1 Algorithms

1.1 The reduction to periodic upper Hessenberg form

The reduction to periodic Hessenberg form is done using Householder reflections. Suppose we have three 5×5-matrices and suppose we have brought the first two columns in the desired form. We have

$$\begin{array}{ccc} M_3 & M_2 & M_1 \\ \begin{array}{ccccc} \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \end{array} & \begin{array}{ccccc} \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \end{array} & \begin{array}{ccccc} \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \end{array} \end{array}.$$

Let $P^{[i]}_{j,k:l}$ denote the Householder reflection that, if applied to the rows of M_i, changes row j and introduces zeros on rows k to l in column j. We first apply the Householder reflection $P^{[1]}_{3,4:5}$ to the rows of M_1 and the columns of M_2. This does not alter the structure of M_2. We get

$$\begin{array}{ccc} M_3 & M_2 & M_1 \\ \begin{array}{ccccc} \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \end{array} & \begin{array}{ccccc} \bullet & \bullet & * & * & * \\ & \bullet & * & * & * \\ & & * & * & * \\ & & * & * & * \\ & & * & * & * \end{array} & \begin{array}{ccccc} \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & * & * & * \\ & & 0 & * & * \\ & & 0 & * & * \end{array} \end{array}$$

where the stars denote values that have changed. Then a second reflection $P^{[2]}_{3,4:5}$ is constructed that if applied to the rows of M_2 zeros the $(4,3)$ and $(5,3)$ elements and leaves the first two rows unchanged. This transformation is applied to the rows of M_2 and the columns of M_3 and reduces the matrices to

$$\begin{array}{ccc} M_3 & M_2 & M_1 \\ \begin{array}{ccccc} \bullet & \bullet & * & * & * \\ \bullet & \bullet & * & * & * \\ & \bullet & * & * & * \\ & & * & * & * \\ & & * & * & * \end{array} & \begin{array}{ccccc} \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & * & * & * \\ & & 0 & * & * \\ & & 0 & * & * \end{array} & \begin{array}{ccccc} \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet \\ & & & \bullet & \bullet \end{array} \end{array}.$$

Next, we construct a Householder transformation $P^{[3]}_{4,5}$ that puts a zero at the $(5,3)$ position of M_3 and leaves its first three rows unchanged. This transformation is applied to the rows of M_3 and the columns of M_1. Note only the last two columns of M_1 change and the structure is left intact. After this transformation we get

$$\begin{array}{ccc} M_3 & M_2 & M_1 \\ \begin{array}{ccccc} \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & * & * & * \\ & & 0 & * & * \end{array} & \begin{array}{ccccc} \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet \\ & & & \bullet & \bullet \end{array} & \begin{array}{ccccc} \bullet & \bullet & \bullet & * & * \\ & \bullet & \bullet & * & * \\ & & \bullet & * & * \\ & & & * & * \\ & & & * & * \end{array} \end{array}.$$

and we see that now the first three columns are in their final shape. Hence we obtain the following algorithm

Algorithm 1.1 *Reduction to periodic upper Hessenberg form.*

Input:

$G_1, \ldots, G_m$

Output:

$H_1, \ldots, H_m$ *and orthogonal matrices* $Q_0, \ldots, Q_{m-1}$ *such that* $Q_i^T G_i Q_{i-1} = H_i$ *(*$Q_m := Q_0$*).*

begin

for $i = 1$ ***to*** m ***do***

$H_i \leftarrow G_i$

$Q_{i-1} \leftarrow I_N$

endfor
for $i = 1$ **to** $N-1$ **do**
for $j = 1$ **to** $m-1$ **do**
Construct the Householder reflection P such that PH_j has zeros at position $(i+1, i)$ to (N, i) and the rows $1, \ldots, i-1$ are unchanged.
$H_j \leftarrow PH_j$
$H_{j+1} \leftarrow H_{j+1}P^T$
$Q_j \leftarrow Q_jP^T$
endfor
if $i < N-1$ **then**
Construct the Householder reflection P such that PH_m has zeros at position $(i+2, i)$ to (N, i) and the rows $1, \ldots, i$ are unchanged.
$H_m \leftarrow PH_m$
$H_1 \leftarrow H_1P^T$
$Q_0 \leftarrow Q_0P^T$
endif
endfor
end

This algorithm requires $\mathrm{O}(mN^3)$ operations.

1.2 Deflation of a zero on the diagonal

A zero at position (i,i) in one of the blocks M_k, $k = 1, \ldots, m-1$ translates in a zero at position $(i+1, i)$ in the product $M_m \cdots M_1$. Our implementation of the QR algorithm implicitly applies double shift QR steps on the product matrix and relies on the implicit Q theorem which requires that all operations are done on an unreduced block of the Hessenberg matrix. Therefore we want to mirror this in the structure of M_m and introduce a zero at position $(i+1, i)$ of that matrix. We can do even better. With the zero on the diagonal of M_k also corresponds a zero eigenvalue and we can isolate an eigenvalue in the upper Hessenberg block M_m, i.e., introduce zeros at position $(i+1, i)$ and $(i, i-1)$. This is done in two phases. First we will introduce a zero at position $(i+1, i)$ of M_m and in the second phase we will introduce a zero at position $(i-1, i)$.

