

Package ‘bcv’

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Title Cross-Validation for the SVD (Bi-Cross-Validation)

Description Methods for choosing the rank of an SVD (singular value decomposition) approximation via cross validation. The package provides both Gabriel-style ``block" holdouts and Wold-style ``speckled" holdouts. It also includes an implementation of the SVDImpute algorithm. For more information about Bi-cross-validation, see Owen & Perry's 2009 AoAS article (at <[doi:10.48550/arXiv.0908.2062](https://doi.org/10.48550/arXiv.0908.2062)>) and Perry's 2009 PhD thesis (at <[doi:10.48550/arXiv.0909.3052](https://doi.org/10.48550/arXiv.0909.3052)>).

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URL <https://github.com/michbur/bcv>

BugReports <https://github.com/michbur/bcv/issues>

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bcv-package	<i>Cross-Validation for the SVD (Bi-Cross-Validation)</i>
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Description

This package implements methods for choosing the rank of an SVD approximation via cross validation. It provides both Gabriel-style "block" holdouts and Wold-style "speckled" holdouts. Also included is an implementation of the SVDImpute algorithm.

Details

Package: bcv
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 License: BSD3

Basic usage is to call either [cv.svd.gabriel](#) or [cv.svd.wold](#).

Author(s)

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See Also

[impute.svd](#), [cv.svd.gabriel](#), [cv.svd.wold](#), [plot.cvsvd](#), [print.cvsvd](#) [summary.cvsvd](#)

cv.svd.gabriel	<i>Cross-Validation for choosing the rank of an SVD approximation.</i>
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Description

Perform Wold- or Gabriel-style cross-validation for determining the appropriate rank SVD approximation of a matrix.

Usage

```
cv.svd.gabriel(
  x,
  krow = 2,
  kcol = 2,
  maxrank = floor(min(n - n/krow, p - p/kcol))
)

cv.svd.wold(x, k = 5, maxrank = 20, tol = 1e-04, maxiter = 20)
```

Arguments

x	the matrix to cross-validate.
krow	the number of row folds (for Gabriel-style CV).
kcol	the number of column folds (for Gabriel-style CV).
maxrank	the maximum rank to cross-validate up to.
k	the number of folds (for Wold-style CV).
tol	the convergence tolerance for impute.svd .
maxiter	the maximum number of iterations for impute.svd .

Details

These functions are for cross-validating the SVD of a matrix. They assume a model $X = U D V' + E$ with the terms being signal and noise, and try to find the best rank to truncate the SVD of x at for minimizing prediction error. Here, prediction error is measured as sum of squares of residuals between the truncated SVD and the signal part.

For both types of cross-validation, in each replicate we leave out part of the matrix, fit an SVD approximation to the left-in part, and measure prediction error on the left-out part.

In Wold-style cross-validation, the holdout set is "speckled", a random set of elements in the matrix. The missing elements are predicted using [impute.svd](#).

In Gabriel-style cross-validation, the holdout set is "blocked". We permute the rows and columns of the matrix, and leave out the lower-right block. We use a modified Schur-complement to predict the held-out block. In Gabriel-style, there are $krow * kcol$ total folds.

Value

call	the function call
msep	the mean square error of prediction (MSEP); this is a matrix whose columns contain the mean square errors in the predictions of the holdout sets for ranks 0, 1, ..., maxrank across the different replicates.
maxrank	the maximum rank for which prediction error is estimated; this is equal to $nrow(msep)+1$.
krow	the number of row folds (for Gabriel-style only).
kcol	the number of column folds (for Gabriel-style only).

rowsets	the partition of rows into krow holdout sets (for Gabriel-style only).
colsets	the partition of the columns into kcol holdout sets (for Gabriel-style only).
k	the number of folds (for Wold-style only).
sets	the partition of indices into k holdout sets (for Wold-style only).

Note

Gabriel's version of cross-validation was for leaving out a single element of the matrix, which corresponds to n-by-p-fold. Owen and Perry generalized Gabriel's idea to larger holdouts, showing that 2-by-2-fold cross-validation often works better.

