ALGORITHM 590
DSUBSP and EXCHQZ: FORTRAN Subroutines for Computing Deflating Subspaces with Specified Spectrum

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1. DESCRIPTION

A reliable and widely available method to compute the generalized eigenvalues of an $n \times n$ real regular (i.e., invertible) pencil $\lambda B - A$ is the so-called QZ-algorithm [1, 3]. This algorithm constructs orthogonal row and column transformations $Q$, and $Z$, such that the transformed pencil

$$\lambda B_1 - A_1 = Q (\lambda B - A) Z,$$

is in "quasi-triangular" form, that is, with $B_1$ in upper triangular form and $A_1$ in lower triangular form, or in block triangular Hessenberg form with $1 \times 1$ and $2 \times 2$ diagonal blocks, as illustrated below:

$$B_1 = \begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{bmatrix}, \quad A_1 = \begin{bmatrix} x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{bmatrix}$$

(2)

The $1 \times 1$ diagonal pencils of $\lambda B_1 - A_1$ contain the real generalized eigenvalues of the pencil $\lambda B - A$, and the $2 \times 2$ diagonal pencils of $\lambda B_1 - A_1$ contain the complex generalized eigenvalues, a conjugate pair to each $2 \times 2$ pencil.
The FORTRAN subroutines DSUBSP and EXCHQZ allow one to update the
decomposition (1) by premultiplying Z by B, and by Q, by Q, such that
\[ \lambda B^* + A = Q B^* Q + Z^* Z. \] (3)
is still in quasi-triangular form, but in addition, a specific ordering of generalized
eigenvalues is obtained in this form. This is important in several applications [6, 7]. Indeed, when the generalized eigenvalues \( \lambda_1, \ldots, \lambda_r \) are ordered such that
\[ \lambda_1, \ldots, \lambda_r \] are inside a region \( \Gamma \) and \( \lambda_{r+1}, \ldots, \lambda_r \) are outside this region, then the
space spanned by the first \( r \) orthonormal columns of \( Z = Z_1 Z \), is the deflating
subspace [4] of \( \lambda B - A \) corresponding to the spectrum inside \( \Gamma \). In several
applications, deflating subspaces have to be computed for different regions \( \Gamma \). Of
course, \( \Gamma \) has to be symmetric with respect to the real axis, since complex pairs
of eigenvalues have to be categorized both outside or inside \( \Gamma \) in order for this
deflating subspace to be real. No further assumptions have to be imposed on \( \Gamma \):
it can be open or not, connected or not.

The user has to provide a function describing the region \( \Gamma \) by testing whether
the generalized eigenvalues of a \( 1 \times 1 \) or \( 2 \times 2 \) (diagonal) pencil lies inside or
outside the region \( \Gamma \). This function must be of the type

**INTEGER FUNCTION PTEST (LSIZE, ALPHA, BETA, S, P)**

with parameters:

- **LSIZE**: An integer containing the size of the considered pencil (1 or 2).
- **ALPHA, BETA**: Two real variables. In case **LSIZE**=1, the generalized eigenvalue of the considered pencil is given by **ALPHA**/**BETA**, which may be infinite when **BETA=0**.
- **S, P**: Two real variables. In case **LSIZE**=2, they contain the sum and product of the two complex conjugate generalized eigenvalues of the considered pencil.
- **PTEST**: The function value, which is put equal to 1 when the general-
edized eigenvalue(s) of the considered pencil is (are) inside the
specified region \( \Gamma \), and equal to -1 otherwise.

Simple examples for such routines are given by the functions FIN, FOINT, FOIHP, and FCRHP, describing the regions inside and outside the unit circle, the open left half-plane, and the closed right half-plane, respectively. Their listings are included below as templates for the user.

This routine is then used as parameter for the subroutine DSUBSP which
orders the \( 1 \times 1 \) and \( 2 \times 2 \) diagonal pencils of the quasi-triangular form \( \lambda B = A \), such that those with generalized eigenvalues inside \( \Gamma \) appear first. The calling sequence for DSUBSP is

**CALL DSUBSP (NMAX, N, A, B, Z, PTEST, EPS, NDIS, FAHL, IND)**

with (parameters preceded by an asterisk are altered by the subroutine):

- **NMAX**: An integer containing the first dimension of the array \( A, B, \) and \( Z \).
- **N**: An integer containing the current order of \( A, B, \) and \( Z \).
Doubly subscripted real arrays containing the pencil to be reordered. On return, \( A \ldots A \) contains the final quasi-triangular pencil rearranged with respect to the region \( I^\prime \) specified by \texttt{FTEST}.

