Package ‘irlba’

Type Package

Title Fast Truncated Singular Value Decomposition and Principal Components Analysis for Large Dense and Sparse Matrices

Version 2.3.5

Date 2021-12-05

Description Fast and memory efficient methods for truncated singular value decomposition and principal components analysis of large sparse and dense matrices.

Depends R (>= 3.6.2), Matrix

LinkingTo Matrix

Imports stats, methods

License GPL-3

BugReports https://github.com/bwlewis/irlba/issues

RoxygenNote 5.0.1

NeedsCompilation yes

Author Jim Baglama [aut, cph],
Lothar Reichel [aut, cph],
B. W. Lewis [aut, cre, cph]

Maintainer B. W. Lewis <blewis@illposed.net>

Repository CRAN

Date/Publication 2021-12-06 14:10:05 UTC

R topics documented:

irlba .......................................................... 2
partial_eigen .............................................. 5
prcomp_irlba .............................................. 7
ssvd .......................................................... 9
summary.irlba_prcomp .................................. 12
svdr ........................................................ 12

Index 15
Find a few approximate singular values and corresponding singular vectors of a matrix.

Description

The augmented implicitly restarted Lanczos bidiagonalization algorithm (IRLBA) finds a few approximate largest (or, optionally, smallest) singular values and corresponding singular vectors of a sparse or dense matrix using a method of Baglama and Reichel. It is a fast and memory-efficient way to compute a partial SVD.

Usage

```r
irlba(A, nv = 5, nu = nv, maxit = 1000, work = nv + 7, reorth = TRUE,
       tol = 1e-05, v = NULL, right_only = FALSE, verbose = FALSE,
       scale = NULL, center = NULL, shift = NULL, mult = NULL,
       fastpath = TRUE, svtol = tol, smallest = FALSE, ...)
```

Arguments

- **A**: numeric real- or complex-valued matrix or real-valued sparse matrix.
- **nv**: number of right singular vectors to estimate.
- **nu**: number of left singular vectors to estimate (defaults to `nv`).
- **maxit**: maximum number of iterations.
- **work**: working subspace dimension, larger values can speed convergence at the cost of more memory use.
- **reorth**: if `TRUE`, apply full reorthogonalization to both SVD bases, otherwise only apply reorthogonalization to the right SVD basis vectors; the latter case is cheaper per iteration but, overall, may require more iterations for convergence. Automatically `TRUE` when `fastpath=TRUE` (see below).
- **tol**: convergence is determined when \[ \| A^T U - V S \| < tol \| A \| , \] and when the maximum relative change in estimated singular values from one iteration to the next is less than `svtol = tol` (see below), where the spectral norm \( \| A \| \) is approximated by the largest estimated singular value, and \( U, V, S \) are the matrices corresponding to the estimated left and right singular vectors, and diagonal matrix of estimated singular values, respectively.
- **v**: optional starting vector or output from a previous run of `irlba` used to restart the algorithm from where it left off (see the notes).
- **right_only**: logical value indicating return only the right singular vectors (`TRUE`) or both sets of vectors (`FALSE`). The `right_only` option can be cheaper to compute and use much less memory when `nrow(A) >> ncol(A)` but note that obtained solutions typically lose accuracy due to lack of re-orthogonalization in the algorithm and that `right_only = TRUE` sets `fastpath = FALSE` (only use this option for really large problems that run out of memory and when `nrow(A) >> ncol(A)`). Consider increasing the `work` option to improve accuracy with `right_only=TRUE`. 

Notes

- The `irlba` function is designed to be fast and memory-efficient, making it suitable for large datasets.
- The `nu` argument defaults to the value of `nv`, allowing for simultaneous estimation of both left and right singular vectors.
- The `maxit` parameter controls the maximum number of iterations the algorithm is allowed to perform. Increasing this value can improve the accuracy of the solution but may also increase computation time and memory usage.
- The `work` parameter determines the size of the working subspace. Larger values can speed up convergence but require more memory.
- The `reorth` parameter controls the level of reorthogonalization applied to the SVD bases. While the default setting of `TRUE` ensures a higher quality of the solution, using `FALSE` can be more memory-efficient for large datasets.
- The `tol` parameter sets the tolerance level for convergence, with smaller values leading to more accurate but slower computations.
- The `right_only` parameter enables selection of only the right singular vectors, which can be useful for certain applications but may result in less accurate solutions.
**verbose** logical value that when TRUE prints status messages during the computation.

