Shifted QR algorithm

Let $\rho \in \mathbb{F}$. If λ_k be the eigenvalue of A closest to ρ, then let the eigenvalue set of A be reordered if necessary such that

$$|\lambda_1 - \rho| \geq |\lambda_2 - \rho| \geq \cdots \geq |\lambda_{n-1} - \rho| > |\lambda_n - \rho|.$$

If the QR iterations are performed on $B = A - \rho I$ to produce iterates B_j, then $b^{(j)}(n, n-1) \to 0$ linearly at the rate $|\lambda_n - \rho|/|\lambda_{n-1} - \rho|$.

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Shifted QR algorithm: Let $A_0 = A$ and $\rho_j \in \mathbb{F}$ for $j = 0, 1, \ldots$.
for j =1,2, . . .
    (i) Find a QR decomposition $A_{j-1} - \rho_{j-1} I = Q_{j-1} R_{j-1}$
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Clearly $A_j = Q_{j-1}^* A_{j-1} Q_{j-1}$ and is again upper Hessenberg !

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Shifted QR algorithm:

for j =1,2, . . .

(i) Find reflectors $Q_{j-1}^{(1)}, Q_{j-1}^{(2)}, \ldots Q_{j-1}^{(n-1)}$ *such that*

$$Q_{j-1}^{(n-1)} \cdots Q_{j-1}^{(2)} Q_{j-1}^{(1)} (A_{j-1} - \rho_{j-1} I) = R_{j-1}$$

(ii) Set $A_j = Q_{j-1}^{(n-1)} \cdots Q_{j-1}^{(2)} Q_{j-1}^{(1)} A_{j-1} Q_{j-1}^{(1)} Q_{j-1}^{(2)} \cdots Q_{j-1}^{(n-1)}$.

This costs $O(n^2)$ flops if A is upper Hessenberg and $O(n)$ flops if A is tridiagonal.

Shifted QR algorithms

Where do we get good shifts ?

Raleigh quotient shifts: $\rho_j = a_{nn}^{(j)}$.

Wilkinson shifts: $\rho_j = \lambda$ where λ is the eigenvalue of

$$\begin{bmatrix} a_{n-1,n-1}^{(j)} & a_{n-1,n}^{(j)} \\ a_{n,n-1}^{(j)} & a_{nn}^{(j)} \end{bmatrix}$$

closest to $a_{n,n}^{(j)}$. In case of a tie, the eigenvalue smallest in magnitude is chosen.

For symmetric tridiagonal matrices *QR* iterations with Wilkinson shifts always converge. With Rayleigh Quotient shifts, they almost always converge. Also, whenever convergence occurs, the rate of convergence is usually cubic.

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However, for general matrices both shifting strategies can fail!

Vera Kublanovskaya
1920-2012

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Theorem If A is a singular properly upper Hessenberg matrix, then the last row of the matrix A_1 obtained after one step of the QR algorithm is zero.

Corollary Let ρ be an eigenvalue of A and B be the matrix obtained after one step of shifted QR with shift ρ. Then the last row of B is $[0, 0, \cdots \rho]$.

Double Shift QR

Let $A \in \mathbb{C}^{n\times n}$ and $\rho, \tau \in \mathbb{C}$. Consider one iteration of Shifted QR with shift ρ followed by another with shift τ :

$$\begin{aligned} A - \rho I &= Q_\rho R_\rho, \hat{A} = R_\rho Q_\rho + \rho I \\ \hat{A} - \tau I &= Q_\tau R_\tau, \tilde{A} = R_\tau Q_\tau + \tau I \end{aligned}$$

Let $Q = Q_\rho Q_\tau$ and $R = R_\tau R_\rho$. Then,

$$(A - \rho I)(A - \tau I) = QR \text{ and } \tilde{A} = Q^* A Q.$$

Also if A is real and $\tau = \bar{\rho}$, then $(A - \rho I)(A - \tau I)$ and $\tilde{A}$ are real.

Additionally, if ρ and τ are not eigenvalues of A, then given *any* QR decomposition $(A - \rho I)(A - \tau I) = Q_1 R_1$ of $(A - \rho I)(A - \tau I)$, if $A_1 := Q_1^* A Q_1$, then there exists diagonal matrix D with $D(i,i) = \pm 1$, $i = 1, \ldots, n$, such that $A_1 = \bar{D}\tilde{A}D$.

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Exercise: Prove the above statements!

Double Shift QR

Let $A_0 = A$ and $\rho_j, \tau_j \in \mathbb{F}$ for $j = 0, 1, \ldots.$

for j = 1,2, . . .

(i) Form $M = (A_{j-1} - \rho_{j-1} I)(A_{j-1} - \tau_{j-1} I)$.

(ii) Find a reflectors $Q_{j-1}^{(1)}, Q_{j-1}^{(2)}, \ldots, Q_{j-1}^{(n-1)}$ *such that*

$$\mathbf{Q_{j-1}^{(n-1)}} \cdots \mathbf{Q_{j-1}^{(2)}} \mathbf{Q_{j-1}^{(1)}} M$$

is upper triangular.

(iii) Find $A_j = \mathbf{Q_{j-1}^{(n-1)}} \cdots \mathbf{Q_{j-1}^{(2)}} \mathbf{Q_{j-1}^{(1)}} A_{j-1} \mathbf{Q_{j-1}^{(1)}} \mathbf{Q_{j-1}^{(2)}} \cdots \mathbf{Q_{j-1}^{(n-1)}}$.

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Generally the shifts ρ_{j-1} and τ_{j-1} are taken to be the eigenvalues of

$$\begin{bmatrix} a_{n-1,n-1}^{(j-1)} & a_{n-1,n}^{(j-1)} \\ a_{n,n-1}^{(j-1)} & a_{nn}^{(j-1)} \end{bmatrix}.$$

This is called generalized Rayleigh Quotient shifting strategy.

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(i) Form $M = (A_{j-1} - \rho_{j-1} I)(A_{j-1} - \tau_{j-1} I)$.

(Costs $O(n^3)$ flops and may be severely affected by rounding error. Also M is not upper Hessenberg!)

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