\(*Z\) A doubly subscripted real array into which the reducing column transformation is postmultiplied.

\texttt{FTEST} The integer function provided by the user to describe the region \( I^\prime \) of interest.

\texttt{EPS} A real number used as the convergence criterion. Maximal accuracy is obtained when \( \texttt{EPS} \) is set equal to \( \text{replr} \times \max(|A_{11}, |B_{11}|) \), where replr is the relative precision of the computer used. Smaller values of \( \texttt{EPS} \) will increase the amount of work without significantly improving the accuracy.

\(*NDM\) An integer giving the dimension of the computed deflating subspace.

\(*FAIL\) A logical variable that on normal return is \texttt{FALSE}. If the iterative part of the algorithm does not converge, \texttt{FAIL} is set to \texttt{TRUE}.

\(*IND\) An integer working array of dimension at least \( N \).

\texttt{DSURSP} is to be used together with the 
EISPACK programs \texttt{QZIES}, \texttt{QZIT}, and \texttt{QZVAL} \cite{1} to reduce a full pencil \( \lambda B - A \) to a quasi-triangular form with the eigenvalues inside the contour \( \Gamma \) appearing first on diagonal. (For the explanation of the parameters \texttt{EPSI}, \texttt{IERR}, \texttt{ALPHAR}, \texttt{ALPHAI}, and \texttt{BETA} in these routines, see \cite{1}).

\begin{align*}
&\text{CALL QZIES}(N, A, B, \text{TRUE, Z})
&\text{CALL QZIT}(N, A, B, \text{EPSI, TRUE, Z, IERR})
&\text{CALL QZVAL}(N, A, B, \text{ALPHAR, ALPHAI, BETA, TRUE, Z})
&\text{CALL DSURSP}(N, A, B, Z, \text{FTEST, EPS, NDM, FAIL, IND})
\end{align*}

Besides the function \texttt{FTEST}, describing the region \( I^\prime \) of interest, \texttt{DSURSP} also uses the subroutines \texttt{EXCHQZ}, \texttt{GIV}, and \texttt{SROT}. \texttt{EXCHQZ} is a FORTRAN subroutine to interchange two adjacent \((1 \times 1) \) or \((2 \times 2)\) pencils of a quasi-triangular form. Specifically, if it is supposed that \( A \) has a block of order \( I^\prime \) starting at the \( i^\prime\)th diagonal element illustrated below for \( n = 5, I^\prime = 2, I_{ii} = 2, I_{i'} = 1\):

\[
B = \begin{bmatrix}
1 & x & x & x & x \\
x & x & x & x & x \\
x & x & x & x & x \\
x & x & x & x & x \\
x & x & x & x & x
\end{bmatrix}, \quad A = \begin{bmatrix}
1 & x & x & x & x \\
x & x & x & x & x \\
x & x & x & x & x \\
x & x & x & x & x \\
x & x & x & x & x
\end{bmatrix}
\]

(4)

\texttt{EXCHQZ} constructs orthogonal row and column transformations \( V \) and \( W \) such that \( V(\lambda B - A)W \) has consecutive blocks of order \( I^\prime \) and \( I_{ii} \) at the \( i^\prime\)th diagonal.

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diagonal element (illustrated for the example above):

\[
\begin{bmatrix}
| x | x | x | x | \\
| x | x | x | x | \\
| x | x | x | x | \\
| x | x | x | x |
\end{bmatrix}
\]

\[
\begin{bmatrix}
| x | x | x | x | \\
| x | x | x | x | \\
| x | x | x | x | \\
| x | x | x | x |
\end{bmatrix}
\]

The generalized eigenvalues associated with each diagonal block are interchanged along with the blocks. The column transformation \( W \) is postmultiplied into the array \( Z \); the row transformation \( V \) is not stored since it is not required in the computation of bases of deflating subspaces.

