Abstract

This manual gives an introduction to the use of JADAMILU, a set of Fortran 77 routines to compute selected eigenvalues and associated eigenvectors of large scale real symmetric or complex Hermitian matrices. Generalized eigenvalue problems with positive definite mass matrix can also be solved. The eigenvalues sought can either be the smallest ones or those closest to some specified target inside the spectrum. The package is based on the Jacobi-Davidson method. Key features are modest memory requirements, robust convergence to accurate solutions, and the automatic setup of an in-built preconditioner. On the other hand, the program is flexible and easy to use by non-experts. If the matrix is sparse and explicitly available, the user can simply pass it to the program and let JADAMILU compute the desired eigenvalues. If not, then a crude sparse approximation which may even be diagonal, can be passed. In the latter case the user only needs to define a routine that performs matrix-vector products.
**Key words.** eigensolver, Jacobi–Davidson, preconditioning, software

**AMS subject classification.** 65F10
1 Introduction

JADAMILU allows to compute selected solutions of standard

\[ A u = \lambda u \]

or generalized

\[ A u = \lambda B u \]

eigenvalue problem, where \(A, B\) are large sparse symmetric or complex Hermitian matrices, with \(B\) being positive definite in case of a generalized eigenvalue problem.

JADAMILU is an inverse free software: neither the inverse of (shifted) \(A\) nor that of \(B\) is used even implicitly. The algorithms used are based on the Jacobi–Davidson method ([13, 14]), one of the state-of-the-art methods for computing a few selected eigenvalues and associated eigenvectors of large sparse matrices. Roughly spoken, Jacobi-Davidson can be viewed as a Newton-like method for computing an eigenvalue and its associated eigenvector. Similar to Newton’s method where one has to solve a system with the Jacobian at every step, in the Jacobi–Davidson method one has to solve a correction equation with the shifted input matrix \(A - sI\) or \(A - sB\) (plus some projection). This system needs not be solved accurately, and, actually, they are solved inside JADAMILU using the conjugate gradient method with state-of-the-art preconditioning [4] based on integrated multilevel incomplete LU (ILU) factorization of the shifted matrix \((A - sI)\) or \((A - sB)\).

1.1 How to use this guide

This guide is self contained, but does not describe methods and algorithms used in JADAMILU, for which we refer to [14]. The latter paper also describes some real life applications. We strongly recommend its reading for an enlightened use of the package.

On the other hand, main driver routines are reproduced in the Appendix with the comment lines describing precisely each parameter. It is a good idea to have a look at the listing of a driver routine while reading a section of this guide describing its usage.

1.2 Main driver routines and versions

JADAMILU has three main driver routines, \(PJD\), \(PJDRVC\) and \(JDREVCOM\), which are declined in different versions. Each driver is available in double precision (prefix \(D\)), double complex (prefix \(Z\)), single precision (prefix \(S\)) and single complex (prefix \(C\)) arithmetic. Each driver has also a variant for standard eigenvalue problems (no suffix) and a variant for generalized eigenvalue problems (suffix \(_{\text{GEP}}\)). In addition, for each arithmetic, JADAMILU provides a routine \(PJDCLEAN\) that releases internal memory (same routine for both generalized and non generalized cases).
Therefore available driver routines are

<table>
<thead>
<tr>
<th>DP JD</th>
<th>ZP JD</th>
<th>SP JD</th>
<th>CP JD</th>
</tr>
</thead>
<tbody>
<tr>
<td>DPJDREVCOM</td>
<td>ZPJDREVCOM</td>
<td>SPJDREVCOM</td>
<td>CPJDREVCOM</td>
</tr>
<tr>
<td>DJDREVCOM</td>
<td>ZJDREVCOM</td>
<td>SJDREVCOM</td>
<td>CJDREVCOM</td>
</tr>
<tr>
<td>DPJD_GEP</td>
<td>ZPJD_GEP</td>
<td>SPJD_GEP</td>
<td>CPJD_GEP</td>
</tr>
<tr>
<td>DPJDREVCOM_GEP</td>
<td>ZPJDREVCOM_GEP</td>
<td>SPJDREVCOM_GEP</td>
<td>CPJDREVCOM_GEP</td>
</tr>
<tr>
<td>DJDREVCOM_GEP</td>
<td>ZJDREVCOM_GEP</td>
<td>SJDREVCOM_GEP</td>
<td>CJDREVCOM_GEP</td>
</tr>
<tr>
<td>DPJDCLAENUP</td>
<td>ZPJDCLAENUP</td>
<td>SPJDCLAENUP</td>
<td>CPJDCLAENUP</td>
</tr>
</tbody>
</table>

The usage of these driver routines is pretty much independent of the version (for standard or generalized eigenvalue problem) and of the arithmetic. Therefore, most of this guide (Sections 2 to 7) describes, by way of example, the usage of the double precision routines for standard eigenproblems DPJD, DPJDREVCOM DJDREVCOM and DPJDCLAENUP. Peculiarities related to generalized eigenvalue problems and to complex arithmetic (for complex Hermitian matrices) are discussed in Sections 8 and 9 respectively.

In the Appendix, we only reproduce driver routines for double precision, because the argument description is the same for all arithmetics, besides of course the argument type of non integer variables. At any rate, the source files of all drivers are provided with the package, see the README file for details.

Note that we do not recommend single precision versions, which are provided for the sake of completeness and should be considered with care. As you may see by running the examples provided with the package, accuracy is limited. Further, for ill-conditioned problems, rounding errors may spoil any accuracy and/or convergence. If saving memory is important and/or if single precision arithmetic is much faster on your machine, we recommend to use the double precision version but with preconditioner in single precision, see the description of parameter ICNTL(5) in Section 4.3.

1.3 Which driver use

PJJD is the major driver of this package and we recommend its use, which is documented in Sections 2 to 7 but Sections 5.3, 6.3 and 4.6. PJDREVCOM has to be used when the matrix is not explicitly available or when passing it to JADAMILU would require excessive memory; its usage is more particularly documented in Sections 5.3 and 6.3 but remarks on PJJD in other sections also apply to PJDREVCOM. Eventually, you should use JDREVCOM if you want to use your own preconditioner instead of the one provided by JADAMILU. Its usage is documented in Section 4.3 remarks on PJJD/PJDREVCOM also apply, except of course those related to preconditioning, mainly in Section 4.

1.4 Release and backward compatibility

This guide describes JADAMILU 2.0 and above. From previous release (the first version, without revision number) the naming of the routines has been changed and some control parameter has been added. We nevertheless provide full backward compatibility, i.e. application programs based on this previous release need not be modified.
If you want nevertheless upgrade a program working with previous release, you just need to add a D as prefix to the driver called, and extend the declared length of control parameter ICNTL from 4 to 5, while initializing ICNTL(5)=0.

1.5 Disclaimer and copyright

THIS MATERIAL IS PROVIDED AS IS, WITH ABSOLUTELY NO WARRANTY EXPRESSED OR IMPLIED. ANY USE IS AT YOUR OWN RISK.

Using JADAMILU is free for non commercial applications (For commercial use, please contact the authors). You can acknowledge, using reference [1], the contribution of this package in any scientific publication dependent upon the use of the package. You shall use reasonable endeavors to notify the authors of the package of this publication.

JADAMILU also uses some external packages. Please check Appendix B for additional copyright notice.

1.6 Running the examples

Source files for all listings in this guide are provided with the package. Therefore, you can run the examples on your own. Please note that some decisions taken inside JADAMILU, like recomputing or not a preconditioner, are based on timing measures that are machine dependant. Therefore, RUNNING THE EXAMPLES ON DIFFERENT MACHINES MAY PRODUCE SLIGHTLY DIFFERENT OUTPUT. This is harmless as long as the computed eigenvalues are the same up to the required accuracy.

In all cases, we give the source files for standard eigenvalue problems in double precision arithmetic, but some source files are also provided for other arithmetics and/or generalized eigenvalue problems. They are not discussed in this guide, but you can run them on your own, and compare the source code with the one of the standard version; you will see that only few straightforward modifications are needed.
2 Getting started

Given your real symmetric matrix, suppose you plan to compute a few eigenvalues closest to the origin and their associated eigenvectors; JADAMILU asks you to do the following steps.

1. Provide the upper triangular part of your matrix in compressed sparse row format. Suppose your matrix is

\[
A = \begin{pmatrix}
0 & 5 \\
5 & 1 & 5 \\
5 & 2 & 5 \\
5 & 3 & 5 \\
5 & 4
\end{pmatrix} \in \mathbb{R}^{5,5},
\]

then the compressed sparse row format of the upper triangular part of \( A \) is given by the following three vectors.

\[
\begin{align*}
IA &= [1 \ 3 \ 5 \ 7 \ 9 \ 10] \\
JA &= [1 \ 2 | 2 \ 3 | 3 \ 4 | 4 \ 5 | 5] \\
A &= [0.0 \ 5.0 | 1.0 \ 5.0 | 2.0 \ 5.0 | 3.0 \ 5.0 | 4.0]
\end{align*}
\]

The first array \( IA \) indicates where every row starts (“10” would be the start of row 6). \( JA \) carries the column indices of the upper triangular part, \( A \) the associated numerical values.

Note that even zero diagonal entries must be stored. For a more detailed description see Appendix [B]. Here is a sample code how one would enter the matrix in FORTRAN if it were a \( 1000 \times 1000 \) matrix.

Listing 1: Sample code for compressed sparse row format

```fortran
INTEGER N PARAMETER (N=1000) INTEGER IA(N+1), JA(2*N-1), I,K DOUBLE PRECISION A(2*N-1)
K=1 DO I=1,N c start of row I IA(I)=K c diagonal entry JA(K)=I A(K)=DBLE(I-1) K=K+1 c entries above the diagonal part in row I IF (I .LT. N) THEN JA(K)=I+1 A(K)=5.0 DO K=K+1 END IF END DO c final reference IA(N+1)=K
```
2. call PJD to compute the eigenvalues and eigenvectors. Here you have to decide how many eigenvalues you want, whether or not you have some initial guesses, how much memory you would like to spend, how to choose the drop tolerance, ...

In the most simple case use the following sample code to compute the five (MAXEIG=5) smallest eigenvalues of your $N \times N$ matrix (say, size $N=1000$).

Listing 2: EXAMPLE1: Simple driver to compute inner eigenvalues

```fortran
INTEGER N, MAXEIG, MAXSP
PARAMETER (N=1000, MAXEIG=5, MAXSP=20)
INTEGER LX
PARAMETER (LX=N*(3*MAXSP+MAXEIG+1)+4*MAXSP*MAXSP)
DOUBLE PRECISION EIGS(MAXEIG), RES(MAXEIG), X(LX)
INTEGER NEIG, MADSPACE, ISEARCH, NINIT, ICNTL(5)
INTEGER ITER, IPRINT, INFO
DOUBLE PRECISION SIGMA, TOL, SHIFT, GAP, MEM, DROPTOL

...  
declare IA, JA and A and initialize matrix
...

standard diagnostic report on standard output
IPRINT=6
we want the eigenvalues near some target sigma
ISEARCH=2
target, where are we seeking for eigenvalues. Here: near origin
SIGMA=0.0d0
tolerance for discarded fill
DROPTOL=1.0d-3
number of wanted eigenvalues
NEIG=MAXEIG
no initial approximate eigenvectors
NINIT=0
desired size of the search space
MADSPACE=MAXSP
maximum number of iteration steps
ITER=1000
tolerance for the eigenvector residual
TOL=1.0d-10
additional parameters set to default
ICNTL(1)=0
ICNTL(2)=0
ICNTL(3)=0
ICNTL(4)=0
ICNTL(5)=0

compute NEIG eigenvalues near SIGMA
CALL DPJD( N, A, IA, EIGS, RES, X, LX, NEIG,
+       SIGMA, ISEARCH, NINIT, MADSPACE, ITER, TOL,
+       SHIFT, DROPTOL, MEM, ICNTL, IPRINT, INFO, GAP)

release internal memory
CALL DPJDRCLEANUP
```

9
If completed successfully, PJD will return the desired eigenvalues in \( \text{EIGS}(1), \ldots, \text{EIGS}(5) \).
\( X(1+N*(i-1):N*i) \), for \( i=1, \ldots, 5 \) contains the associated normalized eigenvectors. Program output is as follows.

**ENTERING PJDREVCOM*******************************

Computing the eigenvalue(s) closest to 0.00000E+00

- Setting up a new ILU preconditioner -------------------
  fill-in factor: 1.18 (=nnz(LU)/nnz(A))
  used droptol: 1.00000E-03
  used shift: 0.00000E+00
  ILU computed: 0.00[sec]

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Res. norm</th>
<th>Error est.</th>
<th>No(Cluster)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-4.1813094904623E+00</td>
<td>1.5E-11</td>
<td>2.8E-22</td>
<td>-2(---) (*)</td>
</tr>
<tr>
<td>-1.8829821916247E+00</td>
<td>1.3E-11</td>
<td>9.1E-23</td>
<td>-1(---)</td>
</tr>
<tr>
<td>1.0315023277911E-01</td>
<td>4.3E-11</td>
<td>1.0E-21</td>
<td>1(---)</td>
</tr>
<tr>
<td>1.8777797389543E+00</td>
<td>2.3E-11</td>
<td>3.2E-22</td>
<td>2(---)</td>
</tr>
<tr>
<td>3.4922682206843E+00</td>
<td>3.7E-11</td>
<td>2.0E-21</td>
<td>3(---)</td>
</tr>
</tbody>
</table>

(Warning: error estimates are subject to several limitations, see documentation for details; for (*), error estimate is indicative only)

Number of MATVEC needed: 85 ; Estimated gap: 7.96E-01 ; INFO: 0

CPU time for eigenvalue computation: 0.02[sec]
CPU time for preconditioning: 0.00[sec]
Total CPU time: 0.02[sec]

(Suggested DROPTOL if restart needed: 2.41E-03)

**LEAVING PJDREVCOM*******************************

The diagnostic output tells you that initially an ILU using your given DROPTOL=1.0D-3 is computed. The fill-in factor here refers to how much of MEM was really used. In this example, apparently MEM=20.0 is much more than you really needed. The output also informs you that the ILU has approximated \( A - sI \), where the shift parameter \( s \) is equal to 0.0 in this example. In addition the computing time is printed. At the end of the eigenvalue computation you will be told about the eigenvalues that have been computed as well as the norm of the associated eigenvector residual \( \| A u - \theta u \| \) (“Res. norm”), which can also be found in output vector RES. In addition, for each eigenvalue JADAMILU will provide a bound (“Error est.”) on the distance to the closest exact eigenvalue. Note that this bound does not take into account rounding error effects, which are of the order \( \varepsilon_{\text{mach}} \| A \| \), where \( \varepsilon_{\text{mach}} \) is the unit roundoff of the machine, and where \( \| A \| \) (the norm of \( A \)) is here equal to its largest eigenvalue in modulus, see \[1\] for details. Hence, in practice, the error bound is the maximum of the indicated error estimate and \( \varepsilon_{\text{mach}} \| A \| \) (see Section \[1\] for additional remarks on the error bound). This information is
followed by the number of the eigenvalue with, in brackets, the index of the cluster to which it belongs, if any. Eigenvalues are sorted in increasing order, and eigenvalues less than the target are assigned a negative number, the closest to the target having number $-1$, whereas eigenvalues greater than the target are assigned positive numbers, starting from $+1$. When eigenvalues are close to each other, JADAMILU treats them as members of a cluster, which implies that the error bound is computed in a special way. If the distance between eigenvalues in a cluster is below the maximum of the printed error bound and $\varepsilon_{\text{mach}}\|A\|$, it is likely that the eigenvalue is multiple.

