multiple of the bottom row of A^{-k}.

Let (again) $|\lambda_1|<|\lambda_2|<\cdots<|\lambda_n|$ and let $\boldsymbol{e}_n^\top=\sum_{j=1}^n\varphi_j\boldsymbol{v}_j^\top$ be the expansion of $\boldsymbol{e}_n^\top$ in the basis of *left eigenvectors* of A, i.e. $\boldsymbol{v}_j^\top A=\lambda_j\boldsymbol{v}_j^\top$. Let r be the least integer so that $\varphi_r\neq0$. Then $\boldsymbol{p}_k^\top$ is a scalar multiple of

$$\boldsymbol{e}_n^\top A^{-k}=\sum_{j=r}^n\varphi_j\boldsymbol{v}_j^\top A^{-k}=\sum_{j=r}^n\varphi_j\lambda_j^{-k}\boldsymbol{v}_j^\top=\lambda_r^{-k}\left[\varphi_r\boldsymbol{v}_r^\top+\sum_{j=r+1}^n\varphi_j\left(\frac{\lambda_r}{\lambda_j}\right)^k\boldsymbol{v}_j^\top\right].\qquad(2.5)$$

Therefore, $\boldsymbol{p}_k^\top$ tends to a multiple of $\boldsymbol{v}_r^\top$: letting $\|\boldsymbol{v}_r\|=1$, we have $\boldsymbol{p}_k=\pm\boldsymbol{v}_r+\boldsymbol{g}_k$, where $\boldsymbol{g}_k\to\boldsymbol{0}$.

Theorem 2.24 *(The bottom row of A_{k+1}) Suppose that the conditions of Remark 2.23 are satisfied. Then, as $k\to\infty$, the bottom row of A_{k+1} tends to $\lambda_r\boldsymbol{e}_n^\top$.*

Proof It follows from Lemma 2.20, Remark 2.23, the eigenvalue equation $\boldsymbol{v}_r^\top A=\lambda_r\boldsymbol{v}_r^\top$ and orthogonality of $\bar{Q}_k$ that

$$\begin{aligned}\boldsymbol{e}_n^\top A_{k+1}&=\boldsymbol{e}_n^\top\bar{Q}_k^\top A\bar{Q}_k=\boldsymbol{p}_{k+1}^\top A\bar{Q}_k=(\pm\boldsymbol{v}_r^\top+\boldsymbol{g}_{k+1}^\top)A\bar{Q}_k=\pm\lambda_r\boldsymbol{v}_r^\top\bar{Q}_k+\boldsymbol{g}_{k+1}^\top A\bar{Q}_k\\&=\lambda_r(\boldsymbol{p}_{k+1}^\top-\boldsymbol{g}_{k+1}^\top)\bar{Q}_k+\boldsymbol{g}_{k+1}^\top A\bar{Q}_k\to\lambda_r\boldsymbol{p}_{k+1}^\top\bar{Q}_k=\lambda_r\boldsymbol{e}_n^\top.\end{aligned}$$

The proof is complete. □

Technique 2.25 (Single shifts). If $|\lambda_r|$ is tiny then usually the rightmost sum in (2.5) tends to zero rapidly as k increases, so the convergence result of Theorem 2.24 can be useful for small values of k. The theorem also shows that $(A_k)_{n,n}$ becomes a good estimate of λ_r. The *single shift technique* combines these remarks in the

[1] Please email all corrections and suggestions to these notes to `A.Iserles@damtp.cam.ac.uk`. All handouts are available on the WWW at the URL `http://www.damtp.cam.ac.uk/user/na/PartII/Handouts.html`.

following way. The matrix A_k is replaced by $A_k - s_k I$, where $s_k = (A_k)_{n,n}$ is our guess of λ_r, before the QR factorization. This reduces the magnitude of the rth eigenvalue of A_k substantially, which accelerates convergence because of the relationship to inverse iteration. The eigenvalues of $R_k Q_k$ now differ from these of A_k by a shift $-s_k$, since $R_k Q_k$ is similar to $A_k - s_k I$. We therefore set $A_{k+1} = R_k Q_k + s_k I$.

To recap, $Q_k R_k = A_k - s_k I$, where $s_k = (A_k)_{n,n}$, therefore

$$A_{k+1} = R_k Q_k + s_k I = (Q_k^\top Q_k) R_k Q_k + s_k I = Q_k^\top (A_k - s_k I) Q_k + s_k I = Q_k^\top A_k Q_k, \qquad (2.6)$$

similarly to the original QR iteration.

