Package 'RSpectra'

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Type Package

Title Solvers for Large-Scale Eigenvalue and SVD Problems

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Description R interface to the 'Spectra' library

<https://spectralib.org/> for large-scale eigenvalue and SVD problems. It is typically used to compute a few eigenvalues/vectors of an n by n matrix, e.g., the k largest eigenvalues, which is usually more efficient than eigen() if k << n. This package provides the 'eigs()' function that does the similar job as in 'Matlab', 'Octave', 'Python SciPy' and 'Julia'. It also provides the 'svds()' function to calculate the largest k singular values and corresponding singular vectors of a real matrix. The matrix to be computed on can be dense, sparse, or in the form of an operator defined by the user.</p>

License MPL (>= 2)

URL https://github.com/yixuan/RSpectra

BugReports https://github.com/yixuan/RSpectra/issues

Depends R (>= 3.0.2)

Imports Matrix (>= 1.1-0), Rcpp (>= 0.11.5)

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eigs

Find a Specified Number of Eigenvalues/vectors of a Square Matrix

Description

Given an n by n matrix A, function eigs() can calculate a specified number of eigenvalues and eigenvectors of A. Users can specify the selection criterion by argument which, e.g., choosing the k largest or smallest eigenvalues and the corresponding eigenvectors.

Currently eigs() supports matrices of the following classes:

```
matrix
              The most commonly used matrix type, defined in the base package.
dgeMatrix
             General matrix, equivalent to matrix, defined in the Matrix package.
dgCMatrix
              Column oriented sparse matrix, defined in the Matrix package.
              Row oriented sparse matrix, defined in the Matrix package.
dgRMatrix
dsyMatrix
              Symmetric matrix, defined in the Matrix package.
              Symmetric column oriented sparse matrix, defined in the Matrix package.
dsCMatrix
dsRMatrix
              Symmetric row oriented sparse matrix, defined in the Matrix package.
function
              Implicitly specify the matrix through a function that has the effect of calculating f(x) = Ax. See section Funct
```

eigs_sym() assumes the matrix is symmetric, and only the lower triangle (or upper triangle, which is controlled by the argument lower) is used for computation, which guarantees that the eigenvalues and eigenvectors are real, and in general results in faster and more stable computation. One exception is when A is a function, in which case the user is responsible for the symmetry of the operator.

eigs_sym() supports "matrix", "dgeMatrix", "dgCMatrix", "dgRMatrix" and "function" typed matrices.

Usage

```
eigs(A, k, which = "LM", sigma = NULL, opts = list(), ...)
## S3 method for class 'matrix'
eigs(A, k, which = "LM", sigma = NULL, opts = list(), ...)
## S3 method for class 'dgeMatrix'
eigs(A, k, which = "LM", sigma = NULL, opts = list(), ...)
## S3 method for class 'dsyMatrix'
eigs(A, k, which = "LM", sigma = NULL, opts = list(), ...)
```

```
## S3 method for class 'dgCMatrix'
eigs(A, k, which = "LM", sigma = NULL, opts = list(), ...)
## S3 method for class 'dsCMatrix'
eigs(A, k, which = "LM", sigma = NULL, opts = list(), ...)
## S3 method for class 'dgRMatrix'
eigs(A, k, which = "LM", sigma = NULL, opts = list(), ...)
## S3 method for class 'dsRMatrix'
eigs(A, k, which = "LM", sigma = NULL, opts = list(), ...)
## S3 method for class '`function`'
eigs(
 Α,
  k,
 which = "LM",
  sigma = NULL,
 opts = list(),
  . . . ,
 n = NULL
  args = NULL
)
eigs_sym(A, k, which = "LM", sigma = NULL, opts = list(),
   lower = TRUE, ...)
## S3 method for class '`function`'
eigs_sym(
 Α,
  k,
 which = "LM",
  sigma = NULL,
  opts = list(),
  lower = TRUE,
  . . . ,
  n = NULL
  args = NULL
```

Arguments

A The matrix whose eigenvalues/vectors are to be computed. It can also be a function which receives a vector x and calculates Ax. See section **Function Interface** for details.

k Number of eigenvalues requested.

which Selection criterion. See **Details** below.

sigma Shift parameter. See section **Shift-And-Invert Mode**.

opts	Control parameters related to the computing algorithm. See Details below.
	Arguments for specialized S3 function calls, for example lower, n and args.
n	Only used when A is a function, to specify the dimension of the implicit matrix. See section Function Interface for details.
args	Only used when A is a function. This argument will be passed to the A function when it is called. See section Function Interface for details.
lower	For symmetric matrices, should the lower triangle or upper triangle be used.

Details

The which argument is a character string that specifies the type of eigenvalues to be computed. Possible values are:

"LM" The k eigenvalues with largest magnitude. Here the magnitude means the Euclidean norm of complex numbers.

"SM" The k eigenvalues with smallest magnitude.