This information is followed by the number of matrix-vector multiplications, which corresponds in some sense to the number of iteration steps. Also the gap between the computed eigenvalues and the remaining spectrum is given; INFO=0 means successful termination. Some timings and suggested drop tolerance finalize the output. We refer to Section 7 for a more detailed description of diagnostic output.

If you want to compute the smallest eigenvalues, just use a different value for ISEARCH.

Listing 3: EXAMPLE2: Simple driver to compute the smallest eigenvalues

Changes with respect to Listing 2
compute the smallest eigenvalues and no a priori information on
the eigenvalues is available
ISEARCH=0
SIGMA need not to be set in this case

Program output is then as follows.

**ENTERING PJDREVCOM************************************
Computing the smallest eigenvalue(s)
------------------------------------
Setting up a new ILU preconditioner ------------------
fill-in factor: 1.06 (=nnz(LU)/nnz(A))
used droptol: 1.00000E-03
used shift: -9.00000E+00
ILU computed: 0.00[sec]
--------------------------------------------------------
Setting up a new ILU preconditioner ------------------
fill-in factor: 1.25 (=nnz(LU)/nnz(A))
used droptol: 1.25000E-04
used shift: -9.00000E+00
ILU computed: 0.00[sec]
--------------------------------------------------------
Setting up a new ILU preconditioner

- fill-in factor: 1.50 (=nnz(LU)/nnz(A))
- used droptol: 1.56250E-05
- used shift: -9.00000E+00
- ILU computed: 0.00[sec]

Eigenvalue     Res. norm     Error est.     No(Cluster)
-7.0552450404553E+00  6.9E-12  1.6E-23  1(---)
-4.1813094904623E+00  3.9E-11  6.8E-22  2(---)
-1.8829821916247E+00  2.4E-11  3.0E-22  3(---)
 1.0315023277911E-01  7.2E-11  3.0E-21  4(---)
 1.8777797389543E+00  7.2E-11  3.0E-21  5(---) (*)

(Warning: error estimates are subject to several limitations, see documentation for details; for (*), error estimate is indicative only)

Number of MATVEC needed: 124 ; Estimated gap: 1.75E+00 ; INFO: 0

CPU time for eigenvalue computation: 0.02[sec]
CPU time for preconditioning: 0.00[sec]
Total CPU time: 0.02[sec]

(Suggested SHIFT if restart needed: -9.00E+00)
(Suggested DROPTOL if restart needed: 1.56E-05)

**LEAVING PJDREVCOM*************************************

Beside the eigenvalues that are computed you will notice that the ILU has been recomputed some steps later with a smaller drop tolerance. This is one of the features of the adaptive preconditioning that is part of JADAMILU. According to some heuristic rules, JADAMILU will recompute automatically the ILU with different parameters if necessary.

Note that here the shift parameter $s$ such that the ILU approximates $A - sI$ does no more corresponds to $\Sigma$, but is determined by JADAMILU according some heuristic rules, and update if necessary. Note also, that beside a suggested drop tolerance, you also get on output a suggested shift parameter, which may be used in combination with $ISEARCH=1$ to speedup somewhat the computation of the smallest eigenvalues, see Section 3.2 below.

3 Detailed Description

As seen in the previous section, JADAMILU offers essentially two different strategies to compute eigenvalues

1. The computation of some eigenvalues at the lower end of the spectrum
2. The computation of a few eigenvalues near a desired target $\Sigma$
If you want to compute eigenvalues at the upper end of the spectrum, you can simply pass $-A$ and compute its eigenvalues at the lower end.

### 3.1 The easy way to compute the smallest eigenvalues

Without any knowledge about the eigenvalues, simply set `ISEARCH=0`. This is precisely the situation considered in Section 2.

### 3.2 Advanced computation of the smallest eigenvalues

As you may have seen in Section 2, computing the smallest eigenvalues in principle is easy. But if you have some information available about the location of the eigenvalues then you may supplement JADAMILU with that information.

Consider the matrix from Section 2. We know from the numerical results that the smallest eigenvalue is approximately $-7$. This is maybe not realistic since we have looked at the computed eigenvalues, but in practice it might be that one has some estimates from the underlying physical problem. Why not providing JADAMILU with this external information? To indicate this we set `ISEARCH=1` and we have to provide an estimate `SIGMA` for the smallest eigenvalue. One then needs to indicate as well a `SHIFT` parameter $s$, telling that one wants a preconditioner that approximates $A - sI$. The ideal shift is slightly less than the smallest eigenvalue, and a rule of thumb consist in setting the gap between the shift and the smallest eigenvalue roughly equal to the distance between the two smallest eigenvalues. However, is one has no information about this gap, one may use `SHIFT` equal to `SIGMA`.

Listing 4: EXAMPLE3: Advanced driver to compute the smallest eigenvalues

```plaintext
... changes with respect to Listing 2 ... compute the smallest eigenvalues and pass an appropriate SHIFT & SIGMA
ISEARCH=1
Suppose that we know a good estimate for the smallest eigenvalue, SIGMA=-7
use a shift close to SIGMA but maybe not an exact eigenvalue
SHIFT=-7 ...
```

Here is an excerpt of program output.

```plaintext
... Setting up a new ILU preconditioner -------------
fill-in factor: 1.06 (=nnz(LU)/nnz(A))
used droptol: 1.00000E-03
used shift: -7.00000E+00
ILU computed: 0.00[sec]
ILU-> pos. def.: 1 negative diag. entries changed to positive ...
```
The given shift is actually too large, and the main effect is that the computed ILU preconditioner has some negative eigenvalues, that is, some negative entries on the diagonal of its factors, often referred to as “pivots”. Then the preconditioner is not positive definite, whereas it should be such when computing the smallest eigenvalues. As seen from the line (ILU-> pos. def.: ...), this is detected and cured by JADAMILU, anyway. JADAMILU converts up to 1% negative pivots into positive ones (default choice ICNTL(3)=0). Nevertheless, we recommend to avoid this situation if possible, using a smaller shift (without being too far from the smallest eigenvalue). This is illustrated in EXAMPLE4; running it, you will however discover that this recommended approach, which is based on heuristics, does not necessarily entail faster convergence. You may also turn the conversion by setting ICNTL(3)=1. This forces JADAMILU to search for a sufficiently small shift, at the price of extra preprocessing cost.

3.3 Computing eigenvalues close to a given target

Here you have to set ISEARCH=2 and SIGMA to your desired area of interest. This is illustrated in detail in Section 2.

3.4 Dense matrices or matrices that are not explicitly available

Many practical application problems lead to large sparse matrices. Often enough, matrix entries are not given explicitly, and only a matrix-vector multiplication routine is available. Hence the matrix cannot be passed to JADAMILU. A similar situation arises if the matrix is dense or nearly dense, hence storing it in the prescribed format would require excessive memory.

Consider the following example.

\[
A = \begin{pmatrix}
0.1 & 5.1 & 0.1 & 0.1 & 0.1 \\
5.1 & 0.1 & 5.1 & 0.1 & 0.1 \\
0.1 & 5.1 & 0.1 & 5.1 & 0.1 \\
0.1 & 0.1 & 5.1 & 0.1 & 5.1 \\
0.1 & 0.1 & 0.1 & 5.1 & 0.1
\end{pmatrix}
= \begin{pmatrix}
0 & 5 \\
5 & 0 & 5 \\
5 & 0 & 5 \\
5 & 0 & 5 \\
5 & 0 & 5
\end{pmatrix}
+ 0.1 \begin{pmatrix}
1 \\
1 \\
1 \\
1 \\
1
\end{pmatrix}
\]

The matrix is dense, but, certainly we have a fast matrix vector multiplication available, since we have a sparse matrix plus a low rank correction. For the preconditioner one can simply use the sparse part. The ideal JADAMILU driver for this situation is PJDREVCOM since it only requires an approximation A,IA,JA to the original matrix, which will be used to build the preconditioner.

Since for the matrix-vector multiplication one has to use the original dense matrix which cannot be passed to JADAMILU, PJDREVCOM returns every time it is needed to perform a matrix-vector multiplication, using a so-called reverse communication protocol. The calling program has then to perform this matrix-vector multiplication with prescribed vectors, and return to PJDREVCOM. Note that upon return to the calling program, PJDREVCOM indicates in the variable IJOB what has to be done, in this case perform matrix-vector multiplication or exit.

Listing 5: EXAMPLE5: Advanced driver using reverse communication

```fortran
INTEGER N, MAXEIG, MAXSP
PARAMETER (N=1000,MAXEIG=5,MAXSP=20)
```
INTEGER  LX
PARAMETER (LX=N*(3*MAXSP+MAXEIG+1)+4*MAXSP*MAXSP)
DOUBLE PRECISION  EIGS(MAXEIG), RES(MAXEIG), X(LX)
INTEGER  NEIG, MADSPACE, ISEARCH, NINIT, ICTL(5)
DOUBLE PRECISION  SIGMA, TOL, SHIFT, GAP, MEM, DROPTOL, VAL

... declare approximation IA, JA and A and initialize matrix

... standard diagnostic report on standard output
IPRINT=6
compute the smallest eigenvalues and no a priori information on
the eigenvalues is available
ISEARCH=0
tolerance for discarded fill
DROPTOL=1.d-3
number of wanted eigenvalues
NEIG=MAXEIG
no initial approximate eigenvectors
NINIT=0
desired size of the search space
MADSPACE=MAXSP
maximum number of iteration steps
ITER=1000
tolerance for the eigenvector residual
TOL=1.0d-10
additional parameters set to default
ICTL(1)=0
ICTL(2)=0
ICTL(3)=0
ICTL(4)=0
ICTL(5)=0

Here we start the computation
IJOB=0

We do not have the exact matrix, which A plus a rank one correction;
we call DPDREVCOM (double precision version)
CALL DPDREVCOM( N,A,JA,IA, EIGS, RES, X, LX, NEIG,
+ SIGMA, ISEARCH, NINIT, MADSPACE, ITER, TOL,
+ SHIFT, DROPTOL, MEM, ICTL, IJOB, NDX1, NDX2,
+ IPRINT, INFO, GAP)

IF (IJOB.NE.1) GOTO 20

IJOB=1: MATVEC including rank-1 correction
X(NDX1) input, X(NDX2) output
(1) MATVEC without rank-1
call matvec(N,IA,JA,A,X(NDX1),X(NDX2))
(2) rank-1 update
inner product needed by the rank-1 correction
VAL = 0.0
\begin{verbatim}
do I = 0, N-1
   VAL = VAL + X(NDX1+I)
\end{verbatim}
end do

**scaling factor**
\begin{verbatim}
VAL = VAL * 0.1
\end{verbatim}

**perform update**
\begin{verbatim}
do I = 0, N-1
   X(NDX2+I) = X(NDX2+I) + VAL
\end{verbatim}
end do

GOTO 10

**continue**

**release internal memory**
\begin{verbatim}
CALL DPJDCLEANUP
\end{verbatim}

Reading the program output below you will notice that JADAMILU computes the ILU a few times with smaller and smaller drop tolerance, trying to improve the factorization. So passing an approximate matrix to JADAMILU should be handled with care if the approximation error between the matrix you pass and the matrix used for matrix-vector multiplication is relatively large. There is, however, a way of preventing JADAMILU from recomputing the ILU, which consists in setting ICNTL(2) = 1, see Section 4.1.

**ENTERING PJDREVCOM************************************

Computing the smallest eigenvalue(s)
------------------------------------

- Setting up a new ILU preconditioner -----------------------
  fill-in factor: 1.57 (=nnz(LU)/nnz(A))
  used droptol: 1.00000E-03
  used shift: -1.00000E+01
  ILU computed: 0.00[sec]

- Setting up a new ILU preconditioner -----------------------
  fill-in factor: 1.57 (=nnz(LU)/nnz(A))
  used droptol: 1.25000E-04
  used shift: -1.00000E+01
  ILU computed: 0.01[sec]

- Setting up a new ILU preconditioner -----------------------
  fill-in factor: 1.57 (=nnz(LU)/nnz(A))
  used droptol: 1.56250E-05
  used shift: -1.00000E+01
  ILU computed: 0.00[sec]

**16**
<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Res. norm</th>
<th>Error est.</th>
<th>No(Cluster)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-9.999950750566E+00</td>
<td>4.7E-12</td>
<td>1.5E-19</td>
<td>1(---)</td>
</tr>
<tr>
<td>-9.9998030024238E+00</td>
<td>9.3E-11</td>
<td>5.8E-17</td>
<td>2(---)</td>
</tr>
<tr>
<td>-9.999567580102E+00</td>
<td>4.6E-11</td>
<td>8.8E-18</td>
<td>3(---)</td>
</tr>
<tr>
<td>-9.9992120174570E+00</td>
<td>5.5E-11</td>
<td>8.9E-18</td>
<td>4(---)</td>
</tr>
<tr>
<td>-9.9987687884203E+00</td>
<td>6.8E-11</td>
<td>1.0E-17</td>
<td>5(---) (*)</td>
</tr>
</tbody>
</table>

(Warning: error estimates are subject to several limitations, see documentation for details; for (*), error estimate is indicative only)

Number of MATVEC needed: 72 ; Estimated gap: 5.42E-04 ; INFO: 0

CPU time for eigenvalue computation: 0.01[sec]
CPU time for preconditioning: 0.01[sec]
Total CPU time: 0.02[sec]

(Suggested SHIFT if restart needed:-1.00E+01)
(Suggested DROPTOL if restart needed: 1.56E-05)

**LEAVING PJDREVCOM******************************************************************

Note that when slow convergence is detected, JADAMILU tries to exploit the given memory as much as possible to improve the preconditioner. The smallest DROPTOL that is used by JADAMILU is \( \sqrt{\varepsilon_{\text{mach}}} \); i.e., the square root of the machine precision. Also, no smaller DROPTOL can be used once the memory limit is reached, as specified in the variable MEM.

### 3.5 Iteration parameters

On input, you need to set in ITER the maximal number of iterations to be performed. If you are sure that you use JADAMILU in the right way, just set ITER large enough so that all desired eigenvalues can be computed. Otherwise, in test phase, ITER may be used as safeguard.

Another parameter that may have influence on the number of iteration steps is MADSPACE. This parameter describes the size of the search space beside the eigenvectors that need to be computed. We recommend to use MADSPACE = 20. Choosing a larger number (say 25) might reduce the overall number of iteration steps but at the cost of more expensive single steps which in the end does not necessarily pay off. A smaller MADSPACE may be needed if only few memory is available for JADAMILU, as MADSPACE influences the minimal size of the array \( X \) that has to be passed to driver routines. On the other hand, for optimal error control, MADSPACE should not be smaller than the maximal number of eigenvalues in a cluster, see Section 6 below.

### 4 More on preconditioning

As written in the Introduction, JADAMILU uses preconditioning; that is, an approximation \( M \) to the shifted matrix \( (A - sI) \) (or \( A - sB \) in case of a generalized eigenvalue problem). This approximation should be such that systems of type \( Mx = y \) are easy to solve, and JADAMILU
uses in fact a multilevel approximate LU factorization of \((A - sI)\) (or \(A - sB\)). Some more details on its usage are given in this section.