The calling sequence for EXCHQZ is

\[
\text{CALL EXCHQZ(NMAX, A, B, Z, L, LS1, LS2, EPS, FAIL)}
\]

with parameters preceded by an asterisk are altered by the subroutine:

- **NM**
  - An integer containing the current dimension of \( A, B \), and \( Z \).
- **N**
  - An integer containing the current dimension of \( A, B \), and \( Z \).
- \( \ast A, \ast B \)
  - Doubly subscripted real arrays containing the pencil to be reordered.
- \( \ast Z \)
  - A doubly subscripted real array into which the updating column transformation is postmultiplied.
- **L**
  - An integer containing the leading diagonal position of the first block to be interchanged.
- **LS1**
  - An integer containing the size of the first block.
- **LS2**
  - An integer containing the size of the second block.
- **EPS**
  - A convergence criterion (cf. EPS is the calling sequence of DSUBSP).
- **FAIL**
  - A logical variable that on normal return is FALSE. If the iterative part of the algorithm does not converge, FAIL is set to .TRUE.

EXCHQZ requires the subroutines GIV and SROT, which are elementary routines that construct and perform, given a rotation on column or rows. SROT is a RLA subroutine and GIV is a modification of SROT of the BLAS package [2] in order to allow a more compact code for EXCHQZ, which contains several calls to these routines.

2. METHOD AND PROGRAMMING DETAILS

The subroutine DSUBSP makes a first pass through the diagonal blocks of the quasi-triangular form \( B \sim A \) in order to determine the size of the diagonal blocks and the locations of their generalized eigenvalues with respect to \( \Gamma \). During this pass the integer vector \( \text{IND}(i) \) is created with entries \( \pm 1 \) or \( \pm 2 \). Here \text{sign} \( (\text{IND}(i)) \) refers to the location of the generalized eigenvalues of block \( I \) with respect to \( \Gamma \): + for inside \( \Gamma \), - for outside \( \Gamma \) and abs(\text{IND}(i)) indicates the size

of this block. The entries of this vector are then rearranged such that the plus signs appear first. This is done using a "bubble sort"; thus, it is each time a plus sign is moved to the plus sign following a minus sign, it is moved in front of all the preceding minus signs via
consecutive permutations. Each permutation, of course, involves an interchange
of two consecutive blocks using the subroutine EXCHQZ.

EXCHQZ works in a fashion similar to the routine EXCHNG, developed for the
reordering of the standard eigenvalue problem [1] (this is also the reason why an
appealing parallelism with that paper has been pursued here). To interchange
two consecutive blocks where at least one of them has order 1, a shift is performed
to the real eigenvalue of a 2 x 1 block (in [3], this was only done for the
interchange of two 1 x 1 blocks). Given rotations are then constructed in a
straightforward manner to interchange the shifted zero eigenvalue to the other
block. The construction of the Givens transformations needed for the
exchange of the blocks is done in such a way as to ensure backward stability.

In the case of two 2 x 2 blocks, an arbitrary 2 x 2 Giv is performed on both
blocks in order to eliminate the uncoupling between them. Then a sequence of
QZ steps uses a previously determined shift is performed on both blocks. A
decoupling with the blocks in the desired order is usually obtained with a few
steps (rarely more than two). If within 30 iterations no decoupling is obtained, the
subroutine gives an error return. The criterion used is that the coupling element of
the two blocks in the Householder form of A is smaller than EPS.

Since it does not make sense to force this coupling element to be smaller than the
elements in the rest of the pencil, one should choose EPS smaller than rdip x
max([A], [B]), where rdip is the relative precision of the computer used. A
reasonable choice for EPS is the "estimated" absolute precision of the (sometimes
measured) data in A and B. Since the pencils used here are of dimension 4 x 4, the
QZ steps are implemented with Givens transformations instead of House-
holder transformations, which turns out to be economical. More details are given
in [7], where a proof of the backward stability of the method is also given.

EXCHQZ uses the routines GIV and SROT, which construct a 2 x 2 Givens
rotation to zero out an element of a 2-vector, and perform it, respectively, on two
columns or rows of a specified matrix.

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REFERENCES
2. Lawson, C.L., Hanson, R.J., Kincaid, D.R., and Krogh, F.T.: Linear algebra subroutines
4. Stewart, G.W.: Eigenvectors and perturbation bounds for subspaces associated with
5. Stewart, G.W.: HQRs and EXCHNG. Fortran subroutines for calculating and ordering the
ALGORITHM

[A part of the listing is printed here. The complete listing is available from the ACM Algorithms Distribution Service (see page 404 for order form).]

