I. CODE FOR ODA

A. For a real symmetric matrix

```
subroutine OPDAVIDSONSR(HN1,n,k,order,b,tol,evec,eval,maxi)
```

Parameters

Argument	***in/out***	***Type***	***Description***
n	[in]	integer	n is the dimension of the matrix HN1
HN1	[in]	real*8	HN1 is an array of dimension (0:n-1,0:n-1)
k	[in]	integer	k is the number of extreme eigenpairs to be found
order	[in]	character*1	order is a string, if order='l', k lowest eigenpairs will be found if order='h', k highest eigenpairs will be found
b	[in]	integer	b is a limit on the number of vectors in the basis set V^i
tol	[in]	real*8	tol is the value of tolerance
evec	[out]	real*8	evec is an array of dimension (0:n-1,0:k-1), which contains the k eigenvectors as columns.
eval	[out]	real*8	eval is an array of dimension (0:k-1), which contains the k eigenvalues in ascending order.
maxi	[in]	integer	maxi is the number of maximum iterations

B. For a complex Hermitian matrix

```
subroutine OPDAVIDSONHC(HN1,n,k,order,b,tol,evec,eval)
```

Parameters

Argument	***in/out***	***Type***	***Description***
n	[in]	integer	n is the dimension of the matrix HN1
HN1	[in]	complex*16	HN1 is an array of dimension (0:n-1,0:n-1)
k	[in]	integer	k is the number of extreme eigenpairs to be found
order	[in]	character*1	order is a string, if order='l', k lowest eigenpairs will be found if order='h', k highest eigenpairs will be found
b	[in]	integer	b is a limit on the number of vectors in the basis set V^i
tol	[in]	real*8	tol is the value of tolerance
evec	[out]	complex*16	evec is an array of dimension (0:n-1,0:k-1), which contains the k eigenvectors as columns.

Argument	*in/out*	*Type*	*Description*
eval	[out]	real*8	eval is an array of dimension (0:k-1), which contains the k eigenvalues in ascending order.
maxi	[in]	integer	maxi is the number of maximum iterations

II. CODE FOR OSDA

A. For a real symmetric matrix A

```
subroutine OSDASR(H,nnz,ia,ja,n,k,tol,eval,evec,b,order)
```

Parameters

Argument	*in/out*	*Type*	*Description*
n	[in]	integer	n is the dimension of the matrix A
nnz	[in]	integer	nnz is the number of non-zero elements in the upper triangle of the matrix A
H	[in]	real*8	H is an array of dimension (0:nnz-1) which contains the non-zero elements of the upper triangle part of the matrix A
ia, ja	[in]	integer	ia and ja are arrays of dimension (0:nnz-1) which contains the row and column indices (one based indexing) respectively.
k	[in]	integer	k is the number of extreme eigenpairs to be found
order	[in]	character*1	order is a string, if order='l', k lowest eigenpairs will be found if order='h', k highest eigenpairs will be found
b	[in]	integer	b is a limit on the number of vectors in the basis set V^i
tol	[in]	real*8	tol is the value of tolerance
evec	[out]	real*8	evec is an array of dimension (0:n-1,0:k-1), which contains the k eigenvectors as columns.
eval	[out]	real*8	eval is an array of dimension (0:k-1), which contains the k eigenvalues in ascending order.
maxi	[in]	integer	maxi is the number of maximum iterations

B. For a complex Hermitian matrix A

```
subroutine OSDAHC(H,nnz,ia,ja,n,k,tol,eval,evec,b,order)
```

Parameters

Argument	***in/out***	***Type***	***Description***
n	[in]	integer	n is the dimension of the matrix A
nnz	[in]	integer	nnz is the number of non-zero elements in the upper triangle of the matrix A
H	[in]	complex*16	H is an array of dimension (0:nnz-1) which contains the non-zero elements of the upper triangle part of the matrix A
ia, ja	[in]	integer	ia and ja are arrays of dimension (0:nnz-1) which contains the row and column indices (one based indexing) respectively.
k	[in]	integer	k is the number of extreme eigenpairs to be found
order	[in]	character*1	order is a string, if order='l', k lowest eigenpairs will be found if order='h', k highest eigenpairs will be found
b	[in]	integer	b is a limit on the number of vectors in the basis set V^i
tol	[in]	real*8	tol is the value of tolerance
evec	[out]	complex*16	evec is an array of dimension (0:n-1,0:k-1), which contains the k eigenvectors as columns.
eval	[out]	real*8	eval is an array of dimension (0:k-1), which contains the k eigenvalues in ascending order.
maxi	[in]	integer	maxi is the number of maximum iterations

III. CODE FOR QR DECOMPOSITION (DEPENDENCY)

A. For a real matrix

```
subroutine QRR(n,k,wi)
```

Parameters

Argument	***in/out***	***Type***	***Description***
n	[in]	integer	n is the number of rows in matrix A
k	[in]	integer	k is the number of columns in matrix A
wi	[in/out]	real*8	wi is an array of dimension (0:n-1,0:k-1), on exit, gives an orthogonal matrix Q.

B. For a complex matrix

```
subroutine QRC(s2,k,wi)
```

Parameters

Argument	***in/out***	***Type***	***Description***
s2	[in]	integer	s2 is the number of rows in matrix A
k	[in]	integer	k is the number of columns in matrix A
wi	[in/out]	complex*16	wi is an array of dimension (0:s2-1,0:k-1), on exit, gives an orthogonal matrix Q.