

Package ‘mpm’

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Title Multivariate Projection Methods

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Depends R (>= 2.10), MASS, KernSmooth

Description Exploratory graphical analysis of multivariate data, specifically gene expression data with different projection methods: principal component analysis, correspondence analysis, spectral map analysis.

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URL <http://mpm.r-forge.r-project.org>

Collate 'export.summary.mpm.R' 'Famin81A.R' 'Golub.R' 'mpm.R' 'plot.mpm.R' 'print.mpm.R' 'print.summary.mpm.R' 'summary.mpm.R' 'zzz.R'

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export	<i>Generic Function to Export Output to Files...</i>
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Description

Generic Function to Export Output to Files

Usage

```
export(x, filename, ...)
```

Arguments

x	object to export to a file
filename	name of the file to which the output should be exported
...	further arguments for the method

Author(s)

Tobias Verbeke

export.summary.mpm	<i>Export the summary output for an mpm object to a text file...</i>
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Description

Export the summary output for an mpm object to a text file Output the mpm summary to a tab-demimited file for processing by other programs (Excel, Spotfire...) If the filename is empty, return the data instead of writing to file (useful for web services).

Usage

```
## S3 method for class 'summary.mpm'
export(x, filename="", ...)
```

Arguments

x	object of class summary.mpm as produced by the function of the same name
filename	prefix used to name the output file following <filename>_xyz.txt
...	further arguments; currently none are used

Details

Polar (spherical) coordinates are added if the summary.spm object contains 2 (3) dimensions.

Value

the output is returned invisibly

Author(s)

Rudi Verbeeck, Tobias Verbeke

See Also

[summary.mpm](#)

Famin81A

Famin81A Data...

Description

Famin81A Data Data with demographic indicators by region of the world

References

Friday, L. and Laskey, R. (1989). *The Fragile Environment, The Darwin College Lecture*. Cambridge University Press, UK.

Golub

Golub (1999) Data...

Description

Golub (1999) Data Golub et al. (1999) data on gene expression profiles of 38 patients suffering from acute leukemia and a validation sample of 34 patients.

Details

The original data of Golub et al. (1999) were preprocessed as follows: genes that were called 'absent' in all samples were removed from the data sets, since these measurements are considered unreliable by the manufacturer of the technology. Negative measurements in the data were set to 1. The resulting data frame contains 5327 genes of the 6817 originally reported by Golub et al. (1999).

Note

Luc Wouters et al. (2003), p. 1134 contains a typo concerning the sample sizes of AML- and ALL-type and erroneously reported

References

Luc Wouters et al. (2003). *Graphical Exploration of Gene Expression Data: A Comparative Study of Three Multivariate Methods*, *Biometrics*, 59, 1131-1139.

mpm

*Spectral Map Analysis...***Description**

Spectral Map Analysis Produces an object of class `mpm` that allows for exploratory multivariate analysis of large data matrices, such as gene expression data from microarray experiments.

Usage

```
mpm(data, logtrans=TRUE, logrepl=1e-09, center=c("double", "row", "column",
"global", "none"), normal=c("global", "row", "column", "none"),
closure=c("none", "row", "column", "global", "double"),
row.weight=c("constant", "mean", "median", "max", "logmean", "RW"),
col.weight=c("constant", "mean", "median", "max", "logmean", "CW"),
CW=rep(1, ncol(data) - 1), RW=rep(1, nrow(data)),
pos.row=rep(FALSE, nrow(data)), pos.column=rep(FALSE, ncol(data) -
1))
```

Arguments

<code>data</code>	a data frame with the row descriptors in the first column. For microarray data rows indicate genes and columns biological samples.
<code>logtrans</code>	an optional logical value. If TRUE, data are first transformed to logarithms (base e) before the other operations. Non-positive numbers are replaced by <code>logrepl</code> . If FALSE, data are left unchanged. Defaults to TRUE.
<code>logrepl</code>	an optional numeric value that replaces non-positive numbers in log-transformations. Defaults to 1e-9.
<code>closure</code>	optional character string specifying the closure operation that is carried out on the optionally log-transformed data matrix. If "double", data are divided by row- and column-totals. If "row" data are divided by row-totals. If "column" data are divided by column-totals. If "none" no closure is carried out. Defaults to "none".
<code>center</code>	optional character string specifying the centering operation that is carried out on the optionally log-transformed, closed data matrix. If "double" both row- and column-means are subtracted. If "row" row-means are subtracted. If "column" column-means are subtracted. If "none" the data are left uncentered. Defaults to "double".
<code>normal</code>	optional character string specifying the normalization operation that is carried out on the optionally log-transformed, closed, and centered data matrix. If "global" the data are normalized using the global standard deviation. If "row" data are divided by the standard deviations of the respective row. If "column" data are divided by their respective column standard deviation. If "none" no normalization is carried out. Defaults to "global".