### 4.1 Adaptive and static preconditioners

By default, JADAMILU recomputes the approximate factorization of \((A - sI)\) as soon as it turns out that outer iterations slow down. As a rule of thumb, first the shift parameter \(s\) is adjusted to be closer to the desired eigenvalues. Once the shift is not altered anymore, as second parameter the drop tolerance is reduced. Note however, if you do not want JADAMILU to adaptively recompute the preconditioner, you can turn off adaptivity by setting \(ICNTL(2)=1\). Occasionally static preconditioning might be useful, e.g. if only a crude approximation to the exact matrix can be passed to the preconditioner and reducing the drop tolerance will not change that. We consider the matrix EXAMPLE5 from Section 3.4, turning off adaptivity.

Listing 6: EXAMPLE6: Advanced driver using reverse communication

```c
... changes with respect to Listing 5
... turn off adaptive preconditioning
ICNTL(2)=1
... additional parameters set to default
ICNTL(1)=0
ICNTL(3)=0
ICNTL(4)=0
ICNTL(5)=0
...
```

In the program output below, you will notice that the preconditioner is computed only once and kept throughout the computation. Since the number of iterations remains the same, this turns out to be more efficient in this example.

**ENTERING PJDREVCOM**************************************************************************

Computing the smallest eigenvalue(s)

- Setting up a new ILU preconditioner ---------------------
  fill-in factor: 1.57 (=nnz(LU)/nnz(A))
  used droptol: 1.00000E-03
  used shift: -1.00000E+01
  ILU computed: 0.00[sec]

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Res. norm</th>
<th>Error est.</th>
<th>No(Cluster)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-9.9995075056666E+00</td>
<td>4.7E-12</td>
<td>1.5E-19</td>
<td>1(---)</td>
</tr>
<tr>
<td>-9.9998030024238E+00</td>
<td>9.3E-11</td>
<td>5.8E-17</td>
<td>2(---)</td>
</tr>
<tr>
<td>-9.9995567580102E+00</td>
<td>4.6E-11</td>
<td>8.8E-18</td>
<td>3(---)</td>
</tr>
<tr>
<td>-9.9992120174570E+00</td>
<td>5.5E-11</td>
<td>8.9E-18</td>
<td>4(---)</td>
</tr>
</tbody>
</table>

18
4.2 Recycling the preconditioner and the eigenvectors

In some applications it might happen that you need to compute sequences of eigenvalue problems, maybe even with a changing matrix. Another situation could be that some of your eigenvectors need to be computed with higher accuracy than others. In any case you are faced with using a routine like PJD or PJDREVCOM a couple of times. If from one call to the next call of, say PJD, the matrices are close enough to each other, why not saving time and recycling the old preconditioner as long as possible? This is certainly a situation where JADAMILU is designed for. Furthermore, the user does not need to do anything else but restarting PJD with the new matrix and changing ICTL(2)=-2. If the ILU is no longer sufficient JADAMILU will automatically detect it and recompute it based on the matrix you passed to PJD.

By way of illustration, consider the matrix

$$A(t) = \begin{pmatrix}
0 & 5 & t & 5 \\
5 & 2t & 5 & t \\
5 & 3t & \ddots \\
\vdots & \ddots & \ddots
\end{pmatrix},$$

for $t = 1.00, 0.05, 1.10, \ldots$ and suppose we are seeking for the eigenvalues near the origin.

Listing 7: EXAMPLE7: Repeated use of JADAMILU

```fortran
! changes with respect to Listing 2
!
!
! do L=0.2
!
! dynamically create matrix entries
!
T=1.0D0+5.0d-2*L
write (6,'(A,1P,E12.4)') 't=',T
K=1
DO 1=1,N
```

---

(Warning: error estimates are subject to several limitations, see documentation for details; for (*), error estimate is indicative only)

Number of MATVEC needed: 72 ; Estimated gap: 5.42E-04 ; INFO: 0

CPU time for eigenvalue computation: 0.02[sec]
CPU time for preconditioning: 0.00[sec]
Total CPU time: 0.02[sec]

(Suggested SHIFT if restart needed: -1.00E+01)
(Suggested DROPTOL if restart needed: 1.00E-03)

**LEAVING PJDREVCOM**************************************************************************
IA(I) = K
JA(K) = I
A(K) = T * DBLE(I - 1)
K = K + 1
IF (I.LT.N) THEN
   JA(K) = I + 1
   A(K) = 5.0 DO
   K = K + 1
END IF
END DO
IA(N + 1) = K

always re-init the following parameters since they are
overwritten by DPJD
ITER = 1000
(ITER set by DPJD to number of iteration steps actually needed)
NEIG = MAXEIG
(NEIG set by DPJD to number of eigenvalues effectively computed)
CALL DPJD((N, A, JA, IA, EIGS, RES, X, LX, NEIG,
+ SIGMA, ISEARCH, NINIT, MADSPACE, ITER, TOL,
+ SHIFT, DROPTOL, MEM, ICNTL,
+ IPRINT, INFO, GAP))

next time we enter DPJD, we continue with adaptive
preconditioning based on the preconditioner that has been used
so far
ICNTL(2) = -2
use previously computed eigenvectors as initial approximation
NINIT = NEIG
end do

release internal memory and discard preconditioner
CALL DPJDCLEANUP

As you can see in the program output, the preconditioner is not recomputed in this example. Note that this can be enforced by setting ICNTL(2) = -1. Then, one re-enters PJD with static preconditioning.

**ENTERING PJDEVCOM**************************************************

Computing the eigenvalue(s) closest to 0.00000E+00
---------------------------------------------------
- Setting up a new ILU preconditioner ------------------
  fill-in factor: 1.18 (=mnz(LU)/mnz(A))
  used droptol: 1.00000E-03
  used shift: 0.00000E+00
  ILU computed: 0.00[sec]
---------------------------------------------------

   Eigenvalue    Res. norm   Error est.   No(Cluster)
<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Res. norm</th>
<th>Error est.</th>
<th>No(Cluster)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-4.0120453498900E+00</td>
<td>6.0E-11</td>
<td>2.6E-21</td>
<td>-2(---) (*)</td>
</tr>
<tr>
<td>-1.6436284668853E+00</td>
<td>7.7E-11</td>
<td>2.9E-21</td>
<td>-1(---)</td>
</tr>
<tr>
<td>4.0080605221695E-01</td>
<td>9.6E-11</td>
<td>5.0E-21</td>
<td>1(---)</td>
</tr>
<tr>
<td>2.2251865872115E+00</td>
<td>7.9E-11</td>
<td>3.7E-21</td>
<td>2(---)</td>
</tr>
<tr>
<td>3.8823846177623E+00</td>
<td>5.5E-11</td>
<td>2.3E-20</td>
<td>3(---)</td>
</tr>
</tbody>
</table>

(Warning: error estimates are subject to several limitations, see documentation for details; for (*), error estimate is indicative only)

Number of MATVEC needed: 85 ; Estimated gap: 7.96E-01 ; INFO: 0

CPU time for eigenvalue computation: 0.02[sec]
CPU time for preconditioning: 0.00[sec]
Total CPU time: 0.02[sec]

(Suggested DROPTOL if restart needed: 2.41E-03)

**LEAVING PJDREVCOM************************************************************************

**ENTERING PJDREVCOM************************************************************************

Computing the eigenvalue(s) closest to 0.00000E+00

---

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Res. norm</th>
<th>Error est.</th>
<th>No(Cluster)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-4.1813094904623E+00</td>
<td>1.5E-11</td>
<td>2.8E-22</td>
<td>-2(---)</td>
</tr>
<tr>
<td>-1.8829821916247E+00</td>
<td>1.3E-11</td>
<td>9.1E-23</td>
<td>-1(---)</td>
</tr>
<tr>
<td>1.031503237911E-01</td>
<td>4.3E-11</td>
<td>1.0E-21</td>
<td>1(---)</td>
</tr>
<tr>
<td>1.8777797389543E+00</td>
<td>2.3E-11</td>
<td>3.2E-22</td>
<td>2(---)</td>
</tr>
<tr>
<td>3.4922682206843E+00</td>
<td>3.7E-11</td>
<td>2.0E-21</td>
<td>3(---)</td>
</tr>
</tbody>
</table>

(Warning: error estimates are subject to several limitations, see documentation for details; for (*), error estimate is indicative only)

Number of MATVEC needed: 53 ; Estimated gap: 1.39E+00 ; INFO: 0

CPU time for eigenvalue computation: 0.00[sec]
CPU time for preconditioning: 0.00[sec]
Total CPU time: 0.00[sec]

(Suggested DROPTOL if restart needed: 1.05E-02)

**LEAVING PJDREVCOM************************************************************************

t= 1.1000E+00

21
Computing the eigenvalue(s) closest to 0.00000E+00

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Res. norm</th>
<th>Error est.</th>
<th>No(Cluster)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-3.8466403861287E+00</td>
<td>6.5E-11</td>
<td>1.0E-20</td>
<td>-2(---)</td>
</tr>
<tr>
<td>-1.4096605995227E+00</td>
<td>2.6E-11</td>
<td>3.1E-22</td>
<td>-1(---)</td>
</tr>
<tr>
<td>6.9159568647511E-01</td>
<td>1.1E-10</td>
<td>6.1E-21</td>
<td>1(---)</td>
</tr>
<tr>
<td>2.5642166391883E+00</td>
<td>3.7E-11</td>
<td>8.2E-22</td>
<td>2(---)</td>
</tr>
<tr>
<td>4.2625293553861E+00</td>
<td>4.3E-11</td>
<td>1.2E-21</td>
<td>3(---) (*)</td>
</tr>
</tbody>
</table>

(Warning: error estimates are subject to several limitations, see documentation for details; for (*), error estimate is indicative only)

Number of MATVEC needed: 57 ; Estimated gap: 1.56E+00 ; INFO: 0

CPU time for eigenvalue computation: 0.01[sec]
CPU time for preconditioning: 0.00[sec]
Total CPU time: 0.01[sec]

(Suggested DROPTOL if restart needed: 4.86E-02)

In listing 7, you can see that some parameters are redefined between successive calls to PJD, because they are overwritten on output. Here is a list of input parameters overwritten on output.

- **ITER.** On input: maximum number of iteration steps; on output: number of steps needed by PJD. *Need always to be reinitialized*

- **DROPTOL.** On input: initial drop tolerance for the ILU; on output: suggested drop tolerance for next run. Hence one may proceed the computation with this new value.

- **NEIG.** On input: number of desired eigenvalues; on output: number of computed eigenvalues. *Need to be reinitialized since it may happen that not all eigenvalues wanted have been computed successfully.*

- **EIGS,X.** On input: if NINIT>0, approximate eigenvalues and eigenvectors (see Section 5 for details); on output: computed eigenvalues and eigenvectors. Hence one may proceed the computation with these, and further set NINIT=NEIG to use them as initial guess for the next run.

- **SIGMA,SHIFT** when ISEARCH ≤ 1. On input, if ISEARCH=1: values supplied by the user for initial eigenvalue approximation and initial shift; on output: parameters suggested by PJD for next run. Hence one may proceed the computation with this new values, and further reset ISEARCH=1 if one had initially ISEARCH=0.

**Remark.** Although it sounds reasonable in a parameter-dependent problem to use the old eigenvectors as initial guesses, this should be considered with care. Indeed, JADAMILU uses
a Newton like process; i.e., it favors convergence towards the solutions in the vicinity of the provided initial guesses. But, as the computation proceeds, these solutions may be no more those really wanted; that is, the smallest or those closest to the given target. For instance, if you run an example similar to EXAMPLE7 but with a matrix \( A = tI + C \), where \( C \) is some symmetric matrix, you will be happy to see that once JADAMILU has computed eigenvalues & eigenvectors for some \( t \), reentering JADAMILU with a different \( t \) gives you the answer with minimal number of matrix vector multiplications. In fact, any inner iteration is skipped, JADAMILU just computes the eigenvalues associated to these initial eigenvectors and the corresponding residual norms. Since they are below \( TOL \), JADAMILU has found solutions to the eigenvalue problem that are accurate enough and exits. But then JADAMILU has no mean to check that the computed eigenvalues are the wanted one. This can be only ensured by restarting the computation from scratch.

4.3 Some advanced preconditioning parameters

Here we will comment on some parameters that you could vary from the default settings if it would improve your application.

**DROPTOL**

We suggest to start with a value \( DROPTOL = 1.0d-3 \), but certainly you may use any value less than 1 based on your experience. \( DROPTOL \) is roughly spoken the drop tolerance which defines “small” entries in absolute values. JADAMILU essentially computes an approximate factorization \( LDL^T \approx A \) such that \( L \) is unit lower triangular (some details concerning multilevel strategies are skipped here for simplicity). During the approximate factorization, in any column \( L \) of the approximate factorization, entries less than \( DROPTOL \) in absolute value are dropped (beside some additional safeguard strategies). Note that the drop tolerance is interpreted in a relative sense, hence it needs not be adapted according to the scaling of the matrix.

Note also that JADAMILU is designed to use adaptive preconditioning, i.e., if the drop tolerance is too rough and if enough memory is available, then the drop tolerance is reduced and a new ILU is computed. So starting with a drop tolerance that is too rough will delay the computation for some time. On the other hand if you start with a drop tolerance that is (maybe) chosen too small, JADAMILU keeps it as long as the preconditioner fits into the memory. So choosing a relatively small drop tolerance should be considered with care. If the drop tolerance is too small to factor the approximate LU within the given memory, JADAMILU automatically increases \( DROPTOL \) in case of adaptive preconditioning.

**MEM**

\( MEM \) describes the memory relative to the number of nonzero entries of the original matrix that the user is willing to spend. E.g. \( MEM = 20 \) means that the ILU is allowed to consume 20 times the memory of the original matrix. In general, using a sufficiently large \( MEM \) parameter is recommended. In particular because this allows JADAMILU to use adaptive preconditioning and reduce the drop tolerance further if necessary. Please note that since JADAMILU computes a multilevel ILU, it may happen that the final fill-in that is printed on the screen is less than the memory that was required in intermediate steps. In particular you should not be confused
that adaptive preconditioning does not compute a new preconditioner, although you may think that there should be enough space left.

**ICNTL(2)**

We have already seen that playing around with ICNTL(2) allows adaptive preconditioning (ICNTL(2) = 0, default), static preconditioning (ICNTL(2) = 1), re-enter with adaptive preconditioning (ICNTL(2) = −2) and re-enter with static preconditioning (ICNTL(2) = −1).

**ICNTL(3)**

Another advanced option that you may alter is given by ICNTL(3). In case of seeking for the smallest eigenvalues (ISEARCH=0, ISEARCH=1), the shifted matrix $A - sI$ is expected to be positive definite, if the SHIFT parameter is sufficiently small. However, it may happen that $s$ is not accurate enough or simply too big. In that case, $A - sI$ will no longer stay positive definite and it is likely that the ILU will encounter negative or indefinite pivots. By default, JADAMILU allows up to 1% negative diagonal diagonal pivots that will be converted to their positive definite counterparts. By setting ICNTL(3)=1 this option is disabled and you force JADAMILU to compute a sufficiently small shift.

**ICNTL(4)**

A rather delicate parameter is ICNTL(4). This parameter is directly connected to the multilevel ILU. In principle the computed ILU includes a strategy to compute $A \approx LDL^T$, where $L$ is unit lower triangular and $D$ is block diagonal, such that $\|L^{-1}\|_\infty \leq 5$. The bound 5 is the default value and since it may happen that this bound is too small, JADAMILU has an internal procedure to raise this bound while it is computing the preconditioner. You may in any case overwrite the initial bound 5 by assigning your desired bound to ICNTL(4), i.e. ICNTL(4)=100 will raise the initial bound to 100 instead of 5.

