Package: RSpectra (via r-universe)

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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.

License MPL (>= 2)

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

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

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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.
`dgRMatrix`	Row oriented sparse matrix, defined in the **Matrix** package.
`dsyMatrix`	Symmetric matrix, defined in the **Matrix** package.
`dsCMatrix`	Symmetric column oriented sparse matrix, defined in the **Matrix** package.
`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(
  A,
  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(
  A,
  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 fro

`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 $k + 2 \leq ncv \leq n$, and for symmetric matrix, the constraint is $k < ncv \leq n$. Default is `min(n, max(2*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/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`.

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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:

`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.
`dgRMatrix`	Row oriented sparse matrix, defined in the **Matrix** package.
`dsyMatrix`	Symmetrix matrix, defined in the **Matrix** package.
`dsCMatrix`	Symmetric column oriented sparse matrix, defined in the **Matrix** package.
`dsRMatrix`	Symmetric row oriented sparse matrix, defined in the **Matrix** package.
`function`	Implicitly specify the matrix through two functions that calculate $f(x) = Ax$ and $g(x) = A'x$. See section **Fun**

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.
...	Arguments for specialized S3 function calls, for example Atrans, dim and args.
Atrans	Only used when A is a function. A is a function that calculates the matrix multiplication Ax, and Atrans is a function that calculates the transpose multiplication $A'x$.
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 $k < ncv \leq p$ 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)
{
    ## 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`.

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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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