QR with single shifts is the method of choice when A has real eigenvalues. However, in the presence of complex conjugate pairs of eigenvalues we require the technique of *double shifts.*

Lemma 2.26 *(Double shifts). Suppose that Technique 2.25 is applied twice: from A_k to A_{k+1} with shift s_k and from A_{k+1} to A_{k+2} with shift s_{k+1}. Let $A_k - s_k I = Q_k R_k$ and $A_{k+1} - s_{k+1} I = Q_{k+1} R_{k+1}$. Then $(A_k - s_{k+1} I)(A_k - s_k I)$ has the QR factorization $(Q_k Q_{k+1})(R_{k+1} R_k)$.*

Proof We have

$$\begin{aligned}(Q_k Q_{k+1})(R_{k+1} R_k) &= Q_k (A_{k+1} - s_{k+1} I) R_k = Q_k (Q_k^\top A_k Q_k - s_{k+1} I) R_k = (A_k - s_{k+1} I) Q_k R_k \\ &= (A_k - s_{k+1} I)(A_k - s_k I)\end{aligned}$$

and the proof is complete. □

Corollary 2.27 *Let A_k be upper Hessenberg. A_{k+2} is calculated from A_k in the way that is the subject of Lemma 2.26. Then A_{k+2} is also upper Hessenberg and $A_{k+2} = Q_*^\top A_k Q_*$, where Q_* is an orthogonal matrix whose first column is a multiple of the first column of $(A_k - s_{k+1} I)(A_k - s_k I)$.*

Proof Replacing A_k by $A_k - s_k I$ in Technique 2.17, it follows that A_{k+1} is upper Hessenberg. Then, increasing k by one, we find that A_{k+2} is also upper Hessenberg.

Using the notation of (2.6), we write A_{k+2} as the product

$$A_{k+2} = Q_{k+1}^\top A_{k+1} Q_{k+1} = Q_{k+1}^\top Q_k^\top A_k Q_k Q_{k+1} = Q_*^\top A_k Q_*,$$

where $Q_* = Q_k Q_{k+1}$. Since $R_{k+1} R_k$ is upper triangular, Lemma 2.26 implies that the first column of Q_* is a multiple of the first column of $(A_k - s_{k+1} I)(A_k - s_k I)$. □

Method 2.28 (Double shifts). Corollary 2.27 suggests the following algorithm for generating A_{k+2} from the upper Hessenberg matrix A_k and the shifts s_k and s_{k+1}, without forming the intermediate matrix A_{k+1}. We retain the notation of Lemma 2.26.

1. Calculate the first column of $(A_k - s_{k+1} I)(A_k - s_k I)$, say $\boldsymbol{v}$;

2. Let Ω_* be an orthogonal matrix whose first column is $\pm \boldsymbol{v}/\|\boldsymbol{v}\|$;

3. Form the matrix $B_k = \Omega_*^\top A_k \Omega_*$;

4. Apply Method 2.15 to transform B_k into an upper Hessenberg matrix A_{k+2} which, being similar to B_k, is also similar to A_k.

It can be shown that only the first three components of $\boldsymbol{v}$ may be nonzero and we can let $\Omega_*^\top = \Omega^{(1,3)} \Omega^{(1,2)}$, where $\Omega^{(i,j)}$ are Given rotations such that $\Omega^{(1,3)} \Omega^{(1,2)} \boldsymbol{v} = \pm \|\boldsymbol{v}\| \boldsymbol{e}_1$. Hence the matrix

$$B_k = \Omega^{(1,3)} \Omega^{(1,2)} A_k \Omega^{(1,2)\top} \Omega^{(1,3)\top}$$

is upper Hessenberg, except that $(B_k)_{3,1}$ and $(B_k)_{4,1}$ might be nonzero. Therefore in Method 2.15 we may restrict q to $\{p+1, p+2\}$ for every $p = 1, 2, \ldots, n-2$ and the total cost of **4** is $\mathcal{O}(n^2)$ for general matrices. The main advantage of Method 2.28 (which is formally equivalent to two steps of Technique 2.25) is that it can be applied in *real arithmetic* when $s_{k+1} = \bar{s}_k \in \mathbb{C}$.