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Eigenproblems

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The QR iteration

Set

$$T_k = Q_k^* \, A \, Q_k \qquad \text{for } k = 0, 1, 2, \ldots .$$

The QR iteration arises when considering how to compute T_k directly from T_{k-1}

From the definition of Q_k and R_k and the relation $Q_{k-1} \, A = R_k \, Q_k$:

$$\begin{aligned} T_{k-1} &= Q_{k-1}^* A \, Q_{k-1} = (Q_{k-1}^* Q_k) \, R_k & (1) \\ T_k &= Q_k^* \, A \, Q_k = (Q_k^* \, A \, Q_{k-1}) \, Q_{k-1}^* Q_k = R_k \, (Q_{k-1}^* Q_k) & (2) \end{aligned}$$

We have that $Q_{k-1}^* Q_k$ is unitary and (1) is the QR factorization of T_{k-1}

Drawbacks

- a single iteration costs $O(n^3)$ flops
- convergence (when it exists) is only linear

The real QR iteration

Matrices arising from applications have real entries! From now

$$\boxed{A \text{ real } n \times n \text{ matrix}}$$

The *real QR iteration* is defined by choosing an orthogonal $n \times n$ matrix Q_0 and setting

$$
\begin{aligned}
& H_0 \leftarrow Q_0^T A\, Q_0 \\
& \text{for } k = 1, 2, \ldots \\
& \qquad H_{k-1} = Q_k\, R_k \ \ \textit{(QR factorization)} \\
& \qquad H_k \leftarrow R_k\, Q_k
\end{aligned}
$$

The real Schur form

If the eigenvalues of A are not real, then T_k cannot converge to an upper triangular matrix

$\rightsquigarrow$ we content ourselves with convergence to the *real Schur form*:

$$A = Q\,T\,Q^T$$

with Q orthogonal and T block upper triangular with 1×1 and 2×2 diagonal blocks, that is

$$T = \begin{bmatrix} T_{1,1} & T_{1,2} & \cdots & T_{1,n} \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & T_{n-1,n} \\ 0 & \cdots & 0 & T_{n,n} \end{bmatrix} \in \mathbb{R}^{n \times n}$$

where each $T_{i,i}$ is a 1×1 block or a 2×2 block with complex conjugate eigenvalues

Hessenberg reduction

To implement the QR iteration, we have to choose Q_0 carefully such that

$$T_0 = Q_0^T A Q_0$$

is an upper Hessenberg matrix, which would lower the complexity to $O(n^2)$ flops

Hessenberg reduction (cont.)

It is a variation of the QR factorization, and can be done with a sequence of Householder reflections

Let $n = 5$ and choose $P_1 = \begin{bmatrix} 1 & \mathbb{0} \\ \mathbb{0} & \widetilde{P}_1 \end{bmatrix}$ with $\widetilde{P}_1$ a Householder 4×4 matrix such that

$$P_1\, A = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \end{bmatrix}, \quad A_1 = P_1\, A\, P_1^T = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \end{bmatrix}$$

- P_1 leaves the first row of $P_1\, A$ unchanged
- P_1^T leaves the first column of $(P_1\, A)\, P_1^T$ unchanged, including the zeros

Hessenberg reduction (cont.)

Choose $P_2 = \begin{bmatrix} \mathbb{1}_2 & \mathbb{0} \\ \mathbb{0} & \widetilde{P}_2 \end{bmatrix}$ with $\widetilde{P}_2$ a 3×3 Householder such that

$$P_2\,A_1 = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & \times & \times & \times \end{bmatrix}, \quad A_2 = P_2\,A_1\,P_2^T = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & \times & \times & \times \end{bmatrix}$$

- P_1 leaves the first and second rows of $P_2\,A_1$ unchanged
- P_2^T leaves the first and second columns of $(P_2\,A_2)\,P_2^T$ unchanged

Hessenberg reduction (cont.)