1.2.1 Phase 1.

Assume we start with the following matrices:

$$\begin{array}{cccc}
M_4 & M_3 & M_2 & M_1 \\
\begin{array}{ccccc}
\bullet & \bullet & \bullet & \bullet & \bullet \\
\bullet & \bullet & \bullet & \bullet & \bullet \\
 & \bullet & \bullet & \bullet & \bullet \\
 & & \bullet & \bullet & \bullet \\
 & & & \bullet & \bullet
\end{array} &
\begin{array}{ccccc}
\bullet & \bullet & \bullet & \bullet & \bullet \\
 & \bullet & \bullet & \bullet & \bullet \\
 & & \bullet & \bullet & \bullet \\
 & & & \bullet & \bullet \\
 & & & & \bullet
\end{array} &
\begin{array}{ccccc}
\bullet & \bullet & \bullet & \bullet & \bullet \\
 & \bullet & \bullet & \bullet & \bullet \\
 & & 0 & \bullet & \bullet \\
 & & & \bullet & \bullet \\
 & & & & \bullet
\end{array} &
\begin{array}{ccccc}
\bullet & \bullet & \bullet & \bullet & \bullet \\
 & \bullet & \bullet & \bullet & \bullet \\
 & & \bullet & \bullet & \bullet \\
 & & & \bullet & \bullet \\
 & & & & \bullet
\end{array}
\end{array}.$$

There is a zero at position $(3,3)$ of M_2 and we want to introduce a zero at position $(4,3)$ of M_4. First we introduce a zero at position $(5,4)$ of M_4 using a Givens rotation operating on columns 4 and 5 of M_4. We also apply this Givens rotation to rows 4 and 5 of M_3 to preserve the eigenvalues. This introduces a nonzero element at position $(5,4)$ of M_3. Using a Givens rotation operating on columns 4 and 5 of M_3 and rows 4 and 5 of M_2, we reintroduce the zero in M_3 and introduce a nonzero element at position $(5,4)$ of M_2. After these rotations, we have

$$\begin{array}{cccc}
M_4 & M_3 & M_2 & M_1 \\
\begin{array}{ccccc}
\bullet & \bullet & \bullet & * & * \\
\bullet & \bullet & \bullet & * & * \\
 & \bullet & \bullet & * & * \\
 & & \bullet & * & * \\
 & & & 0 & *
\end{array} &
\begin{array}{ccccc}
\bullet & \bullet & \bullet & * & * \\
 & \bullet & \bullet & * & * \\
 & & \bullet & * & * \\
 & & & * & * \\
 & & & 0 & *
\end{array} &
\begin{array}{ccccc}
\bullet & \bullet & \bullet & * & * \\
 & \bullet & \bullet & * & * \\
 & & 0 & * & * \\
 & & & * & * \\
 & & & * & *
\end{array} &
\begin{array}{ccccc}
\bullet & \bullet & \bullet & \bullet & \bullet \\
 & \bullet & \bullet & \bullet & \bullet \\
 & & \bullet & \bullet & \bullet \\
 & & & \bullet & \bullet \\
 & & & & \bullet
\end{array}
\end{array}.$$

Next we introduce a zero at position $(4,3)$ of M_4 using a Givens rotation operating on columns 3 and 4. This does not change the zero at position $(5,4)$ of that matrix. We apply the rotation also to the corresponding rows of M_3 and reintroduce the zero at position $(4,3)$ of M_3 by using a Givens rotation operating on the columns of M_3 and the rows of M_2. The result is

$$\begin{array}{ccccc} \multicolumn{5}{c}{M_4} \\ \bullet & \bullet & * & * & \bullet \\ \bullet & \bullet & * & * & \bullet \\ & \bullet & * & * & \bullet \\ & & 0 & * & \bullet \\ & & & & \bullet \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_3} \\ \bullet & \bullet & * & * & \bullet \\ & \bullet & * & * & \bullet \\ & & * & * & * \\ & & 0 & * & * \\ & & & & \bullet \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_2} \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & 0 & * & * \\ & & & * & * \\ & & & \bullet & \bullet \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_1} \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet \\ & & & & \bullet \end{array} .$$

Note that the last transformation did not introduce a nonzero element at position $(4,3)$ of M_2 since the $(3,3)$ element is zero. M_4 does now have the required zero at position $(4,3)$. However, we need to restore M_2 to an upper triangular matrix (i.e., remove the newly introduced nonzeros on the subdiagonal.) In doing so we must take care not to reintroduce a nonzero in M_4 at position $(4,3)$. In our case, there is only one nonzero subdiagonal element in M_2. To remove this element, we apply a Givens rotation to columns 4 and 5 of M_2 and the corresponding rows of M_1. This introduces a nonzero element at position $(5,4)$ of M_1 which is again removed by applying a Givens rotation to columns 4 and 5 of M_1 and rows 4 and 5 of M_4. This does reintroduce a nonzero element at position $(5,4)$ of M_4. We obtain

$$\begin{array}{ccccc} \multicolumn{5}{c}{M_4} \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & 0 & * & * \\ & & & * & * \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_3} \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet \\ & & & & \bullet \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_2} \\ \bullet & \bullet & \bullet & * & * \\ & \bullet & \bullet & * & * \\ & & 0 & * & * \\ & & & * & * \\ & & & 0 & * \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_1} \\ \bullet & \bullet & \bullet & * & * \\ & \bullet & \bullet & * & * \\ & & \bullet & * & * \\ & & & * & * \\ & & & 0 & * \end{array}$$

which is in the desired form.