SUBROUTINE DECOMP(NAX, N, A, B, IPIV, NPIVN, FAIL, IND) FSG DFG
LOGICAL FAIL
REAL AL(RMAX), B(RMAX), ZMAX, EPS

C
C GIVEN THE UPPER TRIANGULAR MATRIX A AND UPPER HESSENBERG MATRIX A
C WITH I31 ON THE DIAGONAL, THIS ROUTINE NUMBERS THE DIAGONAL
C ONCE ALONG WITH THEIR GENERALIZED EIGENVALUES BY CONSTRUCTING EIQUS.
C
C BLOCKS ALONG WITH THEIR GENERALIZED EIGENVALUES BY CONSTRUCTING EQUS.
C
C PERFORMED ON THE GIVEN HESSENBERG TRANSFORMATION 2, RESULTING FROM A
C POSSIBLE PREVIOUS STEP OR INITIALIZED WITH THE IDENTITY MATRIX.
C
C AFTER REORDERING, THE EIGENVALUES INSIDE THE BLOCKS SPECIFIED BY THE
C BLOCKS ARE REORDERED TO THEIR NORM ORDER.
C
C FUNCTION TEEET APPEARS AT THE TOP, IF BOTH ARE THEIR NUMBER THEN THE
C NON FIRST COLUMN OF Z STAYS THE REQUESTED SUBSPACE. ALMOD REQUIRES XYZ.
C
C THE SUBROUTINE ENDS AND THE INDEX FUNCTION FITST WHICH HAS TO BE DUM
C PROVIDED BY THE USER. THE PARAMETERS IF THE CALLING SEQUENCE ARE.
C
C (STARTED PARAMETERS ARE ALTERED BY THE SUBROUTINE)
C
C
C
C RMAX THE FIRST DIMENSION OF A, B AND XYZ
C N THE ORDER OF A, B AND XYZ
C *A,B THE MATRIX PAIR WHERE BLOCKS ARE TO BE REORDERED.
C IPIV IPIV [UPON RETURN THIS ARRAY IS MULTIPLED BY THE COLUMN
C TRANSFORMATION.]
C FITST(ALPHA, BETA, P) IS AN INTEGER FUNCTION IDENTIFYING THE
C SPECTRUM OF THE DELEADING SUBSPACE TO BE COMPUTED
C WHEN LEPT FITST CHECKS IF ALPH/BETA IN THAT SPECTRUM
C WHEN LE=2 FITST CHECKS IF THE TWO COMPLEX CONJUGATE
C ROOTS WITH SUM S AND PRODUCT P ARE IN THAT SPECTRUM
C IF THE ABSOLUTELY POSITIVE, FITST=1
C EPS THE REQUIRED ABSOLUTE ACCURACY OF THE RESULTS
C RMAX AN INTEGER GIVING THE DIMENSION OF THE COMPUTED
C SUBSPACE.
C
C A LOGICAL VARIABLE WHICH IS FALSE ON A NORMAL RETURN.
C
C AN INTEGER WORKING ARRAY OF DIMENSION AT LEAST X
C
C AN INTEGER WORKING ARRAY OF X DIMENSION.

CALL DECOMP(NAX, N, A, B, IPIV, NPIVN, FAIL, IND, I.)

C I IFST, IF1ST
C REAL X, P, Q, ALPHA, BETA
C
C IF A IS THE SIZE OF THE BLOCK I

**C*** SIGN(SD(I)) INDICATES THE LOCATION OF ITS EIGENVALUES

**C*** SUM IS THE NUMBER OF ELEMENTS IN THIS ARRAY

**DO** 30 I=1,10

**IF** (L(I),N) GO TO 40

**IF** (L(I),M) GO TO 10

**C*** HERE A X22 BLOCK IS CHECKED

**I** = 2

**D** = 4(I-1) + K2(I,12)


**F** = (A(I,L) - A(L,L) - A(L,L) - A(L,L)) / D

**I** = 2

**I** = **IF** (I3(L,M),I3(L),I3(M),I3(L))

**GO TO** 30

**C*** HERE A X32 BLOCK IS CHECKED

**I** = 2

**LS** = 1

**I** = **IF** (I3(L,M),I3(L),I3(M),I3(L))

**IF** (LS,EQ,1) **D** = SUM + LS

**J0** CONTINUE

**C*** EIGENBLOCKS SUCH THAT THOSE WITH POSITIVE VALUE

**C*** OF I3(L,M) APPEAR FIRST.