<code>row.weight</code>	optional character string specifying the weights of the different rows in the analysis. This can be "constant", "mean", "median", "max", "logmean", or "RW". If "RW" is specified, weights must be supplied in the vector RW. In other cases weights are computed from the data. Defaults to "constant", i.e. constant weighting.
<code>col.weight</code>	optional character string specifying the weights of the different columns in the analysis. This can be "constant", "mean", "median", "max", "logmean", or "CW". If "CW" is specified, weights must be supplied in the vector CW. In other cases weights are computed from the data. Defaults to "constant", i.e. constant weighting.
<code>CW</code>	optional numeric vector with external column weights. Defaults to 1 (constant weights).
<code>RW</code>	optional numeric vector with external row weights. Defaults to 1 (constant weights).
<code>pos.row</code>	logical vector indicating rows that are not to be included in the analysis but must be positioned on the projection obtained with the remaining rows. Defaults to FALSE.
<code>pos.column</code>	logical vector indicating columns that are not to be included in the analysis but must be positioned on the projection obtained with the remaining columns. Defaults to FALSE.

Details

The function `mpm` presents a unified approach to exploratory multivariate analysis encompassing principal component analysis, correspondence factor analysis, and spectral map analysis. The algorithm computes projections of high dimensional data in an orthogonal space. The resulting object can subsequently be used in the construction of biplots (i.e. `plot.mpm`).

The projection of the pre-processed data matrix in the orthogonal space is calculated using the `La.svd` function.

Value

An object of class `mpm` representing the projection of data after the different operations of transformation, closure, centering, and normalization in an orthogonal space. Generic functions `plot` and `summary` have methods to show the results of the analysis in more detail. The object consists of the following components:

<code>TData</code>	matrix with the data after optional log-transformation, closure, centering and normalization.
<code>row.names</code>	character vector with names of the row elements as supplied in the first column of the original data matrix
<code>col.names</code>	character vector with the names of columns obtained from the column names from the original data matrix
<code>closure</code>	closure operation as specified in the function call
<code>center</code>	centering operation as specified in the function call
<code>normal</code>	normalization operation as specified in the function call

row.weight	type of weighting used for rows as specified in the function call
col.weight	type of weighting used for columns as specified in the function call
Wn	vector with calculated weights for rows
Wp	vector with calculated weights for columns
RM	vector with row means of original data
CM	vector with column means of original data
pos.row	logical vector indicating positioned rows as specified in the function call
pos.column	logical vector indicating positioned columns as specified in the function call
SVD	list with components returned by <code>La.svd</code>
eigen	eigenvalues for each orthogonal factor from obtained from the weighted singular value decomposition
contrib	contributions of each factor to the total variance of the pre-processed data, i.e. the eigenvalues as a fraction of the total eigenvalue.
call	the matched call.

Note

Principal component analysis is defined as the projection onto an orthogonal space of the column-centered and column-normalized data. In correspondence factor analysis the data are pre-processed by double closure, double centering, and global normalization. Orthogonal projection is carried out using the weighted singular value decomposition. Spectral map analysis is in essence a principal component analysis on the log-transformed, double centered and global normalized data. Weighted spectral map analysis has been proven to be successful in the detection of patterns in gene expression data (Wouters et al., 2003).

Author(s)

Luc Wouters, Rudi Verbeeck, Tobias Verbeke

References

Wouters, L., Goehlmann, H., Bijmens, L., Kass, S.U., Molenberghs, G., Lewi, P.J. (2003). Graphical exploration of gene expression data: a comparative study of three multivariate methods. *Biometrics* **59**, 1131-1140.

See Also

[plot.mpm](#), [summary.mpm](#)

Examples

```
data(Golub)
# Principal component analysis
r.pca <- mpm(Golub[,1:39], center = "column", normal = "column")
# Correspondence factor analysis
r.cfa <- mpm(Golub[,1:39], logtrans = FALSE, row.weight = "mean",
col.weight = "mean", closure = "double")
```

```
# Weighted spectral map analysis
r.sma <- mpm(Golub[,1:39], row.weight = "mean", col.weight = "mean")
```

plot.mpm

Spectral Map Plot of Multivariate Data...