**scale** optional column scaling vector whose values divide each column of $A$; must be as long as the number of columns of $A$ (see notes).

**center** optional column centering vector whose values are subtracted from each column of $A$; must be as long as the number of columns of $A$ and may not be used together with the deflation options below (see notes).

**shift** optional shift value (square matrices only, see notes).

**mult** DEPRECATED optional custom matrix multiplication function (default is $\%\%\times\%\%$, see notes).

**fastpath** try a fast C algorithm implementation if possible; set fastpath=FALSE to use the reference R implementation. See the notes for more details.

**svtol** additional stopping tolerance on maximum allowed absolute relative change across each estimated singular value between iterations. The default value of this parameter is to set it to $\text{tol}$. You can set svtol=Inf to effectively disable this stopping criterion. Setting svtol=Inf allows the method to terminate on the first Lanczos iteration if it finds an invariant subspace, but with less certainty that the converged subspace is the desired one. (It may, for instance, miss some of the largest singular values in difficult problems.)

**smallest** set smallest=TRUE to estimate the smallest singular values and associated singular vectors. WARNING: this option is somewhat experimental, and may produce poor estimates for ill-conditioned matrices.

... optional additional arguments used to support experimental and deprecated features.

**Value**

Returns a list with entries:

- **d**: $\max(nu, nv)$ approximate singular values
- **u**: $nu$ approximate left singular vectors (only when right_only=FALSE)
- **v**: $nv$ approximate right singular vectors
- **iter**: The number of Lanczos iterations carried out
- **mprod**: The total number of matrix vector products carried out

**Note**

The syntax of irlba partially follows svd, with an important exception. The usual R svd function always returns a complete set of singular values, even if the number of singular vectors $nu$ or $nv$ is set less than the maximum. The irlba function returns a number of estimated singular values equal to the maximum of the number of specified singular vectors $nu$ and $nv$.

Use the optional scale parameter to implicitly scale each column of the matrix $A$ by the values in the scale vector, computing the truncated SVD of the column-scaled sweep($A, 2, scale, FUN=\%\%\div\%\%$), or equivalently, $A \times diag(1 / scale)$, without explicitly forming the scaled matrix. scale must be a non-zero vector of length equal to the number of columns of $A$. 
Use the optional center parameter to implicitly subtract the values in the center vector from each column of A, computing the truncated SVD of sweep(A,2,center,FUN=`-`). without explicitly forming the centered matrix. center must be a vector of length equal to the number of columns of A. This option may be used to efficiently compute principal components without explicitly forming the centered matrix (which can, importantly, preserve sparsity in the matrix). See the examples.

The optional shift scalar valued argument applies only to square matrices; use it to estimate the partial svd of A + diag(shift,nrow(A),nrow(A)) (without explicitly forming the shifted matrix).

(Deprecated) Specify an optional alternative matrix multiplication operator in the mult parameter. mult must be a function of two arguments, and must handle both cases where one argument is a vector and the other a matrix. This option is deprecated and will be removed in a future version. The new preferred method simply uses R itself to define a custom matrix class with your user-defined matrix multiplication operator. See the examples.

Use the v option to supply a starting vector for the iterative method. A random vector is used by default (precede with set.seed() for reproducibility). Optionally set v to the output of a previous run of irlba to restart the method, adding additional singular values/vectors without recomputing the solution subspace. See the examples.

The function may generate the following warnings:

- "did not converge–results might be invalid!; try increasing work or maxit" means that the algorithm didn't converge – this is potentially a serious problem and the returned results may not be valid. irlba reports a warning here instead of an error so that you can inspect whatever is returned. If this happens, carefully heed the warning and inspect the result. You may also try setting fastpath=FALSE.

- "You're computing a large percentage of total singular values, standard svd might work better!" irlba is designed to efficiently compute a few of the largest singular values and associated singular vectors of a matrix. The standard svd function will be more efficient for computing large numbers of singular values than irlba.