"LR" The k eigenvalues with largest real part.

"SR" The k eigenvalues with smallest real part.

"LI" The k eigenvalues with largest imaginary part.

"SI" The k eigenvalues with smallest imaginary part.

"LA" The k largest (algebraic) eigenvalues, considering any negative sign.

"SA" The k smallest (algebraic) eigenvalues, considering any negative sign.

"BE" Compute k eigenvalues, half from each end of the spectrum. When k is odd, compute more from the high and then from

eigs() with matrix types "matrix", "dgeMatrix", "dgCMatrix" and "dgRMatrix" can use "LM", "SM", "LR", "SR", "LI" and "SI".

eigs_sym() with all supported matrix types, and eigs() with symmetric matrix types ("dsyMatrix", "dsCMatrix", and "dsRMatrix") can use "LM", "SM", "LA", "SA" and "BE".

The opts argument is a list that can supply any of the following parameters:

ncv Number of Lanzcos basis vectors to use. More vectors will result in faster convergence, but with greater memory use. For general matrix, ncv must satisfy $k+2 \le ncv \le n$, and for symmetric matrix, the constraint is $k < ncv \le n$. Default is $\min(n, \max(2 \le k+1, 20))$.

tol Precision parameter. Default is 1e-10.

maxitr Maximum number of iterations. Default is 1000.

retvec Whether to compute eigenvectors. If FALSE, only calculate and return eigenvalues.

initvec Initial vector of length n supplied to the Arnoldi/Lanczos iteration. It may speed up the convergence if initvec is close to an eigenvector of A.

Value

A list of converged eigenvalues and eigenvectors.

values Computed eigenvalues.

vectors Computed eigenvectors. vectors[,j] corresponds to values[j].

nconv Number of converged eigenvalues.

niter Number of iterations used in the computation.

nops Number of matrix operations used in the computation.

Shift-And-Invert Mode

The sigma argument is used in the shift-and-invert mode.

When sigma is not NULL, the selection criteria specified by argument which will apply to

$$\frac{1}{\lambda - \sigma}$$

where λ 's are the eigenvalues of A. This mode is useful when user wants to find eigenvalues closest to a given number. For example, if $\sigma=0$, then which = "LM" will select the largest values of $1/|\lambda|$, which turns out to select eigenvalues of A that have the smallest magnitude. The result of using which = "LM", sigma = 0 will be the same as which = "SM", but the former one is preferable in that eigs() is good at finding large eigenvalues rather than small ones. More explanation of the shift-and-invert mode can be found in the SciPy document, https://docs.scipy.org/doc/scipy/reference/tutorial/arpack.html.

Function Interface

The matrix A can be specified through a function with the definition

```
function(x, args)
{
    ## should return A %*% x
}
```

which receives a vector x as an argument and returns a vector of the same length. The function should have the effect of calculating Ax, and extra arguments can be passed in through the args parameter. In eigs(), user should also provide the dimension of the implicit matrix through the argument n.

Author(s)

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```

See Also

```
eigen(), svd(), svds()
```

Examples

```
library(Matrix)
n = 20
k = 5

## general matrices have complex eigenvalues
set.seed(111)
A1 = matrix(rnorm(n^2), n) ## class "matrix"
A2 = Matrix(A1) ## class "dgeMatrix"
```

```
eigs(A1, k)
eigs(A2, k, opts = list(retvec = FALSE)) ## eigenvalues only
## Sparse matrices
A1[sample(n^2, n^2 / 2)] = 0
A3 = as(A1, "dgCMatrix")
A4 = as(A1, "dgRMatrix")
eigs(A3, k)
eigs(A4, k)
## Function interface
f = function(x, args)
{
    as.numeric(args %*% x)
}
eigs(f, k, n = n, args = A3)
## Symmetric matrices have real eigenvalues
A5 = crossprod(A1)
eigs_sym(A5, k)
## Find the smallest (in absolute value) k eigenvalues of A5
eigs_sym(A5, k, which = "SM")
## Another way to do this: use the sigma argument
eigs_sym(A5, k, sigma = 0)
## The results should be the same,
## but the latter method is far more stable on large matrices
```

svds

Find the Largest k Singular Values/Vectors of a Matrix

Description

Given an m by n matrix A, function svds() can find its largest k singular values and the corresponding singular vectors. It is also called the Truncated SVD or Partial SVD since it only calculates a subset of the whole singular triplets.