1.2.2 Phase 2.

In phase 2, we also introduce a zero at position $(3,2)$ of M_4. The procedure is symmetric with the first phase. First we introduce a zero at position $(2,1)$ of M_4 by operating on rows 1 and 2 of M_4 with a Givens rotation and applying the corresponding rotation to columns 1 and 2 of M_1. This itroduces a nonzero element at position $(2,1)$ of M_1 which is subsequently shifted to M_2 using a Givens rotation operating on rows 1 and 2 of M_1 and columns 1 and 2 of M_2. We obtain the following matrices:

$$\begin{array}{ccccc} \multicolumn{5}{c}{M_4} \\ * & * & * & * & * \\ 0 & * & * & * & * \\ & \bullet & \bullet & \bullet & \bullet \\ & & 0 & \bullet & \bullet \\ & & & \bullet & \bullet \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_3} \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet \\ & & & & \bullet \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_2} \\ * & * & \bullet & \bullet & \bullet \\ * & * & \bullet & \bullet & \bullet \\ & & 0 & \bullet & \bullet \\ & & & \bullet & \bullet \\ & & & & \bullet \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_1} \\ * & * & * & * & * \\ 0 & * & * & * & * \\ & & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet \\ & & & & \bullet \end{array} .$$

Similarly, we introduce a zero element at position $(3,2)$ of M_4 operating on rows 2 and 3 of M_4 and columns 2 and 3 of M_1 and reintroduce the zero in that matrix by operating on rows 2 and 3 of that matrix and columns 2 and 3 of M_2. However, this does not introduce a nonzero element at position $(3,2)$ of M_2 since the $(3,3)$ element is zero. Hence we end up with

$$\begin{array}{ccccc} \multicolumn{5}{c}{M_4} \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ & * & * & * & * \\ & 0 & * & * & * \\ & & & \bullet & \bullet \\ & & & \bullet & \bullet \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_3} \\ \bullet & \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet & \bullet \\ & & \bullet & \bullet & \bullet \\ & & & \bullet & \bullet \\ & & & & \bullet \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_2} \\ \bullet & * & * & \bullet & \bullet \\ \bullet & * & * & \bullet & \bullet \\ & & 0 & \bullet & \bullet \\ & & & \bullet & \bullet \\ & & & & \bullet \end{array} \quad \begin{array}{ccccc} \multicolumn{5}{c}{M_1} \\ \bullet & * & * & \bullet & \bullet \\ & * & * & * & * \\ & 0 & * & * & * \\ & & & \bullet & \bullet \\ & & & & \bullet \end{array} .$$

Now we have to restore the upper triangular structure of M_2 again taking care no to reintroduce a nonzero at position $(3,2)$ of M_4. We reintroduce a zero at position $(2,1)$ of M_2 by applying a Givens rotation to rows 1 and 2 of M_2 and columns 2 and 3 of M_3 and then apply a Givens rotation to rows 1 and 2 of M_3 and columns 1 and 2 of M_4 to reintroduce the zero at position.

1.2.3 Algorithm

Algorithm 1.2 *Deflation of a zero on the diagonal of a matrix M_k.*

Input:

$M_1^{(0)}, \ldots, M_m^{(0)}$ *and orthogonal matrices* $Q_0^{(0)}, \ldots, Q_{m-1}^{(0)}$.

k^*, i^* *such that* $M_{k^*}(i^*, i^*) = 0$.

Output:

$M_1, \ldots, M_m$ *and orthogonal matrices* $Q_0, \ldots, Q_{m-1}$ *such that* $Q_i^T Q_i^{(0)} M_i^{(0)} Q_{i-1}^{(0)^T} Q_{i-1} = M_i$ $(Q_m := Q_0)$ *with* $M_m(i^*+1, i^*) = 0$ *and* $M_m(i^*, i^*-1) = 0$.

```
begin
    for i = 1 to m do
        M_i ← M_i^(0)
        Q_{i-1} ← Q_{i-1}^(0)
    endfor
    /* Phase 1a: introduce a zero at M_m(i*+1, i*). */
    for j = N-1 downto i*
        /* Introduce a zero at M_m(j+1, j). */
        for k = m downto k*+1
            Construct a Givens rotation J such that M_k J^T has a zero at position (j+1, j) changing
            only columns j and j+1 of M_k.
            M_k ← M_k J^T; M_{k-1} ← J M_{k-1}; Q_{k-1} ← Q_{k-1} J^T;
        endfor
    endfor
    /* Phase 1b: restore the upper triangular structure of M_{k*}. */
    for j = N-1 downto i*+1
        /* Introduce a zero at M_{k*}(j+1, j). */
        for k = k* downto 1
            Construct a Givens rotation J such that M_k J^T has a zero at position (j+1, j) changing
            only columns j and j+1 of M_k..
            M_k ← M_k J^T; M_{k-1} ← J M_{k-1} (M_0 := M_m); Q_{k-1} ← Q_{k-1} J^T;
        endfor
    endfor
    /* Phase 2a: introduce a zero at position M_m(i*, i*-1). */
    for i = 2 to i*
        /* Introduce a zero at M_m(i, i-1). */
        for k = 0 to k*-1
            Construct a Givens rotation J such that J M_k(i, i-1) = 0 (M_0 := M_m) changing only
            rows i-1 and i of M_k.
            M_k ← J M_k; M_{k+1} ← M_{k+1} J^T; Q_{k+1} ← J Q_{k+1};
        endfor
    endfor
    /* Phase 2b: restore the upper triangular structure of M_{k*}. */
    for i = 2 to i*-1
        /* Introduce a zero at position M_{k*}(i, i-1). */
        for k = k* to m-1
            Construct a Givens rotation J such that J M_k(i, i-1) = 0 (M_0 := M_m) changing only
            rows i-1 and i of M_k.
            M_k ← J M_k; M_{k+1} ← M_{k+1} J^T; Q_{k+1} ← J Q_{k+1};
        endfor
    endfor
end
```

1.3 Single-shift QR step

We implement a single-shift QR step based on the implicit-Q theorem. Therefore this step should be aplied to an unreduced block in the periodic Hessenberg decomposition. This implies that there should be no zeros on the diagonal of the matrices M_i, $i = 1, \ldots, m-1$ and on the subdiagonal of M_m for the block under consideration.