- "convergence criterion below machine epsilon" means that the product of tol and the largest estimated singular value is really small and the normal convergence criterion is only met up to round off error.

The function might return an error for several reasons including a situation when the starting vector v is near the null space of the matrix. In that case, try a different v.

The fastpath=TRUE option only supports real-valued matrices and sparse matrices of type dgCMatrix (for now). Other problems fall back to the reference R implementation.

References


See Also

svd, prcomp, partial_eigen, svdr
**partial_eigen**

Find a few approximate largest eigenvalues and corresponding eigenvectors of a symmetric matrix.
Description

Use `partial_eigen` to estimate a subset of the largest (most positive) eigenvalues and corresponding eigenvectors of a symmetric dense or sparse real-valued matrix.

Usage

```r
partial_eigen(x, n = 5, symmetric = TRUE, ...)
```

Arguments

- `x`: numeric real-valued dense or sparse matrix.
- `n`: number of largest eigenvalues and corresponding eigenvectors to compute.
- `symmetric`: `TRUE` indicates `x` is a symmetric matrix (the default); specify `symmetric=FALSE` to compute the largest eigenvalues and corresponding eigenvectors of `t(x) %*% x` instead.
- `...`: optional additional parameters passed to the `irlba` function.

Value

Returns a list with entries:

- `values`: `n` approximate largest eigenvalues
- `vectors`: `n` approximate corresponding eigenvectors

Note

Specify `symmetric=FALSE` to compute the largest `n` eigenvalues and corresponding eigenvectors of the symmetric matrix cross-product `t(x) %*% x`.

This function uses the `irlba` function under the hood. See `?irlba` for description of additional options, especially the `tol` parameter.

See the RSpectra package https://cran.r-project.org/package=RSpectra for more comprehensive partial eigenvalue decomposition.

References


See Also

`eigen`, `irlba`
Examples

```r
set.seed(1)
# Construct a symmetric matrix with some positive and negative eigenvalues:
V <- qr.Q(qr(matrix(runif(100), nrow=10)))
x <- V %*% diag(c(10, -9, 8, -7, 6, -5, 4, -3, 2, -1)) %*% t(V)
partial_eigen(x, 3)$values

# Compare with eigen
eigen(x)$values[1:3]

# Use symmetric=FALSE to compute the eigenvalues of t(x) %*% x for general
# matrices x:
x <- matrix(rnorm(100), 10)
partial_eigen(x, 3, symmetric=FALSE)$values
eigen(crossprod(x))$values
```

prcomp_irlba  Principal Components Analysis

Description

Efficient computation of a truncated principal components analysis of a given data matrix using an implicitly restarted Lanczos method from the irlba package.

Usage

`prcomp_irlba(x, n = 3, retx = TRUE, center = TRUE, scale. = FALSE, ...)`

Arguments

- `x`: a numeric or complex matrix (or data frame) which provides the data for the principal components analysis.
- `n`: integer number of principal component vectors to return, must be less than `min(dim(x))`.
- `retx`: a logical value indicating whether the rotated variables should be returned.
- `center`: a logical value indicating whether the variables should be shifted to be zero centered. Alternately, a centering vector of length equal the number of columns of `x` can be supplied.
- `scale.`: a logical value indicating whether the variables should be scaled to have unit variance before the analysis takes place. The default is `FALSE` for consistency with S, but scaling is often advisable. Alternatively, a vector of length equal the number of columns of `x` can be supplied.

The value of `scale` determines how column scaling is performed (after centering). If `scale` is a numeric vector with length equal to the number of columns of `x`, then each column of `x` is divided by the corresponding value from `scale`. 
If \texttt{scale} is \texttt{TRUE} then scaling is done by dividing the (centered) columns of \texttt{x} by their standard deviations if \texttt{center=TRUE}, and the root mean square otherwise. If \texttt{scale} is \texttt{FALSE}, no scaling is done. See \texttt{scale} for more details.

... additional arguments passed to \texttt{irlba}.

