**Mfuzz**

April 19, 2009

---

**acore**  
*Extraction of alpha cores for soft clusters*

**Description**

This function extracts genes forming the alpha cores of soft clusters

**Usage**

```{r}
acore(eset, cl, min.acore=0.5)
```  

**Arguments**

- `eset`: object of the class `ExpressionSet`.
- `cl`: An object of class `flcust` as produced by `mfuzz`.
- `min.acore`: minimum membership values of gene belonging to the cluster core.

**Value**

The function produces an list of alpha cores including genes and their membership values for the corresponding cluster.

**Author(s)**

Matthias E. Futschik ([http://itb.biologie.hu-berlin.de/~futschik](http://itb.biologie.hu-berlin.de/~futschik))

**Examples**

```{r}
if (interactive()){  
  ### Data loading and pre-processing  
  data(yeast)  # data set includes 17 measurements  
  yeastF <- filter.NA(yeast)  
  yeastF <- fill.NA(yeastF)  
  yeastF <- standardise(yeastF)  
  
  ### Soft clustering and visualisation  
  cl <- mfuzz(yeastF, c=20, m=1.25)  
  acore.list <- acore(yeastF, cl=cl, min.acore=0.7)  
}
```
cselection

Repeated soft clustering for detection of empty clusters

Description

This function performs repeated soft clustering for a range of cluster numbers \( c \) and reports the number of empty clusters detected.

Usage

\[
c\text{selection}(\text{eset}, m, \text{crange}=\text{seq}(4,32,4), \text{repeats}=5, \text{visu}=\text{TRUE}, \ldots)
\]

Arguments

- \( \text{eset} \): object of class \( \text{ExpressionSet} \).
- \( m \): value of fuzzy \( c \)-means parameter \( m \).
- \( \text{crange} \): range of number of clusters \( c \).
- \( \text{repeats} \): number of repeated clusterings.
- \( \text{visu} \): If \( \text{visu}=\text{TRUE} \) plot of number of empty clusters is produced.
- \( \ldots \): additional arguments for underlying \( \text{mfuzz} \).

Details

A soft cluster is considered as empty, if none of the genes has a corresponding membership value larger than 0.5.

Value

A matrix with the number of empty clusters detected is generated.

Author(s)

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

References


Examples

```r
if (interactive()){  
data(yeast)  
  # Data pre-processing  
yeastF <- filter.NA(yeast)  
yeastF <- fill.NA(yeastF)  
yeastF <- standardise(yeastF)  

  #### parameter selection  
  # Empty clusters should not appear  
  cl <- mfuzz(yeastF, c=20, m=1.25)
```
mfuzz.plot(yeastF,cl=cl,mfrow=c(4,5))

# Note: The following calculation might take some time

tmp <- cselection(yeastF,m=1.25,crange=seq(5,40,5),repeats=5,visu=TRUE)
# derivation of number of non-empty clusters (crosses) from diagonal line indicate appearance of empty clusters

# Empty clusters might appear
cl <- mfuzz(yeastF,c=40,m=1.25)
mfuzz.plot(yeastF,cl=cl,mfrow=c(4,5))

fill.NA

Replacement of missing values

Description

Methods for replacement of replacing missing values. Missing values should be indicated by NA in the expression matrix.

Usage

fill.NA(eset,mode="mean",k=10)

Arguments

eset

object of the class ExpressionSet.

mode

method for replacement of missing values:

- **mean** - missing values will be replaced by the mean expression value of the gene,
- **median** - missing values will be replaced by the median expression value of the gene,
- **knn** - missing values will be replaced by the averaging over the corresponding expression values of the k-nearest neighbours,
- **knnw** - same replacement method as **knn**, but the expression values averaged are weighted by the distance to the corresponding neighbour

k

Number of neighbours, if one of the **knn** method for replacement is chosen (**knn**, **knnw**).

Value

The function produces an object of the ExpressionSet class with missing values replaced.

Note

The replacement methods **knn** and **knnw** can computationally intensive for large gene expression data sets. It may be a good idea to run these methods as a ‘lunchtime’ or ‘overnight’ job.
Author(s)