Wold's original version of cross-validation did not use the EM algorithm to estimate the SVD. He recommend using the NIPALS algorithm instead, which has since faded into obscurity.

Wold-style cross-validation takes a lot more computation than Gabriel-style. The `maxrank`, `tol`, and `maxiter` have been chosen to give up some accuracy in the name of expediency. They may need to be adjusted to get the best results.

Author(s)

Patrick O. Perry

References

Gabriel, K.R. (2002). Le biplot - outil d'exploration de données multidimensionnelles. *Journal de la Société française de statistique*, Volume 143 (2002) no. 3-4, pp. 5-55. B.

Owen, A.B. and Perry, P.O. (2009). Bi-cross-validation of the SVD and the non-negative matrix factorization. *Annals of Applied Statistics* **3**(2) 564–594.

Wold, S. (1978). Cross-validated estimation of the number of components in factor and principal components models. *Technometrics* **20**(4) 397–405.

See Also

[impute.svd](#), [plot.cvsvd](#), [print.cvsvd](#) [summary.cvsvd](#)

Examples

```
# generate a rank-2 matrix plus noise
n <- 50; p <- 20; k <- 2
u <- matrix( rnorm( n*k ), n, k )
v <- matrix( rnorm( p*k ), p, k )
e <- matrix( rnorm( n*p ), n, p )
x <- u %*% t(v) + e

# perform 5-fold Wold-style cross-validation
(cvw <- cv.svd.wold( x, 5, maxrank=10 ))

# perform (2,2)-fold Gabriel-style cross-validation
(cvg <- cv.svd.gabriel( x, 2, 2, maxrank=10 ))
```

`impute.svd`*Missing value imputation via the SVDImpute algorithm*

Description

Given a matrix with missing values, impute the missing entries using a low-rank SVD approximation estimated by the EM algorithm.

Usage

```
impute.svd(x, k = min(n, p), tol = max(n, p) * 1e-10, maxiter = 100)
```

Arguments

<code>x</code>	a matrix to impute the missing entries of.
<code>k</code>	the rank of the SVD approximation.
<code>tol</code>	the convergence tolerance for the EM algorithm.
<code>maxiter</code>	the maximum number of EM steps to take.

Details

Impute the missing values of `x` as follows: First, initialize all NA values to the column means, or 0 if all entries in the column are missing. Then, until convergence, compute the first `k` terms of the SVD of the completed matrix. Replace the previously missing values with their approximations from the SVD, and compute the RSS between the *non-missing* values and the SVD.

Declare convergence if $\text{abs}(\text{rss}_0 - \text{rss}_1) / (.Machine\$double.eps + \text{rss}_1) < \text{tol}$, where `rss0` and `rss1` are the RSS values computed from successive iterations. Stop early after `maxiter` iterations and issue a warning.

Value

<code>x</code>	the completed version of the matrix.
<code>rss</code>	the sum of squares between the SVD approximation and the non-missing values in <code>x</code> .
<code>iter</code>	the number of EM iterations before algorithm stopped.

Author(s)

Patrick O. Perry

References

Troyanskaya, O., Cantor, M., Sherlock, G., Brown, P., Hastie, T., Tibshirani, R., Botstein, D. and Altman, R.B. (2001). Missing value estimation methods for DNA microarrays. *Bioinformatics* **17**(6), 520–525.

See Also[cv.svd.wold](#)**Examples**

```

# Generate a matrix with missing entries
n <- 20
p <- 10
u <- rnorm( n )
v <- rnorm( p )
xfull <- u %*% rbind( v ) + rnorm( n*p )
miss <- sample( seq_len( n*p ), n )
x      <- xfull
x[miss] <- NA

# impute the missing entries with a rank-1 SVD approximation
xhat <- impute.svd( x, 1 )$x

# compute the prediction error for the missing entries
sum( ( xfull-xhat )^2 )

```

plot.cvsvd

Plot the Result of an SVD Cross-Validation

Description

Plot the result of [cv.svd.gabriel](#) or [cv.svd.wold](#), optionally with error bars.