**ICNTL(5)**

The parameter ICNTL(5) has recently been added to JADAMILU starting from release 2.0. This parameter is meaningless if single precision is used. For double precision, this parameter is used to turn on mixed precision computing. Whenever ICNTL(5) is equal to 1, the computation and the application of the preconditioner is done in single precision only. This should not affect the final accuracy since everything else is kept using double precision.

Note that in this case the MEM parameter refers to the memory available for the ILU relative to the memory of the original matrix as if it were stored in single precision; that is, for the same physical memory available, you may use MEM twice as large when ICNTL(5) = 1.
4.4 Custom preconditioners

If you prefer not to use JADAMILU’s built-in preconditioner, you can use the routine JDREVCOM to apply a private preconditioning routine. Suppose your matrix is given by

\[
A = \begin{pmatrix}
4 & -1 & -1 & \cdots & -1 \\
-1 & 4 & -1 & \cdots & -1 \\
-1 & 4 & -1 & \cdots & -1 \\
\vdots & \vdots & \cdots & \ddots & \vdots \\
-1 & \cdots & \cdots & \cdots & 4 \\
\end{pmatrix}
\]

and you would prefer only to use

\[
A^{-1} \approx B = \frac{1}{64} \begin{pmatrix}
16 & 4 & 1 & 1 & 4 \\
4 & 16 & 4 & 1 & 1 \\
1 & 4 & 16 & 4 & 1 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
1 & 1 & \cdots & 16 & 4 \\
4 & 1 & \cdots & 4 & 16 \\
\end{pmatrix}
\]
as direct sparse approximate inverse preconditioner. In that case you simply have to provide your own matrix-vector multiplication subroutine together with your private preconditioner. The driver JDREVCOM uses reverse-communication subroutine and it stops every time when you have to apply your custom routines. After that you restart JDREVCOM and it will resume with your data.

Listing 8: EXAMPLE8: Advanced driver using reverse communication

```fortran
INTEGER N, MAXEIG, MAXSP PARAMETER (N=1000,MAXEIG=5,MAXSP=20) INTEGER LX PARAMETER (LX=N*(3*MAXSP+MAXEIG+1)+4*MAXSP+MAXSP) DOUBLE PRECISION EIGS(MAXEIG), RES(MAXEIG), X(LX) INTEGER NEIG, MADSPACE, ISEARCH, NINIT, ICNTL(5) INTEGER ITER, IPRINT, INFO DOUBLE PRECISION SIGMA, TOL, SHIFT, GAP, MEM, DROPTOL INTEGER IJOB, NDX1, NDX2
```

```
c
... 
c
standard diagnostic report on standard output
IPRINT=6 
c
we want the smallest eigenvalues
ISEARCH=0 
c
number of wanted eigenvalues
NEIG=MAXEIG 
c
no initial approximate eigenvectors
NINIT=0 
```
desired size of the search space
MADESPACE=MAXSP
maximum number of iteration steps
ITER=1000
tolerance for the eigenvector residual
TOL=1.0d-10
additional parameters set to default
ICNTL(1)=0
ICNTL(2)=0
ICNTL(3)=0
ICNTL(4)=0
ICNTL(5)=0
start reverse communication
IJOB=0
CALL JDREVCOM( N, EIGS, RES, X, LX, NEIG,
+ SIGMA, ISEARCH, NINIT, MADESPACE, ITER, TOL,
+ IJOB, NDX1, NDX2, IPRINT, INFO, GAP)
your private matrix-vector multiplication
IF (IJOB.EQ.1) THEN
  X(NDX1) input, X(NDX2) output
  X(NDX2)=4*X(NDX1)-X(NDX1+1)-X(NDX1+N-1)
  DO I=1,N-2
     X(NDX2+I)=-X(NDX1+I-1)+4*X(NDX1+I)-X(NDX1+I+1)
  END DO
  X(NDX2+N-1)=-X(NDX1)-X(NDX1+N-2)+4*X(NDX1+N-1)
  GOTO 10
ELSE IF (IJOB.EQ.2) THEN
  X(NDX2) input, X(NDX1) output
  X(NDX1)=(16*X(NDX2)+4*X(NDX2+1)+X(NDX2+2)+X(NDX2+N-2)
  +4*X(NDX2+N-1))/64.0
  X(NDX1+1)=(4*X(NDX2)+16*X(NDX2+1)+4*X(NDX2+2)+X(NDX2+3)
  +X(NDX2+N-1))/64.0
  DO I=2,N-3
     X(NDX1+I)=(X(NDX2+I-2)+4*X(NDX2+I-1)+16*X(NDX2+I)
     +4*X(NDX2+I+1)+X(NDX2+I+2))/64.0
  END DO
  X(NDX1+N-2)=(X(NDX2)+X(NDX2+N-4)+4*X(NDX2+N-3)
  +16*X(NDX2+N-2)+4*X(NDX2+N-1))/64.0
  X(NDX1+N-1)=(4*X(NDX2)+X(NDX2+1)+X(NDX2+N-1)
  +4*X(NDX2+N-2)+16*X(NDX2+N-1))/64.0
  GOTO 10
END IF
work done — release internal memory
CALL DPJDCLEANUP

When executing this program, you will notice that two out of five eigenvalues could not be approximated to full precision. Certainly, since there is no adaptive preconditioning, there is no way to improve your preconditioner and thus you should carefully think about the options (e.g. is ITER= 1000 still appropriate?).
4.5 Diagonal preconditioning

In some applications, the matrix may not be explicitly available besides its diagonal entries. When dealing with extremely large systems, it may also happen that no memory is left for computing an ILU preconditioning. To face these situations, JADAMILU offers the possibility to use only diagonal preconditioning. To do this you simply pass \( \text{IA}, \text{JA}, \text{A} \) to \( \text{PJ} \text{DREVCOM} \), but by setting \( \text{JA}(1) \) to a value less than 0, e.g. \( \text{JA}(1)=-1 \), you indicate that your matrix is diagonal. In this case, the other entries of \( \text{JA} \) as well as \( \text{IA} \) are not referenced. Only \( \text{A}(1), \ldots, \text{A}(\text{N}) \) are needed. Here it is important to note that adaptive preconditioning will access the diagonal matrix from time to time in order to set up a new diagonal preconditioner based on a potential new shift parameter. The \text{MEM} \) and \text{DROPTOL} \) parameter are not referenced. Consider as example the matrix

\[
A = \begin{pmatrix}
1 & 5 & 5 & 5 & \\
5 & 2 & 3 & 5 & \\
& 5 & 4 & \ddots & \\
& & \ddots & \ddots & \\
\end{pmatrix}
\]

and suppose we are seeking for the smallest eigenvalues.

Listing 9: EXAMPLE9: Compute the smallest eigenvalues using diagonal preconditioning

```fortran
INTEGER N, MAXEIG, MAXSP
* optimal workspace (here MAXSP+MAXSP-MAXEIG)
INTEGER LX
PARAMETER (LX=N*(3*MAXSP+MAXEIG+1)+4*MAXSP*MAXSP)
DOUBLE PRECISION EIGS(MAXEIG), RES(MAXEIG), X(LX), D(N)
* arguments to pass to the routines
INTEGER NEIG, MADSPECE, ISEARCH, NINIT, Icntl(5)
INTEGER IJOB, NDx1, NDx2, I, J, K

DO I=1,N
  D(I)=0.0
  DO J=IA(I),IA(I+1)-1
    K=JA(J)
    IF (K.EQ.I) D(I)=A(J)
  END DO
END DO

standard diagnostic report on standard output
IPRINT=6
we want the smallest eigenvalues
ISEARCH=0
number of wanted eigenvalues
NEIG=MAXEIG
```
no initial approximate eigenvectors
NINIT=0
desired size of the search space
MADSPACE=MAXSP
maximum number of iteration steps
ITER=1000
tolerance for the eigenvector residual
TOL=1.0d-10
additional parameters set to default
ICNTL(1)=0
ICNTL(2)=0
ICNTL(3)=0
ICNTL(4)=0
ICNTL(5)=0

IJOB=0

CALL DPJDREVCOM( N, D, -1, -1, EIGS, RES, X, LX, NEIG, + SIGMA, ISEARCH, NINIT, MADSPACE, ITER, TOL, + SHIFT, DROPTOL, MEM, ICNTL, + IJOB, NDX1, NDX2, IPRINT, INFO, GAP)

your private matrix-vector multiplication
IF (IJOB.NE.1) GOTO 20
input, output
CALL MYMATVEC(X(NDX1),X(NDX2))

continue
release internal memory

As you will see from the printed output, PJDREVCOM will continue to adapt the shift and the diagonal preconditioner.

**ENTERING PJDREVCOM****************************************************

Computing the smallest eigenvalue(s)

- Setting up a new diagonal preconditioner -----------------
  used shift: 1.0000E-03

- Setting up a new diagonal preconditioner -----------------
  used shift: -5.9139E+00

- Setting up a new diagonal preconditioner -----------------
  used shift: -9.9767E+00
- Setting up a new diagonal preconditioner  
  used shift: \(-8.8221E+00\)  

- Setting up a new diagonal preconditioner  
  used shift: \(-6.2671E+00\)

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Res. norm</th>
<th>Error est.</th>
<th>No(Cluster)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(-6.0552450404553E+00)</td>
<td>8.7E-11</td>
<td>2.6E-21</td>
<td>1(---)</td>
</tr>
<tr>
<td>(-3.1813094904623E+00)</td>
<td>7.0E-11</td>
<td>2.1E-21</td>
<td>2(---)</td>
</tr>
<tr>
<td>(-8.8298219162471E-01)</td>
<td>5.7E-11</td>
<td>1.7E-21</td>
<td>3(---)</td>
</tr>
<tr>
<td>(1.1031502327791E+00)</td>
<td>4.6E-11</td>
<td>1.2E-21</td>
<td>4(---)</td>
</tr>
<tr>
<td>(2.87779797389543E+00)</td>
<td>8.7E-11</td>
<td>4.2E-21</td>
<td>5(---) (*)</td>
</tr>
</tbody>
</table>

(Warning: error estimates are subject to several limitations, see documentation for details; for (*), error estimate is indicative only)

Number of MATVEC needed: 166; Estimated gap: 1.78E+00; INFO: 0

CPU time for eigenvalue computation: 0.02[sec]  
CPU time for preconditioning: 0.00[sec]  
Total CPU time: 0.02[sec]

(Suggested SHIFT if restart needed: \(-6.06E+00\))

**LEAVING PJDREVCOM**********************

Certainly you can reuse the diagonal part after you passed the diagonal entries to PJDREVCOM. To do this, simply set ICNTL(1)=2. By giving away the diagonal part, PJDREVCOM will automatically turn off adaptive preconditioning.

Listing 10: EXAMPLE10: Compute the smallest eigenvalues using diagonal preconditioning, saving memory

c
3 c changes with respect to Listing 9
3 c
3 c use a copy of the diagonal entries to be passed to PJDREVCOM
3 c   DO  I=1,N
8  X(I)=0.0
8  DO  J=IA(I),IA(I+1)-1
13  K=JA(J)
13  IF (K.EQ.I) X(I)=A(J)
13  END DO
13  END DO
3 c
3 c ICNTL(1) set to 2 because the matrix that is passed on input
As you will notice, in contrast to Listing 9, no adaptive preconditioning is performed and the eigenvalues are computed based on the initial diagonal matrix.

**ENTERING PJDREVCOM******************************************

Computing the smallest eigenvalue(s)
------------------------------------
- Setting up a new diagonal preconditioner ------------
used shift:  1.0000E-03
------------------------------------

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Res. norm</th>
<th>Error est.</th>
<th>No(Cluster)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-6.055245040455286E+00</td>
<td>7.1E-11</td>
<td>1.8E-21</td>
<td>1(---)</td>
</tr>
<tr>
<td>-3.181309490462310E+00</td>
<td>3.3E-11</td>
<td>4.7E-22</td>
<td>2(---)</td>
</tr>
<tr>
<td>-8.829821916247098E-01</td>
<td>4.4E-11</td>
<td>9.8E-22</td>
<td>3(---)</td>
</tr>
<tr>
<td>1.103150232779112E+00</td>
<td>8.7E-11</td>
<td>4.3E-21</td>
<td>4(---)</td>
</tr>
<tr>
<td>2.877779738954344E+00</td>
<td>4.0E-11</td>
<td>8.9E-22</td>
<td>5(---)(*)</td>
</tr>
</tbody>
</table>

(Warning: error estimates are subject to several limitations, see documentation for details; for (*), error estimate is indicative only)

Number of MATVEC needed:  185 ; Estimated gap: 1.85E+00 ; INFO:  0

CPU time for eigenvalue computation: 0.04[sec]
CPU time for preconditioning: 0.00[sec]
Total CPU time: 0.04[sec]

(Suggested SHIFT if restart needed:-6.06E+00)

**LEAVING PJDREVCOM**************************************************************************

5 Refined eigenvalue computations

A frequent problem in eigenvalue computations occurs, when given eigenvectors have been computed with some low accuracy and you would like to refine the accuracy. Another related problem could be that you may know some crude approximation to some of the eigenvectors based on the physical background.

The simplest example to illustrate this is to run PJD with some relatively large TOL first and then use PJD to improve the accuracy. Moreover it sounds reasonable that when improving the accuracy, you may keep the old preconditioner and do not need adaptive preconditioning anymore. The JADAMILU routines allow you to pass initial approximate eigenvectors. To do this set NINIT to the number of eigenvectors you provide and overwrite the first N*NINIT components of X with your given approximate eigenvectors. Furthermore, as described in Section 4.1 you can re-enter the routine with the old preconditioner and decide whether to continue with adaptive preconditioning (ICNTL(2)=-2) or simply to stay static (ICNTL(2)=-1). As an example consider A from Section 4.5.

Listing 11: EXAMPLE11: Eigenvector refinement

```fortran
INTEGER N, MAXEIG, MAXSP
PARAMETER (N=1000, MAXEIG=5, MAXSP=20)
* optimal workspace (here MAXSP*MAXSP>MAXEIG)
INTEGER LX
PARAMETER (LX=N*(3*MAXSP+MAXEIG+1)+4*MAXSP*MAXSP)
DOUBLE PRECISION EIGS(MAXEIG), RES(MAXEIG), X(LX)
* arguments to pass to the routines
INTEGER NEIG, MADSPACE, ISEARCH, NINIT, ICNTL(5)
INTEGER ITER, IPRINT, INFO
DOUBLE PRECISION SIGMA, TOL, GAP, MEM, DROPTOL, SHIFT

... declare IA, JA and A and initialize matrix
... standard report on standard output
IPRINT=6

we want the smallest eigenvalues
ISEARCH=0
elbow space factor for the fill computed during the ILU
MEM=20.0
tolerance for discarded fill
DROPTOL=1.d-3
number of wanted eigenvalues
NEIG=MAXEIG
```
On execution you will see that PJD is called twice, once computing the preconditioner and returning the desired eigenvector according to a low accuracy. The second time PJD is invoked, the preconditioner and the old eigenvectors are already present. The accuracy is improved using a smaller TOL.