Description

Spectral Map Plot of Multivariate Data Produces a spectral map plot (biplot) of an object of class `mpm`

Usage

```
## S3 method for class 'mpm'
plot(x, scale=c("singul", "eigen", "uvr", "uvc"), dim=c(1, 2), zoom=rep(1,
  2), show.row=c("all", "position"), show.col=c("all", "position"),
  col.group=rep(1, length(x$col.names)), colors=c("orange1", "red",
  rainbow(length(unique(col.group))), start = 2/6, end = 4/6)),
  col.areas=TRUE, col.symbols=c(1, rep(2,
  length(unique(col.group)))), sampleNames=TRUE, rot=rep(-1,
  length(dim)), labels, label.tol=1, label.col.tol=1, lab.size=0.725,
  col.size=10, row.size=10, do.smoothScatter=FALSE, do.plot=TRUE, ...)
```

Arguments

<code>x</code>	object of class <code>mpm</code> a result of a call to <code>mpm</code> .
<code>scale</code>	optional character string specifying the type of factor scaling of the biplot. This can be either <code>"singul"</code> (singular value scaling), <code>"eigen"</code> (eigenvalue scaling), <code>"uvr"</code> (unit row-variance scaling), <code>"uvc"</code> (unit column-variance scaling). The latter is of particular value when analyzing large matrices, such as gene expression data. Singular value scaling <code>"singul"</code> is customary in spectral map analysis. Defaults to <code>"singul"</code> .
<code>dim</code>	optional principal factors that are plotted along the horizontal and vertical axis. Defaults to <code>c(1, 2)</code> .
<code>zoom</code>	optional zoom factor for row and column items. Defaults to <code>c(1, 1)</code> .
<code>show.row</code>	optional character string indicating whether all rows (<code>"all"</code>) are to be plotted or just the positioned rows <code>"position"</code> .
<code>show.col</code>	optional character string indicating whether all columns (<code>"all"</code>) are to be plotted or just the positioned columns <code>"position"</code> .
<code>col.group</code>	optional vector (character or numeric) indicating the different groupings of the columns, e.g. <code>Golub.grp</code> . Defaults to <code>1</code> .
<code>colors</code>	vector specifying the colors for the annotation of the plot; the first two elements concern the rows; the third till the last element concern the columns; the first element will be used to color the unlabeled rows; the second element for the labeled rows and the remaining elements to give different colors to different groups of columns.

<code>col.areas</code>	logical value indicating whether columns should be plotted as squares with areas proportional to their marginal mean and colors representing the different groups (TRUE), or with symbols representing the groupings and identical size (FALSE). Defaults to TRUE.
<code>col.symbols</code>	vector of symbols when <code>col.areas=FALSE</code> corresponds to the <code>pch</code> argument of the function <code>plot</code> .
<code>sampleNames</code>	Either a logical vector of length one or a character vector of length equal to the number of samples in the dataset. If a logical is provided, sample names will be displayed on the plot (TRUE; default) or not (FALSE); if a character vector is provided, the names provided will be used to label the samples instead of the default column names.
<code>rot</code>	rotation of plot. Defaults to <code>c(-1, -1)</code> .
<code>labels</code>	character vector to be used for labeling points on the graph; if NULL, the row names of <code>x</code> are used instead
<code>label.tol</code>	numerical value specifying either the percentile (<code>label.tol<=1</code>) of rows or the number of rows (<code>label.tol>1</code>) most distant from the plot-center (0,0) that are labeled and are plotted as circles with area proportional to the marginal means of the original data.
<code>label.col.tol</code>	numerical value specifying either the percentile (<code>label.col.tol<=1</code>) of columns or the number of columns (<code>label.col.tol>1</code>) most distant from the plot-center (0,0) that are labeled and are plotted as circles with area proportional to the marginal means of the original data.
<code>lab.size</code>	size of identifying labels for row- and column-items as <code>cex</code> parameter of the <code>text</code> function
<code>col.size</code>	size in mm of the column symbols
<code>row.size</code>	size in mm of the row symbols
<code>do.smoothScatter</code>	use <code>smoothScatter</code> or not instead of plotting individual points
<code>do.plot</code>	produce a plot or not
<code>...</code>	further arguments to <code>eqscaleplot</code> which draws the canvas for the plot; useful for adding a <code>main</code> or a custom <code>sub</code>

Details

Spectral maps are special types of biplots with the area of the symbols proportional to some measure, usually the row or column mean value and an identification of row- and column-items. For large matrices, such as gene expression data, where there is an abundance of rows, this can obscure the plot. In this case, the argument `label.tol` can be used to select the most informative rows, i.e. rows that are most distant from the center of the plot. Only these row-items are then labeled and represented as circles with their areas proportional to the marginal mean value. For the column-items it can be useful to apply some grouping specified by `col.group`. Examples of groupings are different pathologies, such as specified in `Golub.grp`

