THE QR METHOD

Given a square matrix A, form its QR factorization, as

$$A = Q_1 R_1$$

Then define

$$A_2 = R_1 Q_1$$

Continue this process: for $k \geq 1$ (with $A_1 = A$),

$$\begin{aligned} A_k &= Q_k R_k \\ A_{k+1} &= R_k Q_k \end{aligned}$$

Then the sequence $\{A_k\}$ will usually converge to something from which the eigenvalues can be computed easily.

Note first that A_2 is similar to A (and A_{k+1} is similar to A_k):

$$\begin{aligned} R_1 &= Q_1^T A \\ A_2 &= R_1 Q_1 = Q_1^T A Q_1 \end{aligned}$$

Thus A_2 is similar to A with an orthogonal similarity transformation.

EXAMPLE

$$A = \begin{bmatrix} 1 & 3 & 4 \\ 3 & 1 & 2 \\ 4 & 2 & 1 \end{bmatrix}$$

The true eigenvalues are

$$\begin{aligned} \lambda_1 &= 7.07467358251512 \\ \lambda_2 &= -3.18788259626475 \\ \lambda_3 &= -0.88679098625037 \end{aligned}$$

For $k = 20$, we have A_{20} is approximately the matrix

$$\begin{bmatrix} 7.07467 & 0.0 & 0.0 \\ 0.00000 & -3.18788 & 0.0 \\ 0.0 & 0.0 & -0.88679 \end{bmatrix}$$

which gives the correct answers to within an error of 5×10^{-6}.

A complete table of the first 20 iterates is given in the data file on the web page. For later use,

$$\frac{\lambda_2}{\lambda_1} = -.4506, \quad \frac{\lambda_3}{\lambda_1} = -.1253, \quad \frac{\lambda_3}{\lambda_2} = .2782$$

IMPLEMENTATION ISSUES

The repeated QR factorizations can be quite expensive. For that reason it is important to first convert A to a simpler form using orthogonal similarity transformations. For A symmetric, we convert to tridiagonal matrix. For A nonsymmetric, we convert A to an upper *Hessenberg matrix*:

$$U^T A U = H = \begin{bmatrix} * & * & * & \cdots & & * \\ * & * & * & \cdots & & * \\ 0 & * & * & & & \\ 0 & 0 & * & * & & \vdots \\ & & & \ddots & \ddots & \\ 0 & & \cdots & 0 & * & * \end{bmatrix}$$

The QR factorization of H is usually carried out with rotation matrices $R_{k,l}$ rather than with Householder matrices, as using the rotation matrices is generally slightly more efficient. This leads to

$$R = R_{n-1,n} \cdots R_{1,2} H, \quad Q = \left(R_{n-1,n} \cdots R_{1,2}\right)^T$$

$R_{1,2}$ is used to convert to zero the element in the (2,1) position of H; $R_{2,3}$ is used to subsequently convert to zero the element in the (2,3) position of $R_{1,2}H$; and this is continued for each column.

In doing

$$H = QR, \quad H_1 = RQ$$

it is important to know that H_1 is again a Hessenberg matrix. To see this, we must examine carefully the process by which $H = QR$ is computed. Let me consider the case of $n = 4$. Then

$$H = \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \end{bmatrix}$$

Then

$$\begin{aligned} R &= R_{3,4}R_{2,3}R_{1,2}H \\ Q &= \left(R_{3,4}R_{2,3}R_{1,2}\right)^T = R_{1,2}^T R_{2,3}^T R_{3,4}^T \end{aligned}$$

$R_{1,2}$, $R_{2,3}$, $R_{3,4}$ have the form

$$\begin{bmatrix} * & * & 0 & 0 \\ * & * & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & * & * & 0 \\ 0 & * & * & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & * & * \\ 0 & 0 & * & * \end{bmatrix}$$

