Report on Numerical Linear Algebra Coding Assignment
Chapter 6: Unsymmetric Eigenvalue Problems

Hongyi Zhang, 1500017736

December 31, 2017

1 Problem setting

Apply the double implicit shift QR method to the upper Hessenberg matrix

$$H = \begin{bmatrix} 2 & 3 & 4 & 5 & 6 \\ 4 & 4 & 5 & 6 & 7 \\ 0 & 3 & 6 & 7 & 8 \\ 0 & 0 & 2 & 8 & 9 \\ 0 & 0 & 0 & 1 & 10 \end{bmatrix},$$

and observe the convergence behavior of the subdiagonal entries.

2 Double implicit shift QR method

For an upper Hessenberg matrix $H \in \mathbb{R}^{n\times n}$, consider the 2×2 matrix $G = H(n-1 : n, n-1 : n)$ on the bottom right corner. Double shift strategy iterates by

$$M = H^2 - sH + tI, \quad M = QR, \quad H_1 = Q^T HQ,$$

where $s = \mathrm{tr}(G)$ and $t = \det(G)$.

To avoid the high cost on computing M, we compute $\tilde{H}_1 = P^T HP$ instead of H_1. $\tilde{H}_1$ is essentially equal to H_1 as long as P and Q share the same first column, guaranteed by the implicit Q theorem. Pick a Householder matrix P_0 which reflects Me_1 to αe_1, then P_0, M, Q have their first columns colinear. In order to turn $P_0^T HP_0$ into the upper Hessenberg matrix $\tilde{H}_1$, use a series of reflections $P_1, \cdots, P_{n-2}$ (as similarity transformations) to proceed. Let

Table 1: Convergence of subdiagonal entries of H

Steps	h_{21}	h_{32}	h_{43}	h_{54}
1	1.2420e+00	6.9585e-01	3.3880e+00	-4.5561e+00
2	6.4585e-01	4.3761e+00	4.5437e-01	-2.1540e+00
3	4.3430e-01	5.3484e+00	7.1330e-02	-1.9552e-01
4	2.9706e-01	4.3271e+00	1.4366e-03	-3.2546e-03
5	2.0786e-01	3.3686e+00	4.0834e-07	-1.0349e-06
6	1.5164e-01	2.5115e+00	2.4535e-14	-7.3388e-12
7	7.9937e-04	-6.7939e+00	Converged	-7.3388e-12
8	1.3319e-07	-1.8393e+00		
9	9.6667e-15	-1.9757e-02		
10	Converged	-1.9757e-02		

$P = P_0 P_1 \cdots P_{n-2}$, then $Pe_1 = P_0 e_1 = Qe_1$, which renders $P^T HP$ essentially equal to H_1. Such implicit determination from H to $\tilde{H}_1 = P^T HP$ is referred to as a Francis QR step.

Now we describe the overall process of computing the real Schur normal form. At each step, the largest upper quasi-triangular matrix H_{33} on the bottom right corner is considered finished, and an implicit QR step is performed on the largest irreducible upper Hessenberg matrix H_{22} next to H_{33}. Note that not all 2×2 blocks in H_{33} has already converged, that is, do not necessarily have complex eigenvalues, since the subdiagonal entries of H can converge at different time steps, possibly violating the irreducibility of Hessenberg matrix. Hence an additional check on these 2×2 blocks is needed at the end of all iterations.

3 Numerical results

For the given upper Hessenberg matrix H, its eigenvalues all lie on the real axis, so its Schur normal form is an upper triangular matrix. By applying the QR method to H, the convergence of its subdiagonal entries are shown in Table 1.

As can be seen, QR method with shift strategy enjoys quadratic convergence on subdiagonal entries. Numerical error is a critical issue, especially when computing a Householder reflection for a vector fairly close to zero. The tolerance for convergence is set to 10^{-12}.

The output of the algorithm is a quasi-triangular matrix with its diagonal being

$$\tilde{D} = \mathrm{diag}\left\{ -0.3354, \begin{bmatrix} 1.4989 & 1.6234 \\ -0.0198 & 14.1565 \end{bmatrix}, \begin{bmatrix} 9.5248 & 5.3666 \\ -7.3\mathrm{e}{-12} & 5.1552 \end{bmatrix} \right\}.$$

A check on these 2×2 blocks is necessary to bring out all the real eigenvalues hidden by the already converged entries. Direct computation, which takes no more than $O(n)$ operations, gives the final Schur normal form, whose diagonal is

$$D = \mathrm{diag}\{-0.3354,\ 14.1540,\ 1.5014,\ 9.5248,\ 5.1552\},$$

with eigenvalues placed in no particular order.