Let us consider the following set of 3 3-by-3 matrices as an example:

$$\begin{array}{ccccccccccc} & M_3 & & & & M_2 & & & & M_1 & \\ \bullet & \bullet & \bullet & & \bullet & \bullet & \bullet & & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & & & \bullet & \bullet & & & \bullet & \bullet \\ & \bullet & \bullet & & & & \bullet & & & & \bullet \end{array}.$$

First we must construct the first column of the matrix $M_3 M_2 M_1 - \lambda I$ where λ is our shift. Note that this only requires the first column of M_3 and the (1,1)-elements of M_2 and M_1. First we construct a Givens rotation $J(1,2)$ which introduces a zero on the $(2,1)$-position of $M_3 M_2 M_1 - \lambda I$. This transformation is applied to rows 1 and 2 of M_3 and columns 1 and 2 of M_1, introducing a nonzero off-diagonal element at position $(2,1)$ of the latter:

$$\begin{array}{ccccccccccc} & M_3 & & & & M_2 & & & & M_1 & \\ * & * & * & & \bullet & \bullet & \bullet & & * & * & \bullet \\ * & * & * & & & \bullet & \bullet & & * & * & \bullet \\ & \bullet & \bullet & & & & \bullet & & & & \bullet \end{array}.$$

Not that this does not introduce a zero at the $(2,1)$-position of M_3! Now we restore the structure of M_1 by shifting the nozero subdiagonal element to M_2 using a Givens rotation operating on rows 1 and 2 of M_1 and columns 1 and 2 of M_2, and shift the nonzero element now appearing at position $(2,1)$ of M_2 to M_3 in an identical way. This introduces a nonzero element at position $(3,1)$ of M_3:

$$\begin{array}{ccccccccccc} & M_3 & & & & M_2 & & & & M_1 & \\ * & * & \bullet & & * & * & * & & * & * & * \\ * & * & \bullet & & 0 & * & * & & 0 & * & * \\ * & * & \bullet & & & & \bullet & & & & \bullet \end{array}.$$

This element is removed by a Givens rotation $J(2,3)$ applied to M_3 and M_1:

$$\begin{array}{ccccccccccc} & M_3 & & & & M_2 & & & & M_1 & \\ \bullet & \bullet & \bullet & & \bullet & \bullet & \bullet & & \bullet & * & * \\ * & * & * & & & \bullet & \bullet & & & * & * \\ 0 & * & * & & & & \bullet & & & * & * \end{array}.$$

Now we apply a Givens rotation to rows 2 and 3 of M_1 and columns 2 and 3 of M_2 to remove the nozero element $M_1(3,2)$ and next we apply a Givens rotation to rows 2 and 3 of M_2 and columns 2 and 3 of M_3 to remove the nozero element $M_2(3,2)$. The last rotation does not introduce a new nozero element in M_3 and we have restored the periodic upper Hessenberg structure:

$$\begin{array}{ccccccccccc} & M_3 & & & & M_2 & & & & M_1 & \\ \bullet & * & * & & \bullet & * & * & & \bullet & \bullet & \bullet \\ \bullet & * & * & & & * & * & & & * & * \\ & * & * & & & 0 & * & & & 0 & * \end{array}.$$

1.3.1 Algorithm

Algorithm 1.3 *Single-shift periodic QR step.*

Input:

$M_1^{(0)}, \ldots, M_m^{(0)}$ *and orthogonal matrices* $Q_0^{(0)}, \ldots, Q_{m-1}^{(0)}$. $M_m^{(0)}$ *is in upper Hessenberg form, the other matrices* $M_k^{(0)}$ *are all upper triangular.*

L *and* U*, the first and last row of an unreduced block in the periodic Hessenberg form.*

Output:

$M_1, \ldots, M_m$ *and orthogonal matrices* $Q_0, \ldots, Q_{m-1}$ *such that* $Q_i^T Q_i^{(0)} M_i^{(0)} {Q_{i-1}^{(0)}}^T Q_{i-1} = M_i$ $(Q_m := Q_0)$.

begin

for $i = 1$ ***to*** m ***do***

$M_i \leftarrow M_i^{(0)}$

$Q_{i-1} \leftarrow Q_{i-1}^{(0)}$

endfor

Determine the shift λ.

Compute elements L *and* $L+1$ *of column* L *of* $H = M_m \cdots M_1$*:* $H(L:L+1,L) = M_m(L:L+1,:)\,(M_{m-1}(L,L)\cdots M_1(L,L))$.

Compute a Givens transformation $J(L,L{+}1)$ *such that* $J(L,L{+}1)H$ *has a zero at position* $(L+1,L)$.