Then for $RQ = R\,R_{1,2}^T R_{2,3}^T R_{3,4}^T$,

$$\begin{aligned} R\,R_{1,2}^T &= \begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{bmatrix} \begin{bmatrix} * & * & 0 & 0 \\ * & * & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\ &= \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{bmatrix} \end{aligned}$$

$$
\begin{aligned}
R\,R_{1,2}^T R_{2,3}^T &= \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & * & * & 0 \\ 0 & * & * & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\
&= \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & 0 & * \end{bmatrix}
\end{aligned}
$$

$$
\begin{aligned}
R\,R_{1,2}^T R_{2,3}^T R_{3,4}^T &= \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & 0 & * \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & * & * \\ 0 & 0 & * & * \end{bmatrix} \\
&= \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ 0 & * & * & * \\ 0 & 0 & * & * \end{bmatrix}
\end{aligned}
$$

Thus $H_1 = RQ = R\,R_{1,2}^T R_{2,3}^T R_{3,4}^T$ is in upper Hessenberg form. By induction, all of the matrices produced in the iteration are in upper Hessenberg form.

CONVERGENCE

If the eigenvalues of A are distinct and satisfy

$$|\lambda_1| > |\lambda_2| > \cdots > |\lambda_n| > 0$$

Then we can prove for $A_m = Q_m R_m$ that

$$\lim_{n \to \infty} A_m = D$$

as upper triangular matrix. If A is symmetric, then $\{A_m\}$ converges to a diagonal matrix D. In both cases,

$$\|A_m - D\| \leq c \max_{1 \leq i \leq n-1} \left| \frac{\lambda_{i+1}}{\lambda_i} \right|$$

A proof is sketched in the text.

For the case of eigenvalues not distinct, the convergence is more complicated.

EXAMPLE

Recall

$$A = \begin{bmatrix} 1 & 3 & 4 \\ 3 & 1 & 2 \\ 4 & 2 & 1 \end{bmatrix}$$

$$\frac{\lambda_2}{\lambda_1} = -.4506, \quad \frac{\lambda_3}{\lambda_1} = -.1253, \quad \frac{\lambda_3}{\lambda_2} = .2782$$

In that case, look at the ratios of the elements of A_m to the corresponding components of A_{m-1}, for the off-diagonal elements. For the case of A_6 to A_5, we have

$$A_6 \,./\, A_5 = \begin{bmatrix} * & -.4508 & .1254 \\ -.4508 & * & -.2785 \\ .1254 & -.2785 & * \end{bmatrix}$$

SYMMETRIC MATRICES

As shown earlier, if A is symmetric, then we can find an orthogonal U for which

$$U^T AU = T$$

a symmetric tridiagonal matrix. Now consider the QR factorization of T:

$$T = Q_1 R_1, \quad T_2 = R_1 Q_1 = Q_1^T T Q_1$$

This can be used to show T_2 is also symmetric.

Since T is trivially Hessenberg, it follows from our earlier work that T_2 is also Hessenberg. Since T_2 is also symmetric, this implies T_2 is tridiagonal, the same as T. If the eigenvalues of T are distinct, then $T_m \rightarrow D$, a diagonal matrix.

But consider the example

$$T = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Then $T = QR$ implies $Q = T$ and $R = I$, giving the QR factorization of T. Then in the QR method,

$$T_m = T, \quad m \geq 1$$

and $\{T_m\}$ does not converge to a diagonal matrix.

In general,

$$T_m \to \begin{bmatrix} D_1 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \ddots & \vdots \\ \mathbf{0} & \cdots & D_q \end{bmatrix}$$

in which each D_i is either a scalar (and an eigenvalue) or a 2×2 matrix (from which the two eigenvalues can be determined easily).

ACCELERATION

The QR method is too slow as I have defined it, especially if some of the eigenvalues are close together. In practice, the method is *accelerated*. I describe one such acceleration method.

