$\begin{array}{c} {\rm CptSci~440/540:} \\ {\rm Numerical~Computation~I} \end{array}$

Handout #3 April 2, 2013

Problem Set 3

Due Date: April 23

In this problem set, you will implement the QR algorithm with shifts to find the spectrum of a user-provided symmetric matrix.

The algorithm has been discussed in class. It goes as follows (for the sake of clarity, I explain it for the case n = 4).

Step 1. Given a symmetric $n \times n$ matrix A, you feed it into the function upperhes(a, n, u, b) from the previous homework assignment. Note that the result will be a symmetric TRIDIAGONAL matrix B.

Step 2. You perform the shift:

$$\tilde{B} = B - \mu I,\tag{1}$$

where $\mu = B(1,1)$ is the value in the upper left corner.

Step 3. You bring \tilde{B} to the lower triangular form. To do so, you apply n-1 Givens rotation to the rows of \tilde{B} , starting from the bottom and going up. In other words, the order of operations is

$$\tilde{B} = \begin{pmatrix}
\cdot & \cdot & 0 & 0 \\
\cdot & \cdot & \cdot & 0 \\
0 & \cdot & \cdot & \cdot \\
0 & 0 & \cdot & \cdot
\end{pmatrix} \overrightarrow{Q_3} \begin{pmatrix}
\cdot & \cdot & 0 & 0 \\
\cdot & \cdot & \cdot & 0 \\
0 & * & * & 0 \\
0 & * & * & *
\end{pmatrix} \overrightarrow{Q_2} \begin{pmatrix}
\cdot & \cdot & 0 & 0 \\
* & * & 0 & 0 \\
* & * & * & 0 \\
0 & \cdot & \cdot & \cdot
\end{pmatrix} \overrightarrow{Q_1} \begin{pmatrix}
* & 0 & 0 & 0 \\
* & * & 0 & 0 \\
\cdot & \cdot & \cdot & 0 & 0 \\
0 & \cdot & \cdot & \cdot & 0 \\
0 & \cdot & \cdot & \cdot & \cdot
\end{pmatrix} = L, (2)$$

where Q_j is a Givens rotation that combines the rows j and j+1 to put a zero at the position (j, j+1).

Step 4. You apply the adjoints of the Givens rotations from the previous step to L, that is

$$L \to L \cdot Q_3^T \cdot Q_2^T \cdot Q_1^T. \tag{3}$$

Note that the resulting matrix is again tridiagonal and symmetric.

Step 5. You add the shift μ back to the diagonal.

To summarize, the basic iteration of the algorithm transforms B into B_{new} via

$$B \to B - \mu I \to Q(B - \mu I) = L \to LQ^T = Q(B - \mu I)Q^T \to LQ^T + \mu I = QBQ^T = B_{new}, \quad (4)$$

where $Q = Q_1 \cdot Q_2 \cdot Q_3$.

You keep on iterating Steps 2-5 until the value at the position (1,2) (just next to the upper left corner) is very small $(B_{new}(1,2) \sim 0)$. Then you declare the value in the upper left corner to be your approximation of the first eigenvalue of A (why does it make sense?), and apply the same iterations (without upperhes(), of course) to the $(n-1) \times (n-1)$ submatrix obtained from B_{new} by deleting the first column and the first row. You continue until you have found all the eigenvalues of A.

You need to write a code that implements the algorithm described above.

In FORTRAN, your calling sequence should be

$$qr_symmetric(a, n, b)$$
 (5)

where

a(n,n) is a (real) $n \times n$ -matrix to be diagonalized (input parameter). Assume that a is a SYMMET-RIC matrix.

n is the (integer) size of the matrix (input parameter)

b(n,n) is a (real) $n \times n$ -matrix (output parameter). The diagonal of b (i.e. $b(1,1),b(2,2),\ldots$) will contain the spectrum of a.

In C, your calling sequence should be

$$void\ qr_symmetric(double * a, int\ n, double * b),$$
 (6)

where

a points to an array of doubles of size n^2 , containing $a(1,1), a(1,2), \ldots, a(1,n), a(2,1), \ldots, a(n,n)$, a being the $n \times n$ matrix to be diagonalized (input parameter). Assume that a is a SYMMETRIC matrix.

n is the (integer) size of the matrix (input parameter)

b points to an array of doubles of size n^2 , containing $b(1,1), b(1,2), \ldots, b(1,n), b(2,1), \ldots, b(n,n)$, being the $n \times n$ matrix. The diagonal of b ($b(1,1), b(2,2), \ldots$) will contain the spectrum of a (output parameter, memory allocated by the user)

REMARK 1. Make sure that the calling sequence of your function is exactly as specified in the assignment.

REMARK 2. Test your code before submission.