\textbf{Value}

A list with class "prcomp" containing the following components:

- \texttt{sdev} the standard deviations of the principal components (i.e., the square roots of the eigenvalues of the covariance/correlation matrix, though the calculation is actually done with the singular values of the data matrix).
- \texttt{rotation} the matrix of variable loadings (i.e., a matrix whose columns contain the eigenvectors).
- \texttt{x} if \texttt{retx} is \texttt{TRUE} the value of the rotated data (the centred (and scaled if requested) data multiplied by the \texttt{rotation} matrix) is returned. Hence, \texttt{cov(x)} is the diagonal matrix \texttt{diag(sdev^2)}.
- \texttt{center}, \texttt{scale} the centering and scaling used, or \texttt{FALSE}.

\textbf{Note}

The signs of the columns of the rotation matrix are arbitrary, and so may differ between different programs for PCA, and even between different builds of R.

\textbf{NOTE DIFFERENCES WITH THE DEFAULT \texttt{prcomp} FUNCTION!} The \texttt{tol} truncation argument found in \texttt{prcomp} is not supported. In place of the truncation tolerance in the original function, the \texttt{prcomp_irlba} function has the argument \texttt{n} explicitly giving the number of principal components to return. A warning is generated if the argument \texttt{tol} is used, which is interpreted differently between the two functions.

\textbf{See Also}

\texttt{prcomp}

\textbf{Examples}

```r
set.seed(1)
x <- matrix(rnorm(200), nrow=20)
p1 <- prcomp_irlba(x, n=3)
summary(p1)

# Compare with
p2 <- prcomp(x, tol=0.7)
summary(p2)
```
**ssvd**

_Sparse regularized low-rank matrix approximation._

**Description**

Estimate an \( \ell_1 \)-penalized singular value or principal components decomposition (SVD or PCA) that introduces sparsity in the right singular vectors based on the fast and memory-efficient sPCA-rSVD algorithm of Haipeng Shen and Jianhua Huang.

**Usage**

```r
ssvd(x, k = 1, n = 2, maxit = 500, tol = 0.001, center = FALSE,
     scale. = FALSE, alpha = 0, tsvd = NULL, ...)
```

**Arguments**

- **x** A numeric real- or complex-valued matrix or real-valued sparse matrix.
- **k** Matrix rank of the computed decomposition (see the Details section below).
- **n** Number of nonzero components in the right singular vectors. If \( k > 1 \), then a single value of \( n \) specifies the number of nonzero components in each regularized right singular vector. Or, specify a vector of length \( k \) indicating the number of desired nonzero components in each returned vector. See the examples.
- **maxit** Maximum number of soft-thresholding iterations.
- **tol** Convergence is determined when \( \| U_j - U_{j-1} \|_F < tol \), where \( U_j \) is the matrix of estimated left regularized singular vectors at iteration \( j \).
- **center** a logical value indicating whether the variables should be shifted to be zero centered. Alternately, a centering vector of length equal the number of columns of \( x \) can be supplied. Use `center=TRUE` to perform a regularized sparse PCA.
- **scale.** a logical value indicating whether the variables should be scaled to have unit variance before the analysis takes place. Alternatively, a vector of length equal the number of columns of \( x \) can be supplied.
  The value of `scale` determines how column scaling is performed (after centering). If `scale` is a numeric vector with length equal to the number of columns of \( x \), then each column of \( x \) is divided by the corresponding value from `scale`. If `scale` is TRUE then scaling is done by dividing the (centered) columns of \( x \) by their standard deviations if `center=TRUE`, and the root mean square otherwise. If `scale` is FALSE, no scaling is done. See `scale` for more details.
- **alpha** Optional scalar regularization parameter between zero and one (see Details below).
- **tsvd** Optional initial rank-k truncated SVD or PCA (skips computation if supplied).
- **...** Additional arguments passed to `irlba`. 
Details

The `ssvd` function implements a version of an algorithm by Shen and Huang that computes a penalized SVD or PCA that introduces sparsity in the right singular vectors by solving a penalized least squares problem. The algorithm in the rank 1 case finds vectors $u, w$ that minimize

$$\|x - uw^T\|^2_F + \lambda \|w\|_1$$

such that $\|u\| = 1$, and then sets $v = w/\|w\|$ and $d = u^T xv$; see the referenced paper for details. The penalty $\lambda$ is implicitly determined from the specified desired number of nonzero values $n$. Higher rank output is determined similarly but using a sequence of $\lambda$ values determined to maintain the desired number of nonzero elements in each column of $v$ specified by $n$. Unlike standard SVD or PCA, the columns of the returned $v$ when $k > 1$ may not be orthogonal.

