Mathematical Tripos Part II: Michaelmas Term 2024

Numerical Analysis – Lecture 23

Technique 5.15 (The QR iteration for symmetric matrices) We bring A to the upper Hessenberg form, so that QR algorithm commences from a symmetric tridiagonal matrix A_0, and then Technique 5.14 is applied for every k as before. Since both the upper Hessenberg structure and symmetry is retained, each A_{k+1} is also *symmetric tridiagonal* too. It follows that, whenever a Givens rotation $\Omega^{[i,j]}$ combines either two adjacent rows or two adjacent columns of a matrix, the total number of nonzero elements in the new combination of rows or columns is at most five. Thus there is a bound on the work of each rotation that is independent of n. Hence each QR iteration requires just $\mathcal{O}(n)$ operations.

Notation 5.16 To analyse the matrices A_k that occur in the QR algorithm 5.13, we introduce

$$\bar{Q}_k = Q_0 Q_1 \cdots Q_k, \qquad \bar{R}_k = R_k R_{k-1} \cdots R_0, \qquad k = 0, 1, \ldots. \tag{5.3}$$

Note that $\bar{Q}_k$ is orthogonal and $\bar{R}_k$ upper triangular.

Lemma 5.17 (Fundamental properties of $\bar{Q}_k$ and $\bar{R}_k$) *A_{k+1} is related to the original matrix A by the similarity transformation $A_{k+1} = \bar{Q}_k^T A \bar{Q}_k$. Further, $\bar{Q}_k \bar{R}_k$ is the QR factorization of A^{k+1}.*

Proof. We prove the first assertion by induction. By (5.2), we have $A_1 = Q_0^T A_0 Q_0 = \bar{Q}_0^T A \bar{Q}_0$. Assuming $A_k = \bar{Q}_{k-1}^T A \bar{Q}_{k-1}$, equations (5.2)-(5.3) provide the first indentity

$$A_{k+1} = Q_k^T A_k Q_k = Q_k^T (\bar{Q}_{k-1}^T A \bar{Q}_{k-1}) Q_k = \bar{Q}_k^T A \bar{Q}_k \,.$$

The second assertion is true for $k = 0$, since $\bar{Q}_0 \bar{R}_0 = Q_0 R_0 = A_0 = A$. Again, we use induction, assuming $\bar{Q}_{k-1} \bar{R}_{k-1} = A^k$. Thus, using the definition (5.3) and the first statement of the lemma, we deduce that

$$\begin{aligned} \bar{Q}_k \bar{R}_k &= (\bar{Q}_{k-1} Q_k)(R_k \bar{R}_{k-1}) = \bar{Q}_{k-1} A_k \bar{R}_{k-1} = \bar{Q}_{k-1} (\bar{Q}_{k-1}^T A \bar{Q}_{k-1}) \bar{R}_{k-1} \\ &= A \bar{Q}_{k-1} \bar{R}_{k-1} = A \cdot A^k = A^{k+1} \end{aligned}$$

and the lemma is true. □

Remark 5.18 (Relation between QR and the power method) Assume that the eigenvalues of A have different magnitudes,

$$|\lambda_1| < |\lambda_2| < \cdots < |\lambda_n|, \quad \text{and let} \quad \boldsymbol{e}_1 = \textstyle\sum_{i=1}^n c_i \boldsymbol{w}_i = \sum_{i=1}^m c_i \boldsymbol{w}_i \tag{5.4}$$

be the expansion of the first coordinate vector in terms of the normalized eigenvectors of A, where m is the greatest integer such that $c_m \neq 0$.

Consider the first columns of both sides of the matrix equation $A^{k+1} = \bar{Q}_k \bar{R}_k$.

By the power method arguments, the vector $A^{k+1}\boldsymbol{e}_1$ is a multiple of $\sum_{i=1}^m c_i (\lambda_i/\lambda_m)^{k+1} \boldsymbol{w}_i$, so the first column of A^{k+1} tends to be a multiple of $\boldsymbol{w}_m$ for $k \gg 1$. On the other hand, if $\boldsymbol{q}_k$ is the first column of $\bar{Q}_k$, then, since $\bar{R}_k$ is upper triangular, the first column of $\bar{Q}_k \bar{R}_k$ is a multiple of $\boldsymbol{q}_k$.

Therefore $\boldsymbol{q}_k$ tends to be a multiple of $\boldsymbol{w}_m$. Further, because both $\boldsymbol{q}_k$ and $\boldsymbol{w}_m$ have unit length, we deduce that $\boldsymbol{q}_k = \pm \boldsymbol{w}_m + \boldsymbol{h}_k$, where $\boldsymbol{h}_k$ tends to zero as $k \to \infty$. Therefore,

$$A \boldsymbol{q}_k = \lambda_m \boldsymbol{q}_k + o(\mathbf{1}) \,, \quad k \to \infty \,. \tag{5.5}$$

Theorem 5.19 (The first column of A_k) *Let conditions (5.4) be satisfied. Then, as $k \to \infty$, the first column of A_k tends to $\lambda_m \boldsymbol{e}_1$, making A_k suitable for deflation.*

Proof. By Lemma 5.17, the first column of A_{k+1} is $\bar{Q}_k^T A \bar{Q}_k \boldsymbol{e}_1$, and, using (5.5), we deduce that

$$A_{k+1}\boldsymbol{e}_1 = \bar{Q}_k^T A \bar{Q}_k \boldsymbol{e}_1 = \bar{Q}_k^T A \boldsymbol{q}_k \overset{(5.5))}{=} \bar{Q}_k^T[\lambda_m \boldsymbol{q}_k + o(\mathbf{1})] \overset{(*)}{=} \lambda_m \boldsymbol{e}_1 + o(\mathbf{1}),$$

where in $(*)$ we used that $\bar{Q}_k^T \boldsymbol{q}_k = \boldsymbol{e}_1$ by orthogonality of $\bar{Q}$, and that $\bar{Q}_k \boldsymbol{x} = \mathcal{O}(\boldsymbol{x})$ because orthogonal mapping is isometry. □

Remark 5.20 (Relation between QR and inverse iteration) In practice, the statement of Theorem 5.19 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 Remark 5.18, the QR algorithm also enjoys a close relation with *inverse iteration* (Method 5.5).