$M_m \leftarrow J(L,L{+}1)M_m$; $M_1 \leftarrow M_1 J(L,L{+}1)^T$; $Q_0 \leftarrow Q_0 J(L,L{+}1)^T$.

/ Restore the upper Hessenberg structure. */*

for $k=1$ ***to*** $m-1$

  Construct a Givens rotation $J(L,L{+}1)$ *to introduce a zero at position* $(L+1,L)$ *of* M_k.

  $M_k \leftarrow J(L,L{+}1)M_k$; $M_{k+1} \leftarrow M_{k+1}J(L,L{+}1)^T$; $Q_k \leftarrow Q_k J(L,L{+}1)^T$.

endfor

for $j=L$ ***to*** $U-1$ */* Restore the structure of column j. */*

  for $k=1$ ***to*** $m-1$

    Construct a Givens rotation $J(j,j{+}1)$ *to introduce a zero at position* $(j+1,j)$ *of* M_k.

    $M_k \leftarrow J(j,j{+}1)M_k$; $M_{k+1} \leftarrow M_{k+1}J(j,j{+}1)^T$; $Q_k \leftarrow Q_k J(j,j{+}1)^T$.

  endfor

  if $(j<U-1)$ ***then***

    Construct a Givens rotation $J(j{+}1,j{+}2)$ *to introduce a zero at position* $(j+2,j)$ *of* M_m.

    $M_m \leftarrow J(j{+}1,j{+}2)M_m$; $M_1 \leftarrow M_1^T J(j{+}1,j{+}2)^T$; $Q_0 \leftarrow Q_0^T J(j{+}1,j{+}2)^T$.

  endif

endfor

end

There are two points in this algorithm where there is a risk of overflow or underflow: the determination of the shift λ and the computation of the (L,L)- and $(L+1,L)$-elements of $M_m \cdots M_1$. In both cases, we represent the product as a mantissa and exponent (base 2.)

Convergence of single-shift QR iterations is declared if an eigenvalue splits off at the lower right, i.e, if $M_m(U,U-1)$ becomes small compared to $M_m(U-1,U-1)$ and $M_m(U,U)$.

1.4 Double-shift QR step

The double-shift QR step is used as the basic tool in order to compute the eigenvalues and it is also used during the reordering of eigenvalues when a pair of complex conjugate eigenvalues is moved down along the diagonal of the product Hessenberg matrix.

In the double-shift QR step, two single-shift QR steps with shifts λ_1 and λ_2 are combined into a single step such that all arirthmetic is real for real matrices even if the two shifts are complex conjugate numbers. Let H be an unreduced $n \times n$-block of the Hessenberg decomposition. We need to compute the first column of

$$\bar{H} = (H-\lambda_1 I)(H-\lambda_2 I) = H^2 - (\lambda_1+\lambda_2)H + \lambda_1\lambda_2 I. \tag{1}$$

Hence we really only need to know the sum and the product of the shifts. Usually, the eigenvalues of the lower 2×2-block of H are used as the shifts, resulting in

$$\begin{aligned} \lambda_1+\lambda_2 &= H(n\text{-}1,n\text{-}1) + H(n,n), \\ \lambda_1\lambda_2 &= H(n\text{-}1,n\text{-}1)H(n,n) - H(n\text{-}1,n)H(n,n\text{-}1). \end{aligned} \tag{2}$$

However, as explained in [**?**], catastrophic cancellation can occur if (2) is used to compute the sum and product of the shifts and the first column of (1) is then formed using these values. Instead we use the formulas

$$\begin{aligned} \bar{H}(1,1) &= H(2,1)\,[((H(n,n)-H(1,1))\,(H(n\text{-}1,n\text{-}1)-H(1,1)) - H(n,n\text{-}1)\,H(n\text{-}1,n)) \\ &\qquad /H(2,1) + H(1,2)] \\ \bar{H}(2,1) &= H(2,1)\,[H(2,2)-H(1,1)-(H(n,n)-H(1,1))-(H(n\text{-}1,n\text{-}1)-H(1,1))] \\ \bar{H}(3,1) &= H(2,1)H(3,2). \end{aligned}$$

that are obtained by substituting (2) in (1) and reordering the formula's for the first three elements on the first column. Since we really only need the first column up to a constant factor, we can omit the common factor $H(2,1)$.

We will never compute the whole unreduced block H. Instead we only construct its lower right $2{\times}2$-block and upper left 3×2-block since this is all we need for the double-shift periodic QR step. Care is taken to avoid overflow of matrix elements or underflow of all elements while constructing the product: the product is represented as a matrix times a common factor for all elements stored as the 2-logarithm of the actual number. These products can usually be computed with only moderate loss of accuracy. Problems will only occur if the eigenvalues of the unreduced block in the periodic Hessenberg decomposition have largely different moduli. In this case, the shifts will likely be very small and the double-shift QR step will behave very much like two subsequent subspace iteration steps, quickly separating the block in smaller blocks. Convergence is more troublesome than for the usual QR algorithm. We dealt with this by implementing two special shift strategies (based on the EISPACK HQR2 routine and LAPACK code) and if this fails we have yet another backup strategy to be discussed later on.