Value

A list containing the following components:

- $u$ regularized left singular vectors with orthonormal columns
- $d$ regularized upper-triangular projection matrix so that $x \times v = u \times d$
- $v$ regularized, sparse right singular vectors with columns of unit norm
- center, scale the centering and scaling used, if any
- lambda the per-column regularization parameter found to obtain the desired sparsity
- iter number of soft thresholding iterations
- $n$ value of input parameter $n$
- alpha value of input parameter $alpha$

Note

Our `ssvd` implementation of the Shen-Huang method makes the following choices:

1. The l1 penalty is the only available penalty function. Other penalties may appear in the future.
2. Given a desired number of nonzero elements in $v$, value(s) for the $\lambda$ penalty are determined to achieve the sparsity goal subject to the parameter $alpha$.
3. An experimental block implementation is used for results with rank greater than 1 (when $k > 1$) instead of the deflation method described in the reference.
4. The choice of a penalty lambda associated with a given number of desired nonzero components is not unique. The $alpha$ parameter, a scalar between zero and one, selects any possible value of lambda that produces the desired number of nonzero entries. The default $alpha = 0$ selects a penalized solution with largest corresponding value of $d$ in the 1-d case. Think of $alpha$ as fine-tuning of the penalty.
5. Our method returns an upper-triangular matrix $d$ when $k > 1$ so that $x \times v = u \times d$. Nonzero elements above the diagonal result from non-orthogonality of the $v$ matrix, providing a simple interpretation of cumulative information, or explained variance in the PCA case, via the singular value decomposition of $d \times v$.
What if you have no idea for values of the argument n (the desired sparsity)? The reference describes a cross-validation and an ad-hoc approach; neither of which are in the package yet. Both are prohibitively computationally expensive for matrices with a huge number of columns. A future version of this package will include a revised approach to automatically selecting a reasonable sparsity constraint.

Compare with the similar but more general functions SPC and PMD in the PMA package by Daniela M. Witten, Robert Tibshirani, Sam Gross, and Balasubramanian Narasimhan. The PMD function can compute low-rank regularized matrix decompositions with sparsity penalties on both the u and v vectors. The ssvd function is similar to the PMD(*, L1) method invocation of PMD or alternatively the SPC function. Although less general than PMD(*), the ssvd function can be faster and more memory efficient for the basic sparse PCA problem. See https://bwlewis.github.io/irlba/ssvd.html for more information.

(* Note that the s4vd package by Martin Sill and Sebastian Kaiser, https://cran.r-project.org/package=s4vd, includes a fast optimized version of a closely related algorithm by Shen, Huang, and Marron, that penalizes both u and v.)

References


Examples

```r
set.seed(1)
u <- matrix(rnorm(200), ncol=1)
v <- matrix(c(runif(50, min=0.1), rep(0,250)), ncol=1)
u <- u / drop(sqrt(crossprod(u)))
v <- v / drop(sqrt(crossprod(v)))
x <- u %*% t(v) + 0.001 * matrix(rnorm(200*300), ncol=300)
s <- ssvd(x, n=50)
table(actual=v[, 1] != 0, estimated=s$v[, 1] != 0)
oldpar <- par(mfrow=c(2, 1))
plot(u, cex=2, main="u (black circles), Estimated u (blue discs)
points(s$u, pch=19, col=4)
plot(v, cex=2, main="v (black circles), Estimated v (blue discs)
points(s$v, pch=19, col=4)
```

# Let's consider a trivial rank-2 example (k=2) with noise. Like the last example, we know the exact number of nonzero elements in each solution vector of the noise-free matrix. Note the application of different sparsity constraints on each column of the estimated v. # Also, the decomposition is unique only up to sign, which we adjust for below.

```r
set.seed(1)
u <- qr.Q(qr(matrix(rnorm(400), ncol=2)))
v <- matrix(0, ncol=2, nrow=300)
```
svdr

Find a few approximate largest singular values and corresponding singular vectors of a matrix.