Currently svds() supports matrices of the following classes:

```
The most commonly used matrix type, defined in the base package.
matrix
             General matrix, equivalent to matrix, defined in the Matrix package.
dgeMatrix
dgCMatrix
             Column oriented sparse matrix, defined in the Matrix package.
             Row oriented sparse matrix, defined in the Matrix package.
dgRMatrix
dsyMatrix
             Symmetrix matrix, defined in the Matrix package.
dsCMatrix
             Symmetric column oriented sparse matrix, defined in the Matrix package.
             Symmetric row oriented sparse matrix, defined in the Matrix package.
dsRMatrix
             Implicitly specify the matrix through two functions that calculate f(x) = Ax and g(x) = A'x. See section Fun
function
```

Note that when A is symmetric and positive semi-definite, SVD reduces to eigen decomposition, so you may consider using eigs() instead. When A is symmetric but not necessarily positive semi-definite, the left and right singular vectors are the same as the left and right eigenvectors, but the singular values and eigenvalues will not be the same. In particular, if λ is a negative eigenvalue of A, then $|\lambda|$ will be the corresponding singular value.

Usage

```
svds(A, k, nu = k, nv = k, opts = list(), ...)
## S3 method for class 'matrix'
svds(A, k, nu = k, nv = k, opts = list(), ...)
## S3 method for class 'dgeMatrix'
svds(A, k, nu = k, nv = k, opts = list(), ...)
## S3 method for class 'dgCMatrix'
svds(A, k, nu = k, nv = k, opts = list(), ...)
## S3 method for class 'dgRMatrix'
svds(A, k, nu = k, nv = k, opts = list(), ...)
## S3 method for class 'dsyMatrix'
svds(A, k, nu = k, nv = k, opts = list(), ...)
## S3 method for class 'dsCMatrix'
svds(A, k, nu = k, nv = k, opts = list(), ...)
## S3 method for class 'dsRMatrix'
svds(A, k, nu = k, nv = k, opts = list(), ...)
## S3 method for class '`function`'
svds(A, k, nu = k, nv = k, opts = list(), ..., Atrans, dim, args = NULL)
```

Arguments

A	The matrix whose truncated SVD is to be computed.
k	Number of singular values requested.
nu	Number of left singular vectors to be computed. This must be between 0 and k.
nv	Number of right singular vectors to be computed. This must be between 0 and k.
opts	Control parameters related to the computing algorithm. See Details below.
opts	Control parameters related to the computing algorithm. See Details below. Arguments for specialized S3 function calls, for example Atrans, dim and args.

dim	Only used when A is a function, to specify the dimension of the implicit matrix. A vector of length two.
args	Only used when A is a function. This argument will be passed to the A and Atrans functions.

Details

The opts argument is a list that can supply any of the following parameters:

ncv Number of Lanzcos basis vectors to use. More vectors will result in faster convergence, but with greater memory use. ncv must be satisfy $k < ncv \le p$ where p = min(m,n). Default is min(p,max(2*k+1,20)).

tol Precision parameter. Default is 1e-10.

maxitr Maximum number of iterations. Default is 1000.

center Either a logical value (TRUE/FALSE), or a numeric vector of length n. If a vector c is supplied, then SVD is computed on the matrix A-1c', in an implicit way without actually forming this matrix. center = TRUE has the same effect as center = colMeans(A). Default is FALSE.

scale Either a logical value (TRUE/FALSE), or a numeric vector of length n. If a vector s is supplied, then SVD is computed on the matrix (A-1c')S, where c is the centering vector and S=diag(1/s). If scale = TRUE, then the vector s is computed as the column norm of A-1c'. Default is FALSE.

Value

A list with the following components:

d	A vector of the computed singular values.
u	An m by nu matrix whose columns contain the left singular vectors. If $nu == 0$, NULL will be returned.
V	An n by nv matrix whose columns contain the right singular vectors. If $nv == 0$, NULL will be returned.
nconv	Number of converged singular values.
niter	Number of iterations used.
nops	Number of matrix-vector multiplications used.

Function Interface

The matrix A can be specified through two functions with the following definitions

```
A <- function(x, args)
{
    ## should return A %*% x
}
Atrans <- function(x, args)</pre>
```

```
{
    ## should return t(A) %*% x
}
```

They receive a vector x as an argument and returns a vector of the proper dimension. These two functions should have the effect of calculating Ax and A'x respectively, and extra arguments can be passed in through the args parameter. In svds(), user should also provide the dimension of the implicit matrix through the argument dim.

The function interface does not support the center and scale parameters in opts.

Author(s)

```
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```

See Also

```
eigen(), svd(), eigs().
```

Examples

```
m = 100
n = 20
k = 5
set.seed(111)
A = matrix(rnorm(m * n), m)
svds(A, k)
svds(t(A), k, nu = 0, nv = 3)
## Sparse matrices
library(Matrix)
A[sample(m * n, m * n / 2)] = 0
Asp1 = as(A, "dgCMatrix")
Asp2 = as(A, "dgRMatrix")
svds(Asp1, k)
svds(Asp2, k, nu = 0, nv = 0)
## Function interface
Af = function(x, args)
{
    as.numeric(args %*% x)
}
Atf = function(x, args)
{
    as.numeric(crossprod(args, x))
}
svds(Af, k, Atrans = Atf, dim = c(m, n), args = Asp1)
```

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