We proceed in a similar way as for the single-shift QR step. First a Householder transformation is computed to zero all bu the first element of the first column of $\bar{H}$. This transformation is the applied to the corresponding rows of M_m and columns of M_1 and introduces nonzero 3×3-blocks on the diagonal of these matrices. Finally we restore the periodic Hessenberg structure by shifting the nonzero subdiagonal elements in M_1 to M_m and the elements below the subdiagonal of M_m down. We demonstrate this procedure of a product of 3 4×4-matrices. First a Householder transformation P is constructed such that

$$P \begin{bmatrix} \bar{H}(1,1) \\ \bar{H}(2,1) \\ \bar{H}(3,1) \end{bmatrix} = \begin{bmatrix} * \\ 0 \\ 0 \end{bmatrix}. \tag{3}$$

This transformation is applied to rows 1 to 3 of M_m and columns 1 to 3 of M_1. This introduces three nonzero elements in H_1 at the positions $(2,1)$, $(3,1)$ and $(3,2)$ and a nonzero element in the $(3,1)$ position of M_m:.

$$\begin{array}{cccccccccccccc}
\multicolumn{4}{c}{M_3} & & \multicolumn{4}{c}{M_2} & & \multicolumn{4}{c}{M_1} \\
* & * & * & * & & \bullet & \bullet & \bullet & \bullet & & * & * & * & \bullet \\
* & * & * & * & & & \bullet & \bullet & \bullet & & * & * & * & \bullet \\
* & * & * & * & & & & \bullet & \bullet & & * & * & * & \bullet \\
 & & \bullet & \bullet & & & & & \bullet & & & & & \bullet
\end{array}.$$

To restore the structure, we fist build a Householder reflection $P^{[1]}_{1,2:3}$ to zero the $(2,1)$ and $(3,1)$ elements of M_1 and apply the transformation is applied to the rows of M_1 and the columns of M_2 resulting in

$$\begin{array}{cccccccccccccc}
\multicolumn{4}{c}{M_3} & & \multicolumn{4}{c}{M_2} & & \multicolumn{4}{c}{M_1} \\
\bullet & \bullet & \bullet & \bullet & & * & * & * & \bullet & & * & * & * & * \\
\bullet & \bullet & \bullet & \bullet & & * & * & * & \bullet & & 0 & * & * & * \\
\bullet & \bullet & \bullet & \bullet & & * & * & * & \bullet & & 0 & * & * & * \\
 & & \bullet & \bullet & & & & & \bullet & & & & & \bullet
\end{array}.$$

Then the $(2,1)$ and $(3,1)$ elements of M_2 are zeroed using the Householder reflection $P^{[2]}_{1,2:3}$ applied to the rows of M_2 and the columns of M_3. The resulting structure is

$$\begin{array}{cccccccccccccc}
\multicolumn{4}{c}{M_3} & & \multicolumn{4}{c}{M_2} & & \multicolumn{4}{c}{M_1} \\
* & * & * & \bullet & & * & * & * & * & & \bullet & \bullet & \bullet & \bullet \\
* & * & * & \bullet & & 0 & * & * & * & & & \bullet & \bullet & \bullet \\
* & * & * & \bullet & & 0 & * & * & * & & & \bullet & \bullet & \bullet \\
* & * & * & \bullet & & & & & \bullet & & & & & \bullet
\end{array}.$$

Next the $(3,1)$ and $(4,1)$ elements of M_3 are zeroed using a Householder transformation $P^{[3]}_{2,3:4}$. This transformation is applied to the rows of M_3 and the columns of M_1 and does not affect the first column of M_1. We end up with the matrix structure

$$\begin{array}{cccccccccccccc}
\multicolumn{4}{c}{M_3} & & \multicolumn{4}{c}{M_2} & & \multicolumn{4}{c}{M_1} \\
\bullet & \bullet & \bullet & \bullet & & \bullet & \bullet & \bullet & \bullet & & \bullet & * & * & * \\
* & * & * & * & & & \bullet & \bullet & \bullet & & & * & * & * \\
0 & * & * & * & & & \bullet & \bullet & \bullet & & & * & * & * \\
0 & * & * & * & & & & & \bullet & & & * & * & *
\end{array}.$$

The first column of each of the matrices is now in the desired form and we will not touch these columns anymore. In the next phase, we first zero the $(3,2)$ and $(4,2)$ elements of M_1 introducing 2 new nonzero elements in M_2, then zeros the corresponding elements in H_2 and finally zero the $(4,2)$-element in M_3. This results in the matrices

$$\begin{array}{ccc} M_3 & M_2 & M_1 \\ \begin{array}{cccc} \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet \\ & & \bullet & \bullet \end{array} & \begin{array}{cccc} \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet \\ & & \bullet & \bullet \\ & & \bullet & \bullet \end{array} & \begin{array}{cccc} \bullet & \bullet & \bullet & \bullet \\ & \bullet & \bullet & \bullet \\ & & \bullet & \bullet \\ & & \bullet & \bullet \end{array} \end{array}.$$

Finally, we zero the $(4,3)$ elements of M_1 and M_2. This can be done without destroying the structure of M_3 by using transformations that only involve the last two rows/columns of the matrices.