Value

An object of class `plot.mpm` that has the following components:

Rows	a data frame with the X and Y coordinates of the rows and an indication Select of whether the row was selected according to <code>label.tol</code>
Columns	a data frame with the X and Y coordinates of the columns

Note

value is returned invisibly, but is available for further use when an explicit assignment is made

Author(s)

Luc Wouters

References

Wouters, L., Goehlmann, H., Bijmens, L., Kass, S.U., Molenberghs, G., Lewi, P.J. (2003). Graphical exploration of gene expression data: a comparative study of three multivariate methods. *Biometrics* **59**, 1131-1140.

See Also

[mpm](#), [summary.mpm](#)

Examples

```
# Weighted spectral map analysis
data(Golub) # Gene expression data of leukemia patients
data(Golub.grp) # Pathological classes coded as 1, 2, 3
r.sma <- mpm(Golub[,1:39], row.weight = "mean", col.weight = "mean")
# Spectral map biplot with result
r <- plot(r.sma, label.tol = 20, scale = "uvc",
col.group = (Golub.grp)[1:38], zoom = c(1,1.2), col.size = 5)
Golub[r$Rows$Select, 1] # 20 most extreme genes
```

print.mpm

Print Method for mpm Objects...

Description

Print Method for mpm Objects

Usage

```
## S3 method for class 'mpm'
print(x, digits=3, ...)
```

Arguments

<code>x</code>	object of class <code>mpm</code>
<code>digits</code>	minimum number of significant digits to be printed
<code>...</code>	further arguments for the print method (for printing the contributions)

Value

`x` is returned invisibly

See Also

[print.default](#)

`print.summary.mpm` *Print Method for summary...*

Description

Print Method for `summary.mpm` Objects

Usage

```
## S3 method for class 'summary.mpm'
print(x, digits=2, what=c("columns", "rows", "all"), ...)
```

Arguments

<code>x</code>	object of class <code>summary.mpm</code>
<code>digits</code>	minimum number of significant digits to print, defaults to 2
<code>what</code>	one of "columns" (default), "rows" or "all", specifying respectively whether columns, rows or both need to be printed
<code>...</code>	further arguments for the print method

Value

`x` is returned invisibly

See Also

[print.default](#)

summary.mpm

*Summary Statistics for Spectral Map Analysis...***Description**

Summary Statistics for Spectral Map Analysis Summary method for object of class mpm.

Usage

```
## S3 method for class 'mpm'
summary(object, maxdim=4, ...)
```

Arguments

object	an object of class mpm resulting from a call to mpm
maxdim	maximum number of principal factors to be reported. Defaults to 4
...	further arguments; currently none are used

Details

The function `summary.mpm` computes and returns a list of summary statistics of the spectral map analysis given in `x`.

Value

An object of class `summary.mpm` with the following components:

call	the call to mpm
Vxy	sum of eigenvalues
VPF	a matrix with on the first line the eigenvalues and on the second line the cumulative eigenvalues of each of the principal factors (PRF1 to PRFmaxdim) followed by the residual eigenvalues and the total eigenvalue.
Rows	a data frame with summary statistics for the row-items, as described below.
Columns	a data frame with with summary statistics for the column-items, as described below.

The Rows and Columns data frames contain the following columns:

Posit	binary indication of whether the row or column was positioned (1) or not (0).
Weight	weight applied to the row or column in the function mpm.
PRF1-PRFmaxdim	factor scores or loadings for the first maxdim factors using eigenvalue scaling.
Resid	residual score or loading not accounted for by the first maxdim factors.
Norm	length of the vector representing the row or column in factor space.

Contrib	contribution of row or column to the sum of eigenvalues.
Accuracy	accuracy of the representation of the row or column by means of the first maximum principal factors.

Author(s)

Luc Wouters

References

Wouters, L., Goehlmann, H., Bijmens, L., Kass, S.U., Molenberghs, G., Lewi, P.J. (2003). Graphical exploration of gene expression data: a comparative study of three multivariate methods. *Biometrics* **59**, 1131-1140.

See Also

[mpm](#), [plot.mpm](#)

Examples

```
# Example 1 weighted spectral map analysis Golub data
data(Golub)
r.sma <- mpm(Golub[,1:39], row.weight = "mean", col.weight = "mean")
# summary report
summary(r.sma)
# Example 2 using print function
data(Famin81A)
r.fam <- mpm(Famin81A, row.weight = "mean", col.weight = "mean")
r.sum <- summary(r.fam)
print(r.sum, what = "all")
```

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