Finally choose $P_3 = \begin{bmatrix} \mathbb{1}_3 & \mathbb{0} \\ \mathbb{0} & \widetilde{P}_3 \end{bmatrix}$ with $\widetilde{P}_2$ a 2×2 Householder s.t.

$$P_3\, A_2 = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}, \quad A_3 = P_3\, A_2\, P_3^T = \begin{bmatrix} \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & \times & \times \end{bmatrix}$$

This constructs an orthogonal $n \times n$ matrix

$$Q_0 = P_{n-2} \cdots P_1$$

such that $H_0 = Q_0^T\, A\, Q_0$ is Hessenberg

The complexity of this procedure is $5\, n^3 + O(n^2)$ flops

The Hessenberg form through the QR iteration

The Hessenberg form is preserved during the QR iteration: let

$$H = Q\,R \quad \text{and} \quad H_+ = R\,Q$$

with H Hessenberg

Since R is upper triangular, the j-th column of Q is a linear combination of the first columns of H: write

$$H = [h_1 \cdots h_n] \quad \text{and} \quad Q = [q_1 \cdots q_n]$$

Setting $S = R^{-1} = [s_{i,j}]_{i,j}$ we have that

$$q_j = \sum_{k=1}^{j} s_{k,j}\, h_k\,, \quad j = 1, \ldots, n$$

and so Q is Hessenberg

Similarly the j-th row of H_+ is a linear combination of the last j rows of Q, and so H_+ is Hessenberg

The Hessenberg form through the QR iteration (cont.)

The QR factorization of H is computed with $n-1$ Givens rotations:

$$Q^T H = R$$

where R is upper triangular and $Q = G_1 \cdots G_{n-1}$ with

$$G_i = \text{Givens}(i, i+1, \theta_i)$$

Then

$$H_+ = R\,Q = R\,(G_1 \cdots G_{n-1})$$

This requires $6\,n^2 + O(n)$ flops

Deflation

A Hessenberg matrix $H \in \mathbb{R}^{n\times n}$ is *reduced* if it has a zero subdiagonal entry

In this case there is $0 < p < n$ such that

$$H = \begin{array}{cc} & \begin{array}{cc} \scriptstyle p & \scriptstyle n-p \end{array} \\ \begin{array}{c} \scriptstyle p \\ \scriptstyle n-p \end{array} & \begin{bmatrix} H_{1,1} & H_{2,2} \\ \mathbb{0} & H_{2,2} \end{bmatrix} \end{array}$$

and the eigenproblem problem for H decouples into the two smaller problems for $H_{1,1}$ and $H_{2,2}$ *(deflation)*

In practice, this happens when a subdiagonal entry is sufficiently small, for instance when

$$|h_{p+1,p}| \leqslant c\,\varepsilon\,(|h_{p,p}| + |h_{p+1,p+1}|)$$

for ε the machine epsilon and c a small constant

Typically for $p = n-1$ and $p = n-2$

The shifted QR iteration

For $\mu \in \mathbb{R}$ consider the single shift QR iteration

$$
\begin{aligned}
&H_0 \leftarrow Q_0^T A\, Q_0 \ \textit{(Hessenberg reduction)} \\
&\text{for } k = 1, 2, \ldots \\
&\qquad H_{k-1} - \mu\, \mathbb{1}_n = Q_k\, R_k \ \textit{(QR factorization)} \\
&\qquad H_k \leftarrow R_k\, Q_k + \mu\, \mathbb{1}_n
\end{aligned}
$$

Each H is Hessenberg and orthogonally similar to A:

$$\widetilde{H} = R\,Q + \mu\,\mathbb{1}_n = Q^T(Q\,R + \mu\,\mathbb{1}_n)\,Q = Q^T H\,Q$$

The shifted QR iteration (cont.)

If μ is an eigenvalue then deflation occurs in one step

$$\widetilde{h}_{n,n-1} = 0 \quad \text{and} \quad \widetilde{h}_{n,n} = \lambda$$

In practice, we recognize that the QR iteration is converging when $h_{n,n-1}$ is small

When this occurs, we use $\mu = h_{n,n}$ and we obtain a quadratically converging algorithm: if

$$|h_{n,n-1}| \leqslant \eta \, \|H\| \qquad \text{with } 0 \leqslant \eta \ll 1$$

then for $\mu = h_{n,n}$ we have that

$$|\widetilde{h}_{n,n-1}| \leqslant O(\eta^2 \|H\|)$$

$\rightsquigarrow$ the number of correct digits of $h_{n,n} \approx \lambda$ *doubles* at each step