1.4.1 Algorithm

Algorithm 1.4 *Double-shift periodic QR step.*

Input:

$M_1^{(0)}, \ldots, M_m^{(0)}$ *and orthogonal matrices* $Q_0^{(0)}, \ldots, Q_{m-1}^{(0)}$. $M_m^{(0)}$ *is in upper Hessenberg form, the other matrices* $M_k^{(0)}$ *are all upper triangular.*

L *and* U*, the first and last row of an unreduced block in the periodic Hessenberg form.*

Output:

$M_1, \ldots, M_m$ *and orthogonal matrices* $Q_0, \ldots, Q_{m-1}$ *such that* $Q_i^T Q_i^{(0)} M_i^{(0)} Q_{i-1}^{(0)^T} Q_{i-1} = M_i$ *(*$Q_m := Q_0$*).*

begin

for $i = 1$ ***to*** m ***do***

$M_i \leftarrow M_i^{(0)}$

$Q_{i-1} \leftarrow Q_{i-1}^{(0)}$

endfor

Determine the sum and product of the shifts λ_1 *and* λ_2 *anc compute the top 3 elements of the first column of* $\bar{H} = H^2 - (\lambda_1 + \lambda_2)H + \lambda_1\lambda_2 I$ *with* $H = M_m(L{:}U, L{:}U) \cdots M_1(L{:}U, L{:}U)$.

Construct a Householder reflection P *such that* $P\bar{H}(1{:}3, 1) = \begin{bmatrix} * & 0 & 0 \end{bmatrix}^T$.

$M_m(L{:}L{+}2, :) \leftarrow PM_m(L{:}L{+}2, :)$; $M_1(:, L{:}L{+}2) \leftarrow M_1(:, L{:}L{+}2)P$; $Q_0(:, L{:}L{+}2) \leftarrow Q_0(:, L{:}L{+}2)P$

for $j = L$ ***to*** $U - 2$ */* Restore column* j*. */*

for $k = 1$ ***to*** $m - 1$

Construct a Householder transformation P *(operating on rows* j *to* $j+2$*) to introduce zeros in the* $(j+1, j)$*- and* $(j+2, j)$*-positions of* M_k.

$M_k \leftarrow PM_k$; $M_{k+1} \leftarrow M_{k+1}P$; $Q_k \leftarrow Q_k P$

endfor

if $(j < U - 2)$ ***then***

Construct a Householder transformation P *(operating on rows* $j+1$ *to* $j+3$*) to introduce zeros in the* $(j+2, j)$*- and* $(j+3, j)$*-positions of* M_m.

$M_m \leftarrow PM_m$; $M_1 \leftarrow M_1 P$; $Q_0 \leftarrow Q_0 P$

else

Construct a Givens rotation $J(j+1, j+2)$ *to introduce a zero in the* $(j+2, j)$*-position of* M_m.

$M_m \leftarrow J(j+1, j+2)M_m$; $M_1 \leftarrow M_1 J(j+1, j+2)^T$; $Q_0 \leftarrow Q_0 J(j+1, j+2)^T$.

endif

endfor

/ Restore column U-1. */*

for $k = 1$ ***to*** $m - 1$

Construct a Givens rotation $J(U-1, U)$ *to introduce a zero in the* $(U, U-1)$*-position of* M_k.

$M_k \leftarrow J(U-1, U)M_k$; $M_{k+1} \leftarrow M_{k+1} J(U-1, U)^T$; $Q_k \leftarrow Q_k J(U-1, U)^T$.

endfor

end

Note: if the shifts are very large compared to the elements of the first two columns of H, the matrix $H^2 - (\lambda_1 + \lambda_2)H + \lambda_1\lambda_2 I$ will numerically be equal to a multiple of the identity matrix in the first column and therefore QR will not converge. It is not always possible to put the largest eigenvalues down the diagonal using QR steps. The solution to this impasse is to do one or more single-shift or double-shift steps with zero shift(s). This essentially does subspace iteration steps and the largest eigenvalues will appear on the upper left of the Hessenberg block.

Note that our implementation is based on the implicit Q-theorem. This implies that we assume that no subdiagonal elements are "zere" in the active block. Experiments have shown that double-shift QR is more sensitive to the size of subdiagonal elements than single-shift QR iterations.

1.5 Computing eigenvalues of a 2×2-block.

If a 2×2-block in the periodic Hessenberg decomposition corresponds to a pair of complex conjugate eigenvalues, no further reduction is possible. However, if the block corresponds to two real eigenvalues, a further reduction of that block to a periodic upper triangular block is possible. This is done as follows.

- After multiplying all 2×2-blocks together, we compute the eigenvector v_1 for the largest eigenvalue λ_1 of the block. (The largest one since that is the most stable one to compute and since we are usually interested in our applications to have the eigenvalues sorted from largest to smallest along the diagonal.) Next we compute a Givens rotation J such that $Jv_1 = \|v_1\|_2 e_1$. We apply the transformation J to the rows of M_m and columns of M_1 corresponding to the block and restore the upper Hessenberg structure by shifting the nonzero element introduced on the subdiagonal of M_1 to M_m. If no round-off errors were made, the 2×2-block in M_m now becomes upper triangular since assuming $Mv_1 = \lambda v_1$ and $Jv_1 = \|v_1\|_2 e_1$, one has

  $$JMJ^T e_1 = \|v_1\|_2 JMv_1 = \lambda_1 \|v_1\|_2 Jv_1 = \lambda_1 \|v_1\|_2 e_1$$

  or in words, the first column of JMJ^T is a multiple of the first unit vector.

- However, round-off errors occur during the multiplication of the 2×2-blocks and therefore the subdiagonal element in M_m may still be too large. In this case we do one or more single-shift QR iterations using the lower right element as the shift. These iterations usually converge very rapidly since the off-diagonal element is usually very small.