Usage

```

## S3 method for class 'cvsvd'
plot(
  x,
  errorbars = TRUE,
  add = FALSE,
  xlab = "Rank",
  ylab = "Mean Sq. Prediction Error",
  col = "blue",
  col.errorbars = "gray50",
  ...
)

```

Arguments

`x` the result of a [cv.svd.gabriel](#) or `link{cv.svd.wold}` computation.

`errorbars` indicates whether or not to add error bars.

`add` indicates whether or not to add to the current plot.

xlab the label for the x axis.
ylab the label for the y axis.
col the color to use for showing prediction error.
col.errorbars the color to use for the error bars.
... additional arguments for plot.

Details

Plot the result of [cv.svd.gabriel](#) or [cv.svd.wold](#). This plots a the estimated prediction error as a function of rank, optionally with error bars.

If add is TRUE, the current plot is not cleared.

Author(s)

Patrick O. Perry

See Also

[cv.svd.gabriel](#), [cv.svd.wold](#), [print.cvsvd](#) [summary.cvsvd](#)

Examples

```
# generate a rank-2 matrix plus noise
n <- 50; p <- 20; k <- 2
u <- matrix( rnorm( n*k ), n, k )
v <- matrix( rnorm( p*k ), p, k )
e <- matrix( rnorm( n*p ), n, p )
x <- u %%% t(v) + e

# perform 5-fold Wold-style cross-validation
cvw <- cv.svd.wold( x, 5, maxrank=10 )

# perform (2,2)-fold Gabriel-style cross-validation
cvg <- cv.svd.gabriel( x, 2, 2, maxrank=10 )

# plot the results
par( mfrow=c(2,1) )
plot( cvw, main="Wold-style CV" )
plot( cvg, main="Gabriel-style CV" )
```

`print.cvsvd`*Print the Result of an SVD Cross-Validation*

Description

Print the result of `cv.svd.gabriel` or `cv.svd.wold`.

Usage

```
## S3 method for class 'cvsvd'  
print(x, digits = max(3, getOption("digits") - 3), ...)
```

Arguments

<code>x</code>	the result of a <code>cv.svd.gabriel</code> or <code>cv.svd.wold</code> computation.
<code>digits</code>	the digits of precision to show in the output.
<code>...</code>	additional arguments to print.

Details

Print a table of the estimated prediction errors and the standard errors of the estimate. Put an asterisk (*) next to the minimum and a plus (+) next to the "one standard error rule" choice.

Author(s)

Patrick O. Perry

See Also

[cv.svd.gabriel](#), [cv.svd.wold](#), [plot.cvsvd](#) [summary.cvsvd](#)

`summary.cvsvd`*Summarize the Result of an SVD Cross-Validation*

Description

Summarize the result of `cv.svd.gabriel` or `cv.svd.wold`.

Usage

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

Arguments

object the result of a [cv.svd.gabriel](#) or [cv.svd.wold](#) computation.
... additional arguments to `summary`.

Details

Print a table of the estimated prediction errors and the standard errors of the estimate. Put an asterisk (*) next to the minimum and a plus (+) next to the "one standard error rule" choice.

Value

`nfolds` the number of cross-validation folds
`maxrank` the maximum rank for which prediction error is estimated.
`msep.mean` the average mean square error of prediction (MSEP) across all folds for ranks 0, 1, ..., `maxrank`.
`msep.se` the standard errors of the `msep.mean` estimates.
`rank.best` the rank with the minimum `msep.mean` value.
`rank.1se` the smallest rank within one standard error of the minimum `msep.mean` value.

Author(s)

Patrick O. Perry

See Also

[cv.svd.gabriel](#), [cv.svd.wold](#), [plot.cvsvd](#) [print.cvsvd](#)

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