Description

The randomized method for truncated SVD by P. G. Martinsson and colleagues finds a few approximate largest singular values and corresponding singular vectors of a sparse or dense matrix. It is a fast and memory-efficient way to compute a partial SVD, similar in performance for many problems to irlba. The svdr method is a block method and may produce more accurate estimations with less work for problems with clustered large singular values (see the examples). In other problems, irlba may exhibit faster convergence.

summary.irlba_prcomp

Summary method for truncated pca objects computed by prcomp_irlba.

Description

Summary method for truncated pca objects computed by prcomp_irlba.

Usage

## S3 method for class 'irlba_prcomp'
summary(object, ...)

Arguments

object

An object returned by prcomp_irlba.

... Optional arguments passed to summary.
svdr

Usage

svdr(x, k, tol = 1e-05, it = 100L, extra = min(10L, dim(x) - k),
    center = NULL, Q = NULL, return.Q = FALSE)

Arguments

x       numeric real- or complex-valued matrix or real-valued sparse matrix.
k       dimension of subspace to estimate (number of approximate singular values to compute).
tol     stop iteration when the largest absolute relative change in estimated singular values from one iteration to the next falls below this value.
it      maximum number of algorithm iterations.
extra   number of extra vectors of dimension ncol(x), larger values generally improve accuracy (with increased computational cost).
center  optional column centering vector whose values are implicitly subtracted from each column of A without explicitly forming the centered matrix (preserving sparsity). Optionally specify center=TRUE as shorthand for center=colMeans(x). Use for efficient principal components computation.
Q       optional initial random matrix, defaults to a matrix of size ncol(x) by k + extra with entries sampled from a normal random distribution.
return.Q if TRUE return the Q matrix for restarting (see examples).

Details

Also see an alternate implementation (rsvd) of this method by N. Benjamin Erichson in the https://cran.r-project.org/package=rsvd package.

Value

Returns a list with entries:

   d:  k approximate singular values
   u:  k approximate left singular vectors
   v:  k approximate right singular vectors
   mprod: total number of matrix products carried out
   Q:  optional subspace matrix (when return.Q=TRUE)

References


See Also

irlba, svd, rsvd in the rsvd package
**Examples**

```r
set.seed(1)
A <- matrix(runif(400), nrow=20)
svdr(A, 3)$d

# Compare with svd
svd(A)$d[1:3]

# Compare with irlba
irlba(A, 3)$d

## Not run:
# A problem with clustered large singular values where svdr out-performs irlba.
tprolate <- function(n, w=0.25)
{
  a <- rep(0, n)
  a[1] <- 2 * w
  a[2:n] <- sin( 2 * pi * w * (1:(n-1)) ) / ( pi * (1:(n-1)) )
toepilz(a)
}
x <- tprolate(512)
set.seed(1)
tL <- system.time(L <- irlba(x, 20))
tR <- system.time(R <- svdr(x, 20))
S <- svd(x)
plot(S$d)
data.frame(time=c(tL[3], tR[3]),
          error=sqrt(c(crossprod(L$d - S$d[1:20]), crossprod(R$d - S$d[1:20]))),
          row.names=c("IRLBA", "Randomized SVD"))

# But, here is a similar problem with clustered singular values where svdr
# doesn't out-perform irlba as easily...clusters of singular values are,
# in general, very hard to deal with!
# (This example based on https://github.com/bwlewis/irlba/issues/16.)
set.seed(1)
s <- svd(matrix(rnorm(200 * 200), 200))
x <- s$v * (c(exp(-(1:100)^0.3) * 1e-12 + 1, rep(0.5, 100)) * t(s$v))
tL <- system.time(L <- irlba(x, 5))
tR <- system.time(R <- svdr(x, 5))
S <- svd(x)
plot(S$d)
data.frame(time=c(tL[3], tR[3]),
          error=sqrt(c(crossprod(L$d - S$d[1:5]), crossprod(R$d - S$d[1:5]))),
          row.names=c("IRLBA", "Randomized SVD"))

## End(Not run)
```
Index

eigen, 6

irlba, 2, 6–9, 12, 13

partial_eigen, 4, 5
prcomp, 4, 8
prcomp_irlba, 7

scale, 8, 9
ssvd, 9
summary.irlba_prcomp, 12
svd, 4, 13
svdr, 4, 12