The discriminant of the characteristic equation of a matrix

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

is computed using the formula

$$D = (a-d)^2 + 4bc$$

and not using $D = (a+d)^2 + 4(bc - ad)$ for reasons of numerical stability (just check what would happen with the matrix

$$\begin{bmatrix} 1-\varepsilon_1 & \varepsilon_2 \\ \varepsilon_2 & 1-\varepsilon_1 \end{bmatrix}$$

with ε_1 and ε_2 just larger than machine precision.)

1.6 Testing for zeros

Let us define the following constants:

- **sfmin** is the safe minimum, i.e., the smallest number such that $1/$**sfmin** does not overflow. It is computed by the Lapack routine DLAMCH('S').
- ε is the machine precision.
- **smlnum** $= N*$ **sfmin** $/\varepsilon$ where N is the size of the matrices.
- **tol** is an additional tolerance factor allowed.

- Let **SS** be the average of the absolute values just above and just right of the element which we want to test. If both are zero (or outside the matrix), we use the average of the absolute values of all matrix elements.

Then: a number R is consedered to be zero if

$$R < \max(\textbf{tol} * \textbf{SS} * \varepsilon,\ \textbf{smlnum}).$$

1.7 Exceptional shifts

Convergence of the periodic QR iterations is more troublesome as for the traditional QR iterations. Therefore special shift strategies are even more important. Several strategies have been considered. In all cases we build a 2×2-matrix such that its eigenvalues are the exceptional shifts and overwrite the matrix from which the shifts would be determined otherwise. All strategies below start from the product Hessenberg matrix.

- The strategy used by the Lapack routine DLAHQR, the traditional double-shift QR routine in Lapack. Here we have a complex conjugate pair of shifts. If H is the lower 3×3-block of the product Hessenberg matrix, the shifts are

$$s_{1,2} = (|H(2,1)| + |H(3,2)|)\,(0.75 \pm i\sqrt{0.4375}).$$

- The strategy used by the Lapack routine DHSEQR, the multiple shift QR routine. This routine uses two real special shifts,

$$\begin{aligned} s_1 &= 1.5\,(|H(2,1)| + |H(2,2)|)\,, \\ s_2 &= 1.5\,(|H(3,2)| + |H(3,3)|)\,. \end{aligned}$$

- A third possibility is to do a single- or double-shift QR step with zero shift(s), which is essentially one or two subspace iteration steps. We did not withold this strategy, since convergence can be extrememly slow.

If all else fails, some other strategies are also possible. Let H be the product of the currently active blocks in the periodic Hessenberg decomposition. H is an upper Hessenberg matrix. Scalar rescaling of the matrix should be used to avoid overflow problems. Computing its eigenvalues will usually give more accurate results than computing the eigenvalues of the product of the original matrices. We expect best accuracy for the largest eigenvalues. Note that we can still not expect to find all eigenvalues accurately if the difference between the moduli of the largest and smallest eigenvalues is extreme. Underflow may render the smallest eigenvalues inaccurate, even if H would already be in Schur form. Let

$$HQ = QR$$

be the real Schur decomposition of H. We can try the following strategies:

- Since the largest eigenvalues are reliable, we can use them as the new shift(s). Note however that since we are usually interested in getting the largest eigenvalues first on the diagonal of the periodic Schur decomposition, reordering will be needed at the end.
- We can also use the smallest eigenvalues. They are not always very accurate and so the eigenvalue will not split off after one iteration. In case some eigenvalues are very large compared to others, the shift(s) will be essentially zero, but some of the largest eigenvalues should split off at the front of the active block.
- We can multiply the rows of R_m with Q^T and the columns of G_1 with Q and then restore the upper Hessenberg matrix. This might isolate a few eigenvalues in smaller blocks, and will definitely change the periodic Hessenberg matrix a lot so that the next double-shift or single-shift iterations might again converge. However, near-isolation is quite uncommon. This can be understood as follows.
  - Compute G_1Q and compute the QR decomposition $G_1Q = Q_2R_1$. Now we have

$$Q^T G_m \cdots G_2 G_1 Q = Q^T G_m \cdots G_2 Q_2 R_1.$$

    We can now continue by orthogonalising G_2Q_2 and so on until we reach

$$Q^T G_m \cdots G_2 G_1 Q = Q^T G_m Q_m R_{m-1} \cdots R_1.$$

– In the absence of numerical errors in the computation of Q and all further decompositions, $Q^T G_m Q_m$ would be upper Hessenberg. However, because of round-off errors, elements below the subdiagonal will be small but not non-negligible. Assume that the first column of Q is a fairly accurate eigenvector of H for a real eigenvector. After the above steps, the first column will have all near-zero subdiagonal entries. However, entries below the subdiagonal in that columns are not necessarily much smaller than the subdiagonal entry. One should now construct a Householder reflection to put the entries below the subdiagonal to zero and apply that transformation to the rows of G_m and columns of G_1. Since the subdiagonal element and all elements below that one are of comparable size, the transformation matrix is not at all near the identity matrix. After applying it to the columns of R_1 and after restoring the upper triangular structure of the matrices $R_1, \ldots, R_{m-1}$, the new G_m is not at all close to the matrix of the Schur decomposition anymore, and not even close to Hessenberg. If the first two columns of Q would correspond to a pair of complex conjugate eigenvalues, the transformations for the first column would still be close to the identity matrix, but the same story would happen for the second column. We cannot expect to isolate more than one eigenvalue or eigenvalue pair with this procedure, and that block will be at the front of the decomposition and not at the back. It should be combined with the above strategy using another computed eigenvalue (pair) as the shift(s) for the next QR step.

1.8 Exchanging eigenvalues