**ENTERING PJDREVCOM******************************************

Computing the smallest eigenvalue(s)
------------------------------------

- Setting up a new ILU preconditioner -------------------
fill-in factor: 1.06 (=nnz(LU)/nnz(A))
used droptol: 1.00000E-03
used shift: -8.00000E+00
ILU computed: 0.00[sec]

- Setting up a new ILU preconditioner ---------------
fill-in factor: 1.25 (=nnz(LU)/nnz(A))
used droptol: 1.25000E-04
used shift: -8.00000E+00
ILU computed: 0.00[sec]

- Setting up a new ILU preconditioner ---------------
fill-in factor: 1.50 (=nnz(LU)/nnz(A))
used droptol: 1.56250E-05
used shift: -8.00000E+00
ILU computed: 0.00[sec]

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Res. norm</th>
<th>Error est.</th>
<th>No(Cluster)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-6.0552450402030E+00</td>
<td>1.4E-04</td>
<td>7.0E-09</td>
<td>1(---)</td>
</tr>
<tr>
<td>-3.1813094896192E+00</td>
<td>3.0E-04</td>
<td>3.8E-08</td>
<td>2(---)</td>
</tr>
<tr>
<td>-8.8298218873886E-01</td>
<td>4.8E-04</td>
<td>1.2E-07</td>
<td>3(---)</td>
</tr>
<tr>
<td>1.1031502338478E+00</td>
<td>4.5E-04</td>
<td>1.1E-07</td>
<td>4(---)</td>
</tr>
<tr>
<td>2.8777797469109E+00</td>
<td>5.5E-04</td>
<td>1.8E-07</td>
<td>5(---) (*)</td>
</tr>
</tbody>
</table>

(Warning: error estimates are subject to several limitations, see documentation for details; for (*), error estimate is indicative only)

Number of MATVEC needed: 60 ; Estimated gap: 1.65E+00 ; INFO: 0

CPU time for eigenvalue computation: 0.01[sec]
CPU time for preconditioning: 0.00[sec]
Total CPU time: 0.01[sec]

(Suggested SHIFT if restart needed:-8.00E+00)
(Suggested DROPTOL if restart needed: 1.56E-05)

**LEAVING PJDREVCOM************************************

**ENTERING PJDREVCOM************************************

Computing the smallest eigenvalue(s)

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Res. norm</th>
<th>Error est.</th>
<th>No(Cluster)</th>
</tr>
</thead>
</table>

33
(Warning: error estimates are subject to several limitations, 
see documentation for details; for (*), error estimate is indicative only)

Number of MATVEC needed: 68 ; Estimated gap: 1.86E+00 ; INFO: 0

CPU time for eigenvalue computation: 0.01[sec]
CPU time for preconditioning: 0.00[sec]
Total CPU time: 0.01[sec]

(Suggested SHIFT if restart needed: -8.00E+00)
(Suggested DROPTOL if restart needed: 8.52E-05)

**LEAVING PJDREVCOM*****************************************************

You can verify that calling the same routine only once with TOL=1.0d-10 from the very beginning will roughly need the same number of matrix-vector multiplications.

6 Accuracy and missconvergence

Whenever you call one of JADAMILU’s driver you have to prescribe a parameter TOL that describes the desired accuracy. If possible, on exit from JADAMILU the eigenvectors are computed such that the eigenvalue residual \( \|Ax - \theta x\| \) (with \( \|x\| = 1 \)) is less than TOL. However, accuracy is limited by rounding errors, and if TOL is below the attainable accuracy, JADAMILU will detect it and truncate the computation. Roughly, the attainable accuracy is of the order \( \varepsilon_{\text{mach}} \|A\| \), where \( \varepsilon_{\text{mach}} \) is the unit roundoff of the machine, and where \( \|A\| \) (the norm of \( A \)) is here equal to its largest eigenvalue in modulus. Using very small TOL should however be considered with care. The detection of a too small TOL requires several iterations, implying a waste of computing time. It may also fail if TOL is by far too small, in which cases JADAMILU stagnates until the maximum number of iterations is reached. The JADAMILU drivers will return on exit RES to hold the actual norm of the residuals.

TOL is roughly the accuracy of computed eigenvectors. If only the accuracy of eigenvalues matters for you, you are more interested in the printed error bound. You may have noticed that the latter is of the order of the square of TOL, i.e., accuracy of eigenvalues is quadratic with respect to the accuracy of eigenvectors. Hence a moderate TOL is enough to get full accuracy on the eigenvalues. Eigenvalues for which the error bound is not quadratic are eigenvalues that belong to a cluster that cannot be treated as such by JADAMILU because either its size is too large or because it contains eigenvalues that, among the computed ones, are either the largest ones (cases ISEARCH=0,1), or the farthest from the target (case ISEARCH=2). In these cases, a better error bound for these eigenvalues will be obtained by increasing the number of computed eigenvalues. On the other hand, the maximal size of a cluster that JADAMILU can treat as such is equal to the MADSPACE parameter discussed in Section 3.5.
As already written in Section 2, “Error est.” is a bound on the distance to the closest exact eigenvalue, which, however does not take into account some rounding error effects. Hence in practice, the actual error bound is the maximum of the printed error estimate and $\varepsilon_{\text{mach}} \| A \|$. Note also that the printed bound requires in principle to know where uncomputed eigenvalues are located. Hence it becomes untrustable if misconvergence occurred. Misconvergence is a situation where some eigenvalues are missed in the interval between the smallest and the largest of the computed eigenvalues. This may happen incidentally, and missed eigenvalues are in general close to the boundary of the interval. Then, the error bound is wrong for the eigenvalues close to missed eigenvalues, that is, close to the boundary of the interval. Here again, a safeguard consists in computing more eigenvalues than actually needed.

Finally, for either the largest eigenvalue (cases $\text{ISEARCH}=0,1$), or the farthest from the target (case $\text{ISEARCH}=2$), the error bound depends on the estimated gap between computed and uncomputed eigenvalues. Because this gap is only estimated (and not computed accurately) by JADAMILU, the “Error est.” printed for this eigenvalue is no more an error bound, but an indicative estimate.

## 7 Diagnostic Output

The default value of $\text{IPRINT}$ is recommended to be set to 6. This refers to standard output. If, instead, $\text{IPRINT}$ is set to a positive number (different from 5), the information is printed in the file with unit number equal to the indicated value.

The information that is printed tells you how often the ILU has been (re-)computed, how many eigenvalues have been computed and how accurate they are. To be precise, take Listing 2 (EXAMPLE1) and its output.

**ENTERING PJDREVCOM*******************************

Computing the eigenvalue(s) closest to 0.00000E+00

- Setting up a new ILU preconditioner ---------------
  fill-in factor: 1.18 (=nnz(LU)/nnz(A))
  used droptol: 1.00000E-03
  used shift: 0.00000E+00
  ILU computed: 0.00[sec]

<table>
<thead>
<tr>
<th>Eigenvalue</th>
<th>Res. norm</th>
<th>Error est.</th>
<th>No(Cluster)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-4.1813094904623E+00</td>
<td>1.5E-11</td>
<td>2.8E-22</td>
<td>-2(---) (*)</td>
</tr>
<tr>
<td>-1.8829821916247E+00</td>
<td>1.3E-11</td>
<td>9.1E-23</td>
<td>-1(---)</td>
</tr>
<tr>
<td>1.0315023277911E-01</td>
<td>4.3E-11</td>
<td>1.0E-21</td>
<td>1(---)</td>
</tr>
<tr>
<td>1.8777797389543E+00</td>
<td>2.3E-11</td>
<td>3.2E-22</td>
<td>2(---)</td>
</tr>
<tr>
<td>3.4922682206943E+00</td>
<td>3.7E-11</td>
<td>2.0E-21</td>
<td>3(---)</td>
</tr>
</tbody>
</table>

(Warning: error estimates are subject to several limitations, see documentation for details; for (*), error estimate is indicative only)
Number of MATVEC needed: 85 ; Estimated gap: 7.96E-01 ; INFO: 0

CPU time for eigenvalue computation: 0.02[sec]
CPU time for preconditioning: 0.00[sec]
Total CPU time: 0.02[sec]

(Suggested DROPTOL if restart needed: 2.41E-03)

**LEAVING PJDREVCOM*******************************

You start with DROPTOL=1e-3. This leads to an approximate factorization (ILU) of $A$ that has 1.18 as many nonzeros as the initial matrix. Furthermore, the initial shift is chosen to be 0.0; i.e., an ILU of $A-0.0I$ is computed. The computing time is negligible. Since there is no further message concerning any ILU, this will be the only time that an approximate factorization is computed. At the end of the computation you will be faced with the computed eigenvalues. “Res. norm” refers to the norm of the associated eigenvector residual $\|Ax-\theta x\|_2$ in the Euclidean norm, “Error est.” is the error bound (see Section 4) and finally “No(Cluster)” tells you the number of the eigenvalue (see Section 2 for the numbering) and the index of the cluster to which the eigenvalue belongs, if any (see Section 5 for more about clustered eigenvalues).

Furthermore, the number of MATVEC (matrix-vector multiplications) can be considered as a measure for the total number of iteration steps. The estimated gap shows you how far your eigenvalues are with respect to the remaining spectrum. INFO= 0 indicates successful computation. At the end a computation time statistics is given that splits the total time into the time spent in computing the preconditioner (maybe more than one time) and the remaining eigenvalue computation.

If you are sick of all this printed statements, simply set IPRINT=0 and any output is suppressed.

If you would like to have very detailed information you can choose IPRINT=-6 (or a negative number different from -5). In this case you will get detailed information about the multilevel ILU (how many levels, how much fill on each level, ...). In addition, at each outer iteration step you will be told about the progress of the eigenvalue computation.

Step: 0(1); #MV: 1; Rayl. quot.: 5.09490E+02; Res. norm: 2.9E+02
Step: 1(1); #MV: 3; Rayl. quot.: 9.13765E-01; Res. norm: 8.3E+00

... 

Step: 5(1); #MV: 11; Rayl. quot.: 1.03150E-01; Res. norm: 5.7E-07
Step: 6(1); #MV: 15; Rayl. quot.: 1.03150E-01* converged ( 15 MV)

“Step” refers to one outer iteration step and in brackets you are told which eigenvector is computed (here: first eigenvector). Next you will be informed about the total number of matrix-vector multiplications so far (#MV). The difference between two neighboring #MV will tell you how many inner steps were required. “Rayl. quot” describes the size of the current approximate eigenvalue based on the Rayleigh quotient $\theta = \frac{x^TAx}{x^Tx}$. As soon as the method converges you will see that the Rayleigh quotient does not change anymore. Finally “Res.
norm” is the norm of the associated eigenvector residual. Once JADAMILU has successfully computed an eigenvector, it will notify you the success by summarizing the number matrix-vector multiplication instead of the residual norm.

8 Generalized eigenvalue problems

The usage of drivers for generalized eigenvalue problems is pretty similar to that of the corresponding drivers for standard eigenvalue problems; **PJD_GEP** and **PJDREVCOM_GEP** have, as additional arguments, the arrays **B**, **JB** and **IB** in which one should store the mass matrix **B** using the same format as for **A**, described in Appendix B. **Note that B should be positive definite.** Other parameters remain the same and have same meaning.

Similarly to **A**, **JA** and **IA**, when using **PJDREVCOM_GEP**, **B**, **JB** and **IB** need not contain the exact matrix, since matrices are here only used to build the preconditioner (see Section 3.4); if **JA**(1) < 0, diagonal preconditioning is required (see Section 4.5) and **B**(1),...,**B**(N) should contain the diagonal of **B**, whereas neither **JB** nor **IB** is accessed.

For **PJDREVCOM_GEP** and **JDREVCOM_GEP**, the reverse communication protocol is somehow more involved since, on return to the calling program, either a multiplication by **A** or by **B** or both may be required, and there is an additional related parameter **NDX3**; see comments in driver listings (Sections A.5 and A.6) for more details and the source file of EXAMPLE9_GEP for example of use.

Note that, for generalized eigenvalue problems, eigenvectors **x** returned in **X** are normalized in such a way that **x**^∗_i B **x**_i = 1. However, the residual norm used for checking the convergence criterion is \( \frac{||Ax^i - \theta x^i||}{||Bx^i||} \) (that is, JADAMILU tries to find \((\theta, x)\) such that \( \frac{||Ax^i - \theta x^i||}{||Bx^i||} \leq \text{TOL} \)). This is also the quantity returned in vector **RES** and printed in program output.

Program output is similar to that for standard eigenvalue problems, but error estimates have a different meaning. For standard problems JADAMILU tries to deliver an error bound (i.e., a bound on the distance to closest exact eigenvalue), with some limitations explained in Section 6. For generalized eigenvalue problems, the same limitations apply and, in addition, error estimates are indicative in all cases. Indeed, a true bound should be based on \( \frac{||Ax^i - \theta x^i||_B^{-1}}{||Bx^i||_B^{-1}} \), which cannot be computed since the inverse of **B** is not available. The printed error estimate uses therefore \( \frac{||Ax^i - \theta x^i||}{||Bx^i||} \) as approximation to this quantity, and hence should be considered with care.

9 Complex matrices

Complex versions of JADAMILU drivers raise only few comments. All arguments remain real or integer except **A** and **X**, plus **B** in case of a generalized problem. Since **A** (**B**) is supposed Hermitian, it should have real diagonal entries, but this is not checked by JADAMILU. Note that **A** (**B**) has to be a complex array even when passing only the diagonal of **A** (**B**) for diagonal preconditioning.

See Appendix B for a further remark on matrix representation that is specific to the complex case.
A Drivers listings

A.1 DPJD

SUBROUTINE DPJD(N, A, JA, IA, EIGS, RES, X, LX, NEIG,
+ SIGMA, ISEARCH, NINIT, MADSPACE, ITER, TOL,
+ SHIFT, DROPTOL, MEM, ICNTL, IPRINT, INFO,
+ GAP)

implicit none

∗ ∗ ∗ Scalar Arguments ∗ ∗ ∗
integer N, LX, NEIG, ISEARCH, NINIT, MADSPACE
integer ITER, ICNTL(5), IPRINT, INFO
DOUBLE PRECISION SIGMA, TOL, SHIFT, DROPTOL, MEM, GAP

∗ ∗ ∗ Array Arguments ∗ ∗ ∗
integer JA(*), IA(*)
DOUBLE PRECISION A(*), X(*)
DOUBLE PRECISION EIGS(*), RES(*)

∗ ∗ ∗ Purpose ∗ ∗ ∗

Computes selected eigenvalues and eigenvectors of the symmetric matrix A
passed in arrays A, JA, IA, using built-in ILU preconditioning.

∗ ∗ ∗ Arguments ∗ ∗ ∗

∗ ∗ ∗ N (input) INTEGER.
The dimension of the matrix. Should be larger than 1.

∗ ∗ ∗ A (input/output) numerical values
∗ ∗ ∗ IA (input/output) pointers for every column
∗ ∗ ∗ JA (input/output) column indices, if JA(1)<0, then A is assumed
to be diagonal.

∗ ∗ ∗ Detailed description of A,IA,JA

Note first that no more than the diagonal part of A and
EITHER values from the strict upper triangular part OR
values from the strict lower triangular part are needed
to define the full matrix.
DPJD/DPJDREVCOM ASSUMES THAT EACH OFF-DIAGONAL ENTRY IS
REFERENCED ONLY ONCE, in either the upper triangular part
or in the lower triangular part.
(Thus, for instance, A,IA,JA may contain either the upper
triangular part or the lower triangular part – in each
case including diagonal).