Write

$$T_m = \begin{bmatrix} \alpha_1^{(m)} & \beta_1^{(m)} & 0 & 0 & \cdots & 0 \\ \beta_1^{(m)} & \alpha_2^{(m)} & \beta_2^{(m)} & 0 & & \\ 0 & \beta_2^{(m)} & \alpha_3^{(m)} & \beta_3^{(m)} & & \vdots \\ & & \ddots & \ddots & \ddots & \\ \vdots & & & \beta_{n-2}^{(m)} & \alpha_{n-1}^{(m)} & \beta_{n-1}^{(m)} \\ 0 & & \cdots & & \beta_{n-1}^{(m)} & \alpha_n^{(m)} \end{bmatrix}$$

Define

$$\begin{aligned} T_m - \alpha_n^{(m)} I &= Q_m R_m \\ T_{m+1} &= R_m Q_m + \alpha_n^{(m)} I \end{aligned}$$

Then

$$\begin{aligned}
R_m &= Q_m^T \left(T_m - \alpha_n^{(m)} I \right) \\
T_{m+1} &= Q_m^T \left(T_m - \alpha_n^{(m)} I \right) Q_m + \alpha_n^{(m)} I \\
&= Q_m^T T_m Q_m
\end{aligned}$$

Again T_{m+1} is similar to T_m. For convergence, we can show that one of the new coefficients $\beta_{n-1}^{(m)}$ or $\beta_{n-2}^{(m)}$ converges to zero extremely rapidly. If it is $\beta_{n-1}^{(m)}$, then we will have $\alpha_n^{(m)}$ is converging to an eigenvalue of T. When $\beta_{n-1}^{(m)}$ is sufficiently small, set $\lambda_n = \alpha_n^{(m)}$; and then we delete the last row and column of T_m and continue the same process with the new smaller matrix. When $\beta_{n-2}^{(m)}$ is converging to zero, we end up with a 2×2 matrix and we proceed in much the same manner as before.

EXAMPLE

$$T = \begin{bmatrix} 5 & 4 & 0 \\ 4 & 3 & 2 \\ 0 & 2 & 1 \end{bmatrix}$$

$$\begin{aligned} \lambda_1 &= 8.33815817656458 \\ \lambda_2 &= 1.95204720583627 \\ \lambda_3 &= -1.29020538240084 \end{aligned}$$

With acceleration,

$$T_1 = \begin{bmatrix} 8.000000 & -1.732051 & 0.0 \\ -1.732051 & -0.666667 & 0.942809 \\ 0.0 & 0.942809 & 1.666667 \end{bmatrix}$$

$$T_2 = \begin{bmatrix} 8.278350 & 0.756310 & 0.0 \\ 0.756310 & -1.227440 & 0.098342 \\ 0.0 & 0.098342 & 1.949090 \end{bmatrix}$$

$$T_3 = \begin{bmatrix} 8.322734 & -0.385058 & 0.0 \\ -0.385058 & -1.274781 & 0.000090 \\ 0.0 & 0.000090 & 1.952047 \end{bmatrix}$$

$$T_4 = \begin{bmatrix} 8.334178 & 0.195728 & 0.0 \\ 0.195728 & -1.286225 & 0.0 \\ 0.0 & 0.0 & 1.952047 \end{bmatrix}$$

In contrast, without acceleration,

$$T_4 = \begin{bmatrix} 8.338132 & -0.012854 & 0.0 \\ -0.012854 & 1.757031 & 0.770931 \\ 0.0 & 0.770931 & -1.095164 \end{bmatrix}$$

ERROR CONSIDERATIONS

For the error resulting from dropping out an element of the matrix, let T be a tridiagonal matrix and let $\widehat{T}$ the matrix obtained by deleting the element β_{n-1} from the $(n-1, n)$ and $(n, n-1)$ positions of T. Let $\left\{\lambda_j\right\}$ and $\left\{\widehat{\lambda}_j\right\}$ denote the associated eigenvalues. Then from the Wielandt-Hoffman theorem,

$$\left[\sum_{j=1}^{n}\left(\lambda_j-\widehat{\lambda}_j\right)^2\right]^{\frac{1}{2}} \leq F\left(T-\widehat{T}\right)=\mathsf{sqrt}(2)\left|\beta_{n-1}\right|$$

Thus there is not much difference in the eigenvalues if β_{n-1} is a small number.