The double shift strategy

When the eigenvalue λ of A is not real, we might perform two complex single shifts QR steps in succession:

$$\begin{aligned} H - \lambda \mathbb{1}_n &= Q_1 R_1 \\ H_1 &\leftarrow R_1 Q_1 + \lambda \mathbb{1}_n \\ H_1 - \overline{\lambda} \mathbb{1}_n &= Q_2 R_2 \\ H_2 &\leftarrow R_2 Q_2 + \overline{\lambda} \mathbb{1}_n \end{aligned}$$

Set

$$Q = Q_1 Q_2 \quad \text{and} \quad R = R_2 R_1$$

It can be shown that these $n \times n$ matrices are *real* and that

$$H_2 = Q^T H Q \in \mathbb{R}^{n \times n}$$

The double shift strategy (cont.)

To avoid complex arithmetics altogether, we would like to pass from H to H_2 directly and using only real numbers

Set $M = Q\,R$, which verifies that

$$M = H^2 - 2\,\mathrm{Re}(\lambda)\,H + |\lambda|^2\,\mathbb{1}_n$$

Then the strategy is:

- compute $M = H^2 - 2\,\mathrm{Re}(\lambda)\,H + |\lambda|^2\,\mathbb{1}_n$
- compute the QR factorization $M = Q\,R$
- set $H_2 = Q^T H\,Q$

The first step requires $O(n^3)$ flops and so it is still not practical...

The implicit double shift

The *implicit double shift* (or *Francis QR step*) computes this double shift in $O(n^2)$ flops:

- compute $M\, e_1 =$ multiple of e_1,
- determine Householder matrices $P_0, P_1, \ldots, P_{n-2}$ such that if $Z = P_0\, P_1 \cdots P_{n-2}$ then $Z^T\, H\, Z$ is Hessenberg and the first columns of Q and of Z are equal.

Why does it work?

The implicit QR theorem

If both

$$Q^T A\, Q = H \quad \text{and} \quad Z^T A\, Z = Q$$

are Hessenberg, H is unreduced, and Q and Z have the same first column, then

$$G = D^{-1} H\, D$$

with $D = \mathrm{diag}(\pm 1, \ldots, \pm 1)$

- If both $Q^T H\, Q$ and $Z^T H\, Z$ are unreduced, then they are essentially equal
- Else the problem decouples into smaller unreduced subproblems

Implementing the implicit double shift

Set $s = \mathrm{Re}(\lambda)$ and $t = |\lambda|^2$, write

$$M\, e_1 = \begin{bmatrix} x \\ y \\ z \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

with

$$\begin{aligned} x &= h_{1,1}^2 + h_{1,2}\, h_{2,1} - s\, h_{1,1} + t \\ y &= h_{2,1}\,(h_{1,1} + h_{2,2} - s) \\ z &= h_{2,1}\, h_{3,2} \end{aligned}$$

Implementing the implicit double shift

The computation of $M\,e_1$ and P_0 takes $O(1)$ flops

A similarity with P_0 only changes rows and columns 1, 2 and 3:

$$P_0^T H\, P_0 = \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}$$

Implementing the implicit double shift (cont.)

The mission of $P_1, \ldots, P_{n-2}$ is to restore this matrix to Hessenberg form:

$$\begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix} \to \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \end{bmatrix}$$

$$\to \begin{bmatrix} \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \end{bmatrix} \to \ldots$$

Hence

$$P_0 \quad \text{and} \quad Z = P_0 \, P_1 \cdots P_{n-2}$$

have the same first column

$\rightsquigarrow$ $Z\, e_1 = Q\, e_1$ and so Z and Q coincide, up to signs

Implementing the implicit double shift (cont.)

To implement this strategy, we check when $h_{n-1,n-2}$ is small, in which case the eigenvalues of

$$\begin{bmatrix} h_{n-1,n-1} & h_{n-1,n} \\ h_{n,n-1} & h_{n,n} \end{bmatrix}$$

approximate the eigenvalues of A

In this case

$$\begin{aligned} s &= h_{n-1,n-1} + h_{n,n} \qquad \text{(trace)} \\ t &= h_{n-1,n-1}\, h_{n,n} - h_{n-1,n}\, h_{n,n-1} \qquad \text{(determinant)} \end{aligned}$$

gives quadratic convergence

On the average, two QR iterations are needed per eigenvalue, and the overall process costs

$$O(n^3) \text{ flops}$$