DPJD ASSUMES IN ADDITION THAT ALL DIAGONAL ELEMENTS ARE
REFERENCED, EVEN WHEN SOME OF THEM ARE EQUAL TO ZERO.
On input, \( IA(I), I=1, \ldots, N+1 \) refers to the physical start of row \( I \). In this case the entries of row \( I \) are located in \( A(K) \), where \( K=IA(I), \ldots, IA(I+1)-1 \). \( JA(K) \) carries the associated column indices. According what is written above, DPJD assumes that some of these \( JA(K) \) (for \( IA(I) \leq K < IA(I+1) \)) is equal to \( I \) with corresponding \( A(K) \) carrying the value of the diagonal element, possibly equal to zero.

\( A, IA, JA \) are "output" parameters because on exit the entries of each row may occur in a different order (the matrix is mathematically the same, but stored in different way).

\section*{EIGS} \hspace{1cm} \textit{(input/output) DOUBLE PRECISION array, dimension NEIG.}

On input, eigenvalue estimates corresponding to provided initial guesses (EIGS(i) corresponds to approximate eigenvector number i); used only if \( \text{NINIT} > (\text{MADSPACE}+1)/2 \) to make sure that initial approximate eigenvectors are processed in the right order.

Sorting is skipped if \( \text{EIGS}(1)=\text{EIGS}(2)= \ldots =\text{EIGS}(\text{NINIT}) \). Then, if \( \text{NINIT} > (\text{MADSPACE}+1)/2 \), initial approximations should be stored in increasing order of eigenvalues if \( \text{ISEARCH} \leq 1 \), or in increasing distance of eigenvalues to SIGMA if \( \text{ISEARCH} \geq 2 \).

On output, eigenvalues as they are computed (EIGS(i) corresponds to approximate eigenvector number i).

\section*{RES} \hspace{1cm} \textit{(output) DOUBLE PRECISION array, dimension NEIG.}

Residual norms: \( \text{RES}(i)=||A \times(i)-\text{EIGS}(i) \times(i)|| \), where \( A \) is the matrix, || is the two norm, and \( \times(i) \) is the approximate eigenvector number i.

\section*{X} \hspace{1cm} \textit{(input/output+workspace) DOUBLE PRECISION array, dimension LX.}

On input, the initial guess(es) (not required, see \text{NINIT}).

On output (input), approximate eigenvector(s).

On output (input), approximate eigenvector number i is (or should be) stored in \( X(1+N* (i-1):N*i) \) for \( i=1, \ldots, \text{NEIG} \) (for \( i=1, \ldots, \text{NINIT} \)).

\section*{LX} \hspace{1cm} \textit{(input) INTEGER}

Dimension of \( X \). Should be at least
\[
N*(2*\text{MADSPACE}+\text{NEIG}+4)+3*\text{MADSPACE}*2+\text{MAX(}\text{MADSPACE}*2,\text{NEIG})
\]
If \( \text{MADSPACE} \geq 3 \), use \( \text{LX} \) not smaller than
\[
N*(3*\text{MADSPACE}+\text{NEIG}+1)+3*\text{MADSPACE}*2+\text{MAX(}\text{MADSPACE}*2,\text{NEIG})
\]

to guarantee optimal performance.

\section*{NEIG} \hspace{1cm} \textit{(input/output) INTEGER}

On input, the number of eigenvalue(s) to be computed; should be positive.

On output, the number of eigenvalues effectively computed with the required accuracy.
SIGMA (input) DOUBLE PRECISION
If ISEARCH <= 0: not used
If ISEARCH = 1: estimation of the smallest eigenvalue
    (may speed up somewhat the algorithm if not too
     inaccurate)
If ISEARCH >= 2: the "target", see ISEARCH

ISEARCH (input) INTEGER
If ISEARCH <= 0: compute the smallest eigenvalue(s)
If ISEARCH = 1: compute the smallest eigenvalue(s) and use
    SIGMA as initial guess. If one searches for the
    smallest eigenvalue(s) and has to rerun the
    algorithm for the same problem (or a problem with
    similar eigenvalues at the lower end), it is a good
    idea to set ISEARCH=1 and SIGMA=EIGS(1) (as obtained
    from the first run).
If ISEARCH >= 2: compute the eigenvalues closest to SIGMA

NINIT (input) INTEGER
Number of initial guess(es) provided. May be set to 0.

MADSPACE (input) INTEGER
Maximal dimension of the search space (usually between 10
    and 20). Should be at least 2.

ITER (input/output) INTEGER
On input, the maximum number of matrix vector multiplications;
    should be positive.
On output, actual number of matrix vector multiplications.

TOL (input) DOUBLE PRECISION
The tolerance on residual norm. Iterations to compute
    eigenvector number i are stopped whenever
    \| A x(i) - EIGS(i) x(i) \| <= TOL, where \| x(i) \| = 1.
    Should be positive.

SHIFT (input/output) DOUBLE PRECISION
used only if ISEARCH = 1
On input, SHIFT is used to shift the input matrix by a
    multiple of the identity matrix in order to compute the
    preconditioner. A good heuristic is obtained by setting
    SHIFT equal to SIGMA (the smallest eigenvalue estimate)
    minus the estimated gap between this smallest eigenvalue
    and the next one (i.e., SHIFT approximates 2 \lambda_1 - \lambda_2, where \lambda_1 \lambda_2 is smallest (second
    smallest) eigenvalue). If one has no idea of this gap,
    SHIFT may be set equal to SIGMA.
On output: suggested new value for the SHIFT parameter (not
    necessarily equal to the current estimation of 2 \lambda_1
    - \lambda_2). If one searches for the smallest eigenvalue(s)
    and has to rerun the algorithm for the same problem (or
    a problem with similar eigenvalues at the lower end), it
    is a good idea to set ISEARCH=1, SIGMA=EIGS(1) and SHIFT
    equal to the value on output from DPJD/DPJREVCOM.
On input, drop tolerance for the multilevel incomplete factorization. A small drop tolerance will typically lead to more fill-in, i.e. more memory will be consumed and the application of the preconditioner is more costly. On the other hand, the number of iteration steps is expected to be less for a smaller drop tolerance.

On output: suggested new value for the DROPTOL parameter, that might be useful to if one has to rerun the algorithm for a similar problem.

MEM (input) DOUBLE PRECISION

MEM prescribes the amount of memory the user is willing to spend for the preconditioner. MEM is relative to the number of nonzero of the input matrix. If it turns out the preconditioner that is computed does not fit into the memory area that is offered by the user, DPJD will terminate with an error message. In this case one can either increase MEM (if there is more memory available) or one has to increase DROPTOL.

ICNTL (input) INTEGER

some control parameters

ICNTL(1) Not used (kept for compatibility with DPJDREVCOM).

ICNTL(2) If equal to zero, then adaptive preconditioning is used, i.e., during the eigenvector computation the ILU may be recomputed (with different SHIFT and DROPTOL), if useful and possible.

If not equal to zero, then the preconditioner computed initially is kept throughout. If, in addition, ICNTL(2) is equal to -1, the existing preconditioner is reused in a static way (this option presumes that DPJD was called previously and successful for the same problem). Finally, ICNTL(2) set to -2 will cause that a previously existing preconditioner will be reused in a adaptive fashion.

ICNTL(3) If ICNTL(2) is equal to zero and ISEARCH <= 2, then ICNTL(3) states whether negative diagonal entries that show up in the ILU will be changed to positive ones. If set to zero (default), then up to 1% of the negative diagonal entries are converted. If more negative diagonal are discovered then the algorithm searches for a new shift (and possibly a different DROPTOL if adaptive preconditioning is used).

If ICNTL(3) is set to 1, then no negative diagonal entries are permitted forcing the algorithm to compute a different shift.

ICNTL(4) If set to zero, default estimate for norm of the inverse factor is used. Otherwise use ICNTL(4) as bound.

ICNTL(5) If ICNTL(5) is equal to 1, the preconditioner is computed with single precision arithmetic (all other computation remain in double precision).
IPRINT (input) INTEGER
Its absolute value indicates the unit number where
information is to be printed (N.B.: 5 is converted to 6).
If zero, only error messages are printed on standard
output. Otherwise, its sign indicates the level of output:
if negative, extensive information (for expert) is
provided; most users should be satisfied with the
information provided for positive IPRINT.

INFO (output) INTEGER
INFO=0 if normal termination.
INFO>0 if allowed maximum number of matrix vector
multiplications performed without finding all
wanted eigenvalues & eigenvectors.
INFO<0 if an error occurred – see printed output for
details
(INFO=-54321: the computation of the preconditioner
failed).

GAP (output) DOUBLE PRECISION
The estimated distance between the set of NEIG computed
eigenvalues and the remaining part of the spectrum; may be
inaccurate.

A.2 DPJDREVCOM

SUBROUTINE DPJDREVCOM( N, A, JA, IA, EIGS, RES, X, LX, NEIG,
+ SIGMA, ISEARCH, NINIT, MADSPACE, ITER,
+ TOL, SHIFT, DROPTOL, MEM, ICNTL,
+ IJOB, NDX1, NDX2, IPRINT, INFO, GAP)

implicit none

.. Scalar Arguments ..
integer N, LX, NEIG, ISEARCH, NINIT, MADSPACE, INFO
integer ITER, ICNTL(5), IJOB, NDX1, NDX2, IPRINT
DOUBLE PRECISION SIGMA, TOL, SHIFT, DROPTOL, MEM, GAP

.. Array Arguments ..
integer JA(*), IA(*)
DOUBLE PRECISION A(*), X(*)
DOUBLE PRECISION EIGS(*), RES(*)

Purpose
-------
Computes selected eigenvalues and eigenvectors of a symmetric matrix A
using built-in ILU or diagonal preconditioning.
Matrix multiplication by A is carried out in a user defined routine
that is called through a reverse communication protocol.

Arguments
----------
N, A, JA, IA, | see comments in subroutine DPJD

In addition:

A, JA, IA need not to define exactly the matrix whose eigenvalues are wanted; instead it may be some approximation; this is consistent because the matrix passed to DPJDSREVCOM is only used to define a preconditioner, whereas matrix vector multiplications are performed by a user provided routine via the reverse communication protocol (see below).

A, JA, IA should be compliant with the format described in DPJD

However:

zero diagonal entries need not to be referenced in the structure (although they may):
if a diagonal preconditioning is wanted, one should set JA(1) negative;
if JA(1)<0, A(1),...,A(N) is supposed to carry the diagonal of the matrix;
then, JA does not need to have a length greater than 1, IA is neither referenced, and A, JA, IA are unchanged on output.

SIGMA, ISEARCH, NINIT, MSPACE, | see comments in subroutine DPJD
ITER, TOL, SHIFT, DROP TOL, MEM, |
IPRINT, INFO, GAP |

ICNTL (input/output) INTEGER
some control parameters
ICNTL(1) should be set to zero (default value), except if X overwrites the arrays in A, JA, IA, in which case one should set ICNTL(1)=2 (this tells that the matrix cannot be refactored once the eigenvalue computation started)
other entries in ICNTL: see comments in subroutine DPJD

IJOB (input/output) INTEGER,
Used to communicate job code between the levels.
Input: one should use IJOB=0 on the first call, and leave IJOB unchanged on subsequent calls
Output: IJOB=0: work done – terminate IJOB=1: compute X(NDX2:NDX2+N-1)= A*X(NDX1:NDX1+N-1) (call to matrix vector multiplication routine: MATVECM) and return to DPJDSREVCOM leaving IJOB (and other parameters) unchanged.

NDX1 (output) INTEGER.
NDX2 Indicate indices into X() for the needed MATVECM when IJOB=1.
A.3 DJDREVCOM

SUBROUTINE DJDREVCOM( N, EIGS, RES, X, LX, NEIG, SIGMA,
+ ISEARCH, NINIT, MADSPACE, ITER, TOL,
+ IJOB, NDX1, NDX2, IPRINT, INFO, GAP)

implicit none

.. Scalar Arguments ..
integer N, LX, NEIG, ISEARCH, NINIT, MADSPACE
integer ITER, IJOB, NDX1, NDX2, IPRINT, INFO
DOUBLE PRECISION SIGMA, TOL, GAP

.. Array Arguments ..
DOUBLE PRECISION X( * ), EIGS( * ), RES(*)

Purpose
--------
Computes selected eigenvalues and eigenvectors of a symmetric matrix A.
Matrix multiplication by A and preconditioner solve are carried out
in user defined routines that are called through a reverse
communication protocol.

Arguments
---------
N, EIGS, RES, X, LX, NEIG, SIGMA, ISEARCH, NINIT, MADSPACE, ITER, TOL,
IPRINT, INFO, GAP

IJOB (input/output) INTEGER.
Used to communicate job code between the levels.
Input: one should use IJOB=0 on the first call, and leave
IJOB unchanged on subsequent calls
Output:
IJOB=0: work done -- terminate
IJOB=1: compute X(NDX2:NDX2+N-1)= A*X(NDX1:NDX1+N-1)
(called to matrix vector multiplication routine: MATVEC) and return to DJDREVCOM leaving IJOB
(and other parameters) unchanged.
IJOB=2: solve Prec*X(NDX1:NDX1+N-1) = X(NDX2:NDX2+N-1)
(called to preconditioner solve routine: PSOLVE) and return to DJDREVCOM leaving IJOB
(and other parameters) unchanged.

NDX1 (output) INTEGER.
NDX2 Indicate indices into X() for the needed MATVEC when IJOB=1,
or for the needed PSOLVE when IJOB=2.
A.4 DPJD_GEP

SUBROUTINE DPJD_GEP( N, A, JA, IA, B, JB, IB, EIGS, RES, X, LX, 
+ NEIG, SIGMA, ISEARCH, NINIT, MADSPACE, ITER, 
+ TOL, SHIFT, DROPTOL, MEM, ICNTL, IPRINT, 
+ INFO, GAP)

implicit none

* .. Scalar Arguments ..
integer N, LX, NEIG, ISEARCH, NINIT, MADSPACE
integer ITER, ICNTL(5), IPRINT, INFO
DOUBLE PRECISION SIGMA, TOL, SHIFT, DROPTOL, MEM, GAP

* .. Array Arguments ..
integer JA(*), IA(*), JB(*), IB(*)
DOUBLE PRECISION A(*), B(*), X(*)
DOUBLE PRECISION EIGS(*), RES(*)

Purpose
--------
Computes selected eigenvalues and eigenvectors of the generalized 
eigenvalue problem defined by the symmetric matrix A and the symmetric 
positive definite mass matrix B, passed in arrays A, JA, IA, and 
arrays B, JB, IB, respectively; built-in ILU preconditioning is used.

Arguments
----------
N, A, JA, IA; | see comments in subroutine DPJD
B, JB, IB (input/output) define the mass matrix B, using the same 
storage scheme as for A (see comments in subroutine DPJD). 
The same restriction on diagonal entries apply. 
In addition, B should be positive definite.