Let again

$$|\lambda_1| < |\lambda_2| < \cdots < |\lambda_n|, \quad \text{and let} \quad \boldsymbol{e}_n^T = \textstyle\sum_{i=1}^n c_i \boldsymbol{v}_i^T = \sum_{i=s}^n c_i \boldsymbol{v}_i^T \tag{5.6}$$

be the expansion of the last coordinate row vector $\boldsymbol{e}_n^T$ in the basis of normalized *left eigenvectors* of A, i.e. $\boldsymbol{v}_i^T A = \lambda_i \boldsymbol{v}_i^T$, where s is the least integer such that $c_s \neq 0$.

Assuming that A is nonsingular, we can write the equation $A^{k+1} = \bar{Q}_k \bar{R}_k$ in the form $A^{-(k+1)} = \bar{R}_k^{-1} \bar{Q}_k^T$. Consider the bottom rows of both sides of this equation: $\boldsymbol{e}_n^T A^{-(k+1)} = (\boldsymbol{e}_n^T \bar{R}_k^{-1}) \bar{Q}_k^T$.

By the inverse iteration arguments, the vector $\boldsymbol{e}_n^T A^{-(k+1)}$ is a multiple of $\sum_{i=s}^n c_i (\lambda_s/\lambda_i)^{k+1} \boldsymbol{v}_i^T$, so the bottom row of $A^{-(k+1)}$ tends to be multiple of $\boldsymbol{v}_s^T$. On the other hand, let $\boldsymbol{p}_k^T$ be the bottom row of $\bar{Q}_k^T$. Since $\bar{R}_k$ is upper triangular, its inverse $\bar{R}_k^{-1}$ is upper triangular too, hence the bottom row of $\bar{R}_k^{-1} \bar{Q}_k^T$, is a multiple of $\boldsymbol{p}_k^T$.

Therefore, $\boldsymbol{p}_k^T$ tends to a multiple of $\boldsymbol{v}_s^T$, and, because of their unit lengths, we have $\boldsymbol{p}_k^T = \pm \boldsymbol{v}_s^T + \boldsymbol{h}_k^T$, where $\boldsymbol{h}_k \to 0$, i.e.,

$$\boldsymbol{p}_k^T A = \lambda_s \boldsymbol{p}_k^T + o(\mathbf{1}), \quad k \to \infty. \tag{5.7}$$

Theorem 5.21 (The bottom row of A_k) *Let conditions (5.6) be satisfied. Then, as $k \to \infty$, the bottom row of A_k tends to $\lambda_s \boldsymbol{e}_n^T$, making A_k suitable for deflation.*

Proof. By Lemma 5.17, the bottom row of A_{k+1} is $\boldsymbol{e}_n^T \bar{Q}_k^T A \bar{Q}_k$, and similarly to the previous proof we obtain

$$\boldsymbol{e}_n^T A_{k+1} = \boldsymbol{e}_n^T \bar{Q}_k^T A \bar{Q}_k = \boldsymbol{p}_k^T A \bar{Q}_k \overset{(5.7)}{=} [\lambda_s \boldsymbol{p}_k^T + o(\mathbf{1})]\, \bar{Q}_k = \lambda_s \boldsymbol{e}_n^T + o(\mathbf{1}). \tag{5.8}$$

the last equality by orthogonality of $\bar{Q}_k$. □

Technique 5.22 (Single shifts) As we saw in Method 5.5, there is a huge difference between power iteration and inverse iteration: the latter can be accelerated arbitrarily through the use of shifts. The better we can estimate $s_k \approx \lambda_s$, the more we can accomplish by a step of inverse iteration with the shifted matrix $A_k - s_k I$. Theorem 5.21 shows that the bottom right element $(A_k)_{nn}$ becomes a good estimate of λ_s. So, in the *single shift technique*, the matrix A_k is replaced by $A_k - s_k I$, where $s_k = (A_k)_{nn}$, before the QR factorization:

$$\begin{aligned} A_k - s_k I &= Q_k R_k, \\ A_{k+1} &= R_k Q_k + s_k I. \end{aligned}$$

A good approximation $s_k = (A_k)_{nn}$ to the eigenvalue λ_s generates even better approximation of $s_{k+1} = (A_{k+1})_{nn}$ to λ_s, and convergence is accelerating at a higher and higher rate (it will be the so-called cubic convergence $|\lambda_s - s_{k+1}| \le \gamma |\lambda_s - s_k|^3$). Note that, similarly to the original QR iteration, we have

$$A_{k+1} = Q_k^T (Q_k R_k + s_k I) Q_k = Q_k^T A_k Q_k,$$

hence $A_{k+1} = \bar{Q}_k^T A \bar{Q}_k$, but note also that $\bar{Q}_k \bar{R}_k \neq A^{k+1}$, but we have instead

$$\bar{Q}_k \bar{R}_k = \textstyle\prod_{m=0}^k (A - s_m I)$$