EIGS, RES, X

NEIG, SIGMA, ISEARCH, NINIT, 
MADSPACE, ITER, | see comments in subroutine DPJD
SHIFT, DROPTOL, MEM, 
ICNTL, IPRINT, INFO, GAP

LX (input) INTEGER
Dimension of X. If ISEARCH <= 1, should be at least 
N*(3*MADSPACE+2*NEIG+4)+3*MADSPACE+2+MAX(MADSPACE**2,NEIG) 
and, if ISEARCH >= 2, should be at least 
N*(3*MADSPACE+2*NEIG)+MAX(4*N,6*MADSPACE)+3*MADSPACE+2 
+MAX(MADSPACE**2,NEIG) 
(which amounts the same except for very small N)
If MADSPACE >= 3, use LX not smaller than
A.5 DPJDREVCOM_GEP

SUBROUTINE DPJDREVCOM_GEP( N, A, JA, IA, B, JB, IB, EIGS, RES, X, +
  Lx, NEIG, SIGMA, ISEARCH, NINIT, +
  MADSPACE, ITER, TOL, SHIFT, DROPTOL, +
  MEM, ICNTL, IJOB, NDX1, NDX2, NDX3, +
  IPRINT, INFO, GAP) implicit none

.. Scalar Arguments ..
integer N, LX, NEIG, ISEARCH, NINIT, MADSPACE, ITER
integer ICNTL(5), IJOB, NDX1, NDX2, NDX3, IPRINT, INFO
DOUBLE PRECISION SIGMA, TOL, SHIFT, DROPTOL, MEM, GAP

.. Array Arguments ..
integer JA(*), IA(*), JB(*), IB(*)
DOUBLE PRECISION A(*), B(*), X(*)
DOUBLE PRECISION EIGS(*), RES(*)

Purpose

Computes selected eigenvalues and eigenvectors of the generalized
eigenvalue problem defined by a symmetric matrix A and a symmetric
positive definite mass matrix B, using a built-in ILU preconditioning.
Matrix multiplication by A and B is carried out in user defined
routine(s) that are called through a reverse communication protocol.

Arguments

N, A, JA, IA, B, JB, IB (input/output) define the mass matrix B, using the same
storage scheme as for A (see comments in subroutine DPJD).
The same restriction on diagonal entries apply.
In addition, B should be positive definite.

In addition:
A, JA, IA & B, JB, IB need not to define exactly the matrices
A and B; this is consistent because the matrix
passed to DPJDREVCOM_GEP is only used to define a
preconditioner, whereas matrix vector multiplications
are performed by a user provided routine via the reverse communication protocol (see below).

A, JA, IA and B, JB, IB should be compliant with the format described in DPJD. However:

- zero diagonal entries need not to be referenced in the structure (although they may);
- if a diagonal preconditioning is wanted, one should set ja(1) negative;
- if JA(1)<0, A(1),...,A(N) is supposed to carry the diagonal of the matrix A, and B(1),...,B(N) the diagonal of the matrix B;
- then, JA does not need to have a length greater than 1, IA, IB, JB are neither referenced, and A,JA,IA & B,JB,IB are unchanged on output.

EIGS, RES, X,

NEIG, SIGMA, ISEARCH, NINIT,
MADSPACE, ITER,
SHIFT, DROPTOL, MEM,
IPRINT, INFO, GAP

LX (input) INTEGER
Dimension of X. If ISEARCH <= 1, should be at least
N*(3*MADSPACE+2*NEIG)+3*MADSPACE+2+MAX(MADSPACE*2,NEIG)
and, if ISEARCH >= 2, should be at least
N*(3*MADSPACE+2*NEIG)+MAX(4*N,6*MADSPACE)+3*MADSPACE+2
+MAX(MADSPACE*2,NEIG)
(which amounts the same except for very small N)
If MADSPACE >= 3, use LX not smaller than
N*(4*MADSPACE+2*NEIG+1)+3*MADSPACE+2+MAX(MADSPACE*2,NEIG)
to guarantee optimal performance.

TOL (input) DOUBLE PRECISION
The tolerance on residual norm. Iterations to compute eigenvector number i are stopped whenever
|| A*x(i) - EIGS(i)*B*x(i) || <= TOL * ||B*x(i)||.
Should be positive.

ICNTL (input/output) INTEGER
some control parameters
ICNTL(1) should be set to zero (default value), except if X overwrites the arrays in A,JA,IA, in which case one should set ICNTL(1)=2 (this tells that the matrix cannot be refactored once the eigenvalue computation started)
other entries in ICNTL: see comments in subroutine DPJD

IJOB (input/output) INTEGER,
Used to communicate job code between the levels.
Input: one should use IJOB=0 on the first call, and leave IJOB unchanged on subsequent calls.

Output:

- **IJOB=0:** work done - terminate
- **IJOB=1:** compute \( X(NDX2:NDX2+N-1) = AX(NDX1:NDX1+N-1) \)
  and \( X(NDX3:NDX3+N-1) = BX(NDX1:NDX1+N-1) \)
  (call to matrix vector multiplication routine: MATVEC) and return to DJDREVCOM_GEP leaving IJOB (and other parameters) unchanged.
- **IJOB=3:** compute \( X(NDX2:NDX2+N-1) = AX(NDX1:NDX1+N-1) \)
  (call to matrix vector multiplication routine: MATVEC) and return to DJDREVCOM_GEP leaving IJOB (and other parameters) unchanged.
- **IJOB=4:** compute \( X(NDX3:NDX3+N-1) = BX(NDX1:NDX1+N-1) \)
  (call to matrix vector multiplication routine: MATVEC) and return to DJDREVCOM_GEP leaving IJOB (and other parameters) unchanged.

**NDX1** (output) INTEGER.
**NDX2** indicates indices into \( X() \) for the needed MATVEC when IJOB=1, 3 or 4.

### A.6 DJDREVCOM_GEP

```fortran
SUBROUTINE DJDREVCOM_GEP(N, EIGS, RES, X, LX, NEIG, SIGMA,
+ ISEARCH, NINIT, MADSPACE, ITER, TOL,
+ IJOB, NDX1, NDX2, NDX3, IPRINT, INFO,
+ GAP)

implicit none

.. Scalar Arguments ..
integer N, LX, NEIG, ISEARCH, NINIT, MADSPACE
integer ITER, IJOB, NDX1, NDX2, NDX3, IPRINT, INFO
DOUBLE PRECISION SIGMA, TOL, GAP

.. Array Arguments ..
DOUBLE PRECISION X( * )
DOUBLE PRECISION EIGS( * ), RES(*)
```

**Purpose**

Computes selected eigenvalues and eigenvectors of the generalized eigenvalue problem defined by a symmetric matrix \( A \) and a symmetric positive definite mass matrix \( B \), using a built-in ILU preconditioning. Matrix multiplication by \( A \) and \( B \) and preconditioner solve are carried out in user defined routines that are called through a reverse communication protocol.

**Arguments**

---
**EIGS, RES, X**

**NEIG, SIGMA, ISEARCH, NINIT, MADSPACE, ITER,**

see comments in subroutine DPJD

**IPRINT, INFO, GAP**

---

**LX (input) INTEGER**

Dimension of X. If ISEARCH <= 1, should be at least

\[ N(3*\text{MADSPACE} + 2*\text{NEIG}) + 3*\text{MADSPACE} + 2 + \text{MAX}(\text{MADSPACE}^2, \text{NEIG}) \]

and, if ISEARCH >= 2, should be at least

\[ N(3*\text{MADSPACE} + 2*\text{NEIG}) + \text{MAX}(4*N, 6*\text{MADSPACE}) + 3*\text{MADSPACE} + 2 + \text{MAX}(\text{MADSPACE}^2, \text{NEIG}) \]

(which amounts the same except for very small N)

If MADSPACE >= 3, use LX not smaller than

\[ N(4*\text{MADSPACE} + 2*\text{NEIG}) + 3*\text{MADSPACE} + 2 + \text{MAX}(\text{MADSPACE}^2, \text{NEIG}) \]

to guarantee optimal performance.

---

**TOL (input) DOUBLE PRECISION**

The tolerance on residual norm. Iterations to compute eigenvector number i are stopped whenever

\[ ||A*x(i) - EIGS(i)*B*x(i)|| <= TOL * ||B*x(i)||. \]

Should be positive.

---

**IJOB (input/output) INTEGER.**

Used to communicate job code between the levels.

Input: one should use IJOB=0 on the first call, and leave IJOB unchanged on subsequent calls.

Output:

**IJOB=1:** compute X(NDX2:NDX2+N-1) = A*X(NDX1:NDX1+N-1) AND X(NDX3:NDX3+N-1) = B*X(NDX1:NDX1+N-1)

(call to matrix vector multiplication routine: MATVEC) and return to DPJDREVCMLGEP leaving IJOB (and other parameters) unchanged.

**IJOB=2:** solve Prec*X(NDX1:NDX1+N-1) = X(NDX2:NDX2+N-1)

(call to preconditioner solve routine: PSOLVE) and return to DPJDREVCMLGEP leaving IJOB (and other parameters) unchanged.

**IJOB=3:** compute X(NDX2:NDX2+N-1) = A*X(NDX1:NDX1+N-1)

(call to matrix vector multiplication routine: MATVEC) and return to DPJDREVCMLGEP leaving IJOB (and other parameters) unchanged.

**IJOB=4:** compute X(NDX3:NDX3+N-1) = B*X(NDX1:NDX1+N-1)

(call to matrix vector multiplication routine: MATVEC) and return to DPJDREVCMLGEP leaving IJOB (and other parameters) unchanged.

---

**NDX1 (output) INTEGER.**

**NDX2** Indicate indices into X() for the needed MATVEC when

**NDX3** IJOB=1, 3 or 4, or for the needed PSOLVE when IJOB=2.
A.7 PJDCLEANUP

SUBROUTINE DPJDCLEANUP

Purpose

Releases memory allocated by JADAMILU routines.
B Sparse matrix representation

We describe the representation of $A$ (arrays $A$, $JA$ and $IA$); in case of a generalized eigenvalue problem, $B$ must be stored similarly in arrays $B$, $JB$ and $IB$.

Consider the symmetric matrix

$$A = \begin{pmatrix} 0 & 5 & 0 & 4 & 0 \\ 5 & 1 & 0 & 0 & -4 \\ 0 & 0 & 0 & 5 & 0 \\ 4 & 0 & 5 & 1 & 0 \\ 0 & -4 & 0 & 0 & 0 \end{pmatrix} \in \mathbb{R}^{5,5},$$

In order to interact with PJD or PJDREVCOM only half of the matrix should be passed, i.e. you can either pass the diagonal part plus the strict upper triangular part or the diagonal part plus the strict lower triangular part. You may also pass any mixture of both; e.g., a symmetric permutation of the the upper triangular part. In all cases, you should avoid duplicated entries: if an entry from the lower triangular part is passed, the associated upper triangular part must not be passed. On the other hand, all diagonal entries must be explicitly passed, even when they are equal to zero. These two requirements should be met: **otherwise the code will not run properly**.

The following examples are legal possibilities, missing entries are those that will not be passed.

$$\begin{pmatrix} 0 & 5 & 4 \\ 1 & 0 & -4 \\ 0 & 5 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 5 & 1 \\ 4 & 0 & -4 \\ 4 & 5 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 5 & 1 & -4 \\ 0 & 5 & 1 & 0 \\ 4 & 5 & 1 & 0 \end{pmatrix}.$$ 

Note that in the complex case the matrix is Hermitian instead of simply symmetric. Again only half of the offdiagonal entries should be passed, and this should be interpreted as follows: if, say $A_{34} = 2 + 3i$ and hence $A_{43} = 2 - 3i$, you should either pass $2 + 3i$ as entry in position $(3,4)$ or $2 - 3i$ as entry in position $(4,3)$. On the other hand, diagonal entries must be real but nevertheless stored as complex numbers.

The data structures that are required by JADAMILU are based on the so–called compressed sparse row format (CSR).

We kindly refer to the SPARSKIT package [http://www-users.cs.umn.edu/~saad](http://www-users.cs.umn.edu/~saad) for some tools to convert various sparse matrix formats to CSR format.

For every row only the nonzero entries need to be stored, except for the diagonal entries that always have to be stored. The rows are stored one after another. To do that there are three arrays. The first array is used as pointer array to separate the single rows, i.e. if the first row has three nonzero entries and the second row has two nonzero entries, then the pointer array starts with $1, 4, 6, \ldots$. If you have an $N \times N$ matrix, then this pointer array needs $N + 1$ entries. The last entry is used for compatibility and indicates the first spot behind the matrix.
Consider the following matrix

$$
\begin{pmatrix}
0 & 5 & 4 \\
1 & -4 & \\
0 & 5 & 1 \\
0 & &
\end{pmatrix}
$$

Next there are two arrays that hold the column indices of the nonzero and diagonal entries as well as their numerical values

<table>
<thead>
<tr>
<th>pointer IA</th>
<th>index JA</th>
<th>values A</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1 2 4</td>
<td>0.0 5.0 4.0</td>
</tr>
<tr>
<td>4</td>
<td>2 5</td>
<td>1.0 -4.0</td>
</tr>
<tr>
<td>6</td>
<td>3 4</td>
<td>0.0 5.0</td>
</tr>
<tr>
<td>8</td>
<td>4</td>
<td>1.0</td>
</tr>
<tr>
<td>9</td>
<td>5</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Altogether we have to pass the following arrays

$$
\begin{align*}
\text{IA} & = [ 1 4 6 8 9 10 ] \\
\text{JA} & = [ 1 2 4 2 5 3 4 4 5 ] \\
\text{A} & = [ 0.0 5.0 4.0 1.0 -4.0 0.0 5.0 1.0 0.0 ]
\end{align*}
$$
C JADAMILU parameters in alphabetical order

A

Only used in PJD, PJDEVCOM, PJDGEPR and PJDEVCOMGEPR
(input/output) REAL / DOUBLE PRECISION / COMPLEX / DOUBLE COMPLEX array
On input, entries of matrix A, see Appendix [1] for a detailed description.
PJDEVCOM and PJDEVCOMGEPR only: if JA(1)<0, diagonal preconditioning is wanted and
A(1),...,A(N) should carry the diagonal of A.
A is an output parameter because on exit the entries of each row may occur in a different order
(The matrix is mathematically the same, but stored in different way).

B

Only used in PJDGEPR and PJDEVCOMGEPR
(input/output) REAL / DOUBLE PRECISION / COMPLEX / DOUBLE COMPLEX array
On input, entries of matrix B, see Appendix [1] for a detailed description.
PJDEVCOMGEPR only: if JA(1)<0, diagonal preconditioning is wanted and B(1),...,B(N)
should carry the diagonal of B.
B is an output parameter because on exit the entries of each row may occur in a different order
(The matrix is mathematically the same, but stored in different way).

DROPTOL

Only used in PJD, PJDEVCOM, PJDGEPR and PJDEVCOMGEPR
(input/output) REAL / DOUBLE PRECISION
On input, drop tolerance for the multilevel incomplete factorization. A small drop tolerance
will typically lead to more fill-in, i.e. more memory will be consumed and the application of
the preconditioner is more costly. On the other hand, the number of iteration steps is expected
to be less for a smaller drop tolerance.
On output: suggested new value for the DROPTOL parameter, that might be useful to if one
has to rerun the algorithm for a similar problem.

EIGS

(input/output) REAL / DOUBLE PRECISION array, dimension NEIG
On input, eigenvalue estimates corresponding to provided initial guesses (EIGS(i)) corresponds
to approximate eigenvector number i; used only if NINIT>(MADSPACE+1)/2 to make sure
that initial approximate eigenvectors are processed in the right order. Sorting is skipped if
EIGS(1)=EIGS(2)=...=EIGS(NINIT). Then, if NINIT>(MADSPACE+1)/2 , initial approxima-
tions should be in stored in increasing order of eigenvalues if ISEARCH≤1, or in increasing
distance of eigenvalues to SIGMA if ISEARCH≥2.
On output, eigenvalues as they are computed (EIGS(i) corresponds to approximate eigenvector
number i).
GAP

(output) REAL / DOUBLE PRECISION
The estimated distance between the set of NEIG computed eigenvalues and the remaining part of the spectrum; may be inaccurate.

IA

Only used in PJD, PJDREVCOM, PJD_GEP and PJDREVCOM_GEP
(input) INTEGER array, dimension N+1
Pointer for rows in matrix A, see Appendix B for a detailed description.
PJDREVCOM and PJDREVCOM_GEP only: not accessed if if JA(1)<0 (diagonal preconditioning).

IB

Only used in PJD_GEP and PJDREVCOM_GEP
(input) INTEGER array, dimension N+1
Pointer for rows in matrix B, see Appendix B for a detailed description.
PJDREVCOM_GEP only: not accessed if if JA(1)<0 (diagonal preconditioning).

ICNTL

Only used in PJD, PJDREVCOM, PJD_GEP and PJDREVCOM_GEP
(input) INTEGER array, dimension 5.
Some control parameters:
  ICNTL(1) Only used in PJDREVCOM and PJDREVCOM_GEP .
      ICNTL(1) should be set to zero (default value), except if X overwrites the arrays in A, JA, IA, in which case one should set ICNTL(1)=2 (this tells that the matrix cannot be re-factored once the eigenvalue computation started).
  ICNTL(2) If equal to zero, then adaptive preconditioning is used, i.e., during the eigenvector computation the ILU may be recomputed (with different SHIFT and DROPTOL), if useful and possible. If not equal to zero, then the preconditioner computed initially is kept throughout. If, in addition, ICNTL(2)=−1, the existing preconditioner is reused in a static way (this option presumes that PJD was called previously and successful for the same problem). Finally, ICNTL(2) set to −2 will cause that a previously existing preconditioner will be reused in an adaptive fashion.
  ICNTL(3) If ICNTL(2) is equal to zero and ISEARCH≠ 2, then ICNTL(3) states whether negative diagonal entries that show up in the ILU will be changed to positive ones. If set to zero (default), then up to 1% of the negative diagonal entries are converted. If more negative diagonal are discovered then the algorithm searches for a new shift (and possibly a different DROPTOL if adaptive preconditioning is used).
      If ICNTL(3) is set to 1, then no negative diagonal entries are permitted forcing the algorithm to compute a different shift.
ICNTL(4) If set to zero, default estimate for norm of the inverse factor is used. Otherwise use ICNTL(4) as bound.

ICNTL(5) Ignored by single precision versions.
For double precision versions, when ICNTL(5)= 1, then the preconditioner is computed with single precision arithmetic (other computation remain in double precision).

IJOB

Only used in PJDREVCOM, JDREVCOM, PJDREVCOM_GEP and JDREVCOM_GEP
(input/output) INTEGER
Used to control reverse communication protocol.
Input: one should use IJOB=0 on the first call, and leave IJOB unchanged on subsequent calls
Output: IJOB=0: work done – terminate
IJOB=1: compute \( \mathbf{X}(\text{NDX2} : \text{NDX2} + N - 1) = A \mathbf{X}(\text{NDX1} : \text{NDX1} + N - 1) \) (call to matrix vector multiplication routine) and return to PJDREVCOM leaving IJOB (and other parameters) unchanged.
PJDREVCOM_GEP and JDREVCOM_GEP only: in addition, compute also \( \mathbf{X}(\text{NDX3} : \text{NDX3} + N - 1) = B \mathbf{X}(\text{NDX1} : \text{NDX1} + N - 1) \) before returning.
IJOB=2: (JDREVCOM and JDREVCOM_GEP only) solve \( M \mathbf{X}(\text{NDX1} : \text{NDX1} + N - 1) = \mathbf{X}(\text{NDX2} : \text{NDX2} + N - 1) \) (call to preconditioner solve routine) and return to PJDREVCOM leaving IJOB (and other parameters) unchanged.
IJOB=3: (PJDERVCOM_GEP and JDREVCOM_GEP only) compute \( \mathbf{X}(\text{NDX2} : \text{NDX2} + N - 1) = A \mathbf{X}(\text{NDX1} : \text{NDX1} + N - 1) \) (call to matrix vector multiplication routine) and return to PJDREVCOM leaving IJOB (and other parameters) unchanged.
IJOB=4: (PJDERVCOM_GEP and JDREVCOM_GEP only) compute \( \mathbf{X}(\text{NDX3} : \text{NDX3} + N - 1) = B \mathbf{X}(\text{NDX1} : \text{NDX1} + N - 1) \) (call to matrix vector multiplication routine) and return to PJDREVCOM leaving IJOB (and other parameters) unchanged.

INFO

(output) INTEGER
INFO= 0 if normal termination.
INFO> 0 if allowed maximum number of matrix vector multiplications performed without finding all wanted eigenvalues & eigenvectors.
INFO< 0 if an error occurred - see printed output for details
INFO= -54321 (PJDERVCOM, PJDERVCOM_GEP and PJDERVCOM_GEP only)
the computation of the preconditioner failed.

IPRINT

(input) INTEGER
Its absolute value indicates the unit number where information is to be printed (N.B.: 5 is converted to 6). If zero, only error messages are printed on standard output. Otherwise, its
sign indicates the level of output: if negative, extensive information (for expert) is provided; most users should be satisfied with the information provided for positive IPRINT.

**ISEARCH**

(input) INTEGER

ISEARCH \leq 0  compute the smallest eigenvalue(s)
ISEARCH = 1  compute the smallest eigenvalue(s) and use SIGMA as initial guess. If one searches for the smallest eigenvalue(s) and has to rerun the algorithm for the same problem (or a problem with similar eigenvalues at the lower end), it is a good idea to set ISEARCH = 1 and SIGMA=EIGS(1) (as obtained from the first run).
ISEARCH = 2  compute the eigenvalues closest to SIGMA

**ITER**

(input/output) INTEGER

On input, the maximum number of matrix vector multiplications; should be positive.
On output, actual number of matrix vector multiplications.

**JA**

Only used in PJD, PJDREVCOM, PJD_GEP and PJDREVCOM_GEP

(input/output) INTEGER array

Column indices of entries in matrix A, see Appendix for a detailed description.
PJDREVCOM and PJDREVCOM_GEP only: if JA(1) < 0, further entries are not accessed (diagonal preconditioning).
JA is an output parameter because on exit the entries of each row may occur in a different order (The matrix is mathematically the same, but stored in different way).

**JB**

Only used in PJD_GEP and PJDREVCOM_GEP

(input/output) INTEGER array

Column indices of entries in matrix B, see Appendix for a detailed description.
PJDREVCOM_GEP only: not accessed if if JA(1) < 0 (diagonal preconditioning).
JB is an output parameter because on exit the entries of each row may occur in a different order (The matrix is mathematically the same, but stored in different way).

**LX**

(input) INTEGER

Dimension of X.
PJD, PJDREVCOM and JDREVCOM: should be at least

\[ N(2 \text{MADSPACE} + \text{NEIG} + 4) + 3 \text{MADSPACE}^2 + \max(\text{MADSPACE}^2, \text{NEIG}) \]
if $\text{MADSPACE} \geq 3$, use $LX$ not smaller than
\[
N(3 \text{MADSPACE} + \text{NEIG} + 1) + 3\text{MADSPACE}^2 + \max(\text{MADSPACE}^2, \text{NEIG})
\]
to guarantee optimal performance.

$\text{PJD\_GEP}$, $\text{PJDREVCOM\_GEP}$ and $\text{JDREVCOM\_GEP}$: should be at least
\[
N(3\text{MADSPACE} + 2\text{NEIG} + 4) + 3\text{MADSPACE}^2 + \max(\text{MADSPACE}^2, \text{NEIG})
\]
if $\text{ISEARCH} \geq 2$, should be also not less than
\[
N(3\text{MADSPACE} + 2\text{NEIG}) + 6\text{MADSPACE} + 3\text{MADSPACE}^2 + \max(\text{MADSPACE}^2, \text{NEIG})
\]
if $\text{MADSPACE} \geq 3$, use $LX$ not smaller than
\[
N(4\text{MADSPACE} + 2\text{NEIG} + 1) + 3\text{MADSPACE}^2 + \max(\text{MADSPACE}^2, \text{NEIG})
\]
to guarantee optimal performance.

**MADSPACE**

(input) INTEGER
Maximal dimension of the search space (usually between 10 and 20). Should be at least 2.

**MEM**

Only used in $\text{PJD}$, $\text{PJDREVCOM}$, $\text{PJD\_GEP}$ and $\text{PJDREVCOM\_GEP}$
MEM prescribes the amount of memory the user is willing to spend for the preconditioner. MEM is relative to the number of nonzero of the input matrix. If it turns out the preconditioner that is computed does not fit into the memory area that is offered by the user, $\text{PJDINIT}$ will terminate with an error message. In this case one can either increase MEM (if there is more memory available) or one has to increase DROPTOL.

**N**

(input) INTEGER.
The dimension of the matrix. Should be larger than 1.

**NDX1**

Only used in $\text{PJDREVCOM}$, $\text{JDREVCOM}$, $\text{PJDREVCOM\_GEP}$ and $\text{JDREVCOM\_GEP}$
(output) INTEGER
See description of IJOB.

**NDX2**

Only used in $\text{PJDREVCOM}$, $\text{JDREVCOM}$, $\text{PJDREVCOM\_GEP}$ and $\text{JDREVCOM\_GEP}$
(output) INTEGER
See description of IJOB.
**NDX3**

Only used in `PJDEVRVCOM_GEP` and `PJDEVRVCOM_GEP` (output) `INTEGER`  
See description of `IJOB`.

**NEIG**

(input/output) `INTEGER`  
On input, the number of eigenvalue(s) to be computed; should be positive.  
On output, the number of eigenvalues effectively computed with the required accuracy.

**NINIT**

(input) `INTEGER`  
Number of initial guess(es) provided. May be set to 0.

**RES**

(output) `REAL / DOUBLE PRECISION` array, dimension `NEIG`.  
Residual norms.  
**PJD, PJDEVRVCOM and JDREVCOM:**  
\[ RES(i) = \|Ax_i - \text{EIGS}(i)x_i\|, \]  
where \( A \) is the matrix, \( \| \) is the two norm, and \( x_i \) is the approximate eigenvector number \( i \) stored in \( X(1+N*(i-1):N*i) \) (normalized such that \( \|x_i\| = 1 \)).  
**PJD_GEP, PJDEVRVCOM_GEP and JDREVCOM_GEP:**  
\[ RES(i) = \frac{\|Ax_i - \text{EIGS}(i)Bx_i\|}{\|Bx_i\|}, \]  
where \( A \) is the matrix, \( B \) is the mass matrix, \( \| \) is the two norm, and \( x_i \) is the approximate eigenvector number \( i \) stored in \( X(1+N*(i-1):N*i) \).

**SHIFT**

Only used in `PJD, PJDEVRVCOM, PJDEVRVCOM_GEP` and `PJDEVRVCOM_GEP` (input/output) `REAL / DOUBLE PRECISION`  
On input (ISEARCH= 1), `SHIFT` is used to shift the input matrix by a multiple of the identity matrix in order to compute the preconditioner. A good heuristic is obtained by setting `SHIFT` equal to `SIGMA` (the smallest eigenvalue estimate) minus the estimated gap between this smallest eigenvalue and the next one (i.e., `SHIFT` approximates \( 2\lambda_1 - \lambda_2 \), where \( \lambda_1 \) (\( \lambda_2 \)) is smallest (second smallest) eigenvalue). If one has no idea of this gap, `SHIFT` may be set equal to `SIGMA`.  
On output (ISEARCH≤ 1): suggested new value for the `SHIFT` parameter (not necessarily equal to the current estimation of \( 2\lambda_1 - \lambda_2 \)). If one searches for the smallest eigenvalue(s) and has to rerun the algorithm for the same problem (or a problem with similar eigenvalues at the lower end), it is a good idea to set ISEARCH= 1, SIGMA=EIGS(1) and `SHIFT` equal to the value on output from `PJD/PJDEVRVCOM`. 

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**SIGMA**

Only used in PJD, PJDREVCOM, PJD\_GEP and PJDREVCOM\_GEP

*(input) REAL / DOUBLE PRECISION*

- **ISEARCH** $\leq 0$ not used
- **ISEARCH** $= 1$ estimation of the smallest eigenvalue (may speed up somewhat the algorithm if not too inaccurate)
- **ISEARCH** $\geq 2$ the “target”, see **ISEARCH**

**TOL**

*(input) DOUBLE PRECISION*

The tolerance on residual norm. Should be positive.

**PJD, PJDREVCOM and JDREVCOM:**

Iterations to compute eigenvector number $i$ are stopped whenever $\|Ax_i - \text{EIGS}(i)x_i\| \leq \text{TOL}$ (with $\|x_i\| = 1$).

**PJD\_GEP, PJDREVCOM\_GEP and JDREVCOM\_GEP:** Iterations to compute eigenvector number $i$ are stopped whenever $\|Ax_i - \text{EIGS}(i)Bx_i\| \leq \text{TOL} \|Bx_i\|$.

**X**

*(input/output+workspace) REAL / DOUBLE PRECISION / COMPLEX / DOUBLE COMPLEX* array, dimension LX.

On input, the initial guess(es) (not required, see **NINIT**).

On output, the iterated approximate eigenvector(s).

On output (input), approximate eigenvector number $i$ is (or should be) stored in $X(1+i-1):N\_i$, for $i=1,\ldots,N\_\text{INIT}$.
D  Acknowledgments and Copyrights

Using JADAMILU is free for non commercial applications (For commercial use, please contact the authors). You can acknowledge, using reference [4], the contribution of this package in any scientific publication dependent upon the use of the package. You shall use reasonable endeavors to notify the authors of the package of this publication.

Note that JADAMILU also contains code that is not owned by the authors. If you plan to use it in different way please contact the authors. In particular, JADAMILU uses BLAS, LAPACK, MC64 and AMD.

D.1 MC64

We kindly thank Prof. Iain S. Duff for the permission to add MC64 to this library. We refer to [11] if the user is interested in the mathematical background. Please note the following copyright.

```
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PACKAGEMC64A/AD
AUTHORS Iain Duff (i.duff@rl.ac.uk) and Jacko Koster (jak@ii.uib.no)
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D.2 AMD

AMD is a set of routines for ordering a sparse matrix prior to Choleski factorization (or for LU factorization with diagonal pivoting).

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D.3 BLAS

The reference BLAS is a freely-available software package. It is available from netlib via anonymous ftp and the World Wide Web. Thus, it can be included in commercial software packages (and has been). We only ask that proper credit be given to the authors.

Like all software, it is copyrighted. It is not trademarked, but we do ask the following:

If you modify the source for these routines we ask that you change the name of the routine and comment the changes made to the original.

We will gladly answer any questions regarding the software. If a modification is done, however, it is the responsibility of the person who modified the routine to provide support.

Publications/references for the BLAS, see [12, 11, 9, 8, 7], new BLAS see [3, 6].

D.4 LAPACK

The complete LAPACK package or individual routines from LAPACK are freely available on netlib and can be obtained via the World Wide Web or anonymous ftp.

The LAPACK homepage can be accessed on the World Wide Web via the URL address:

http://www.netlib.org/lapack/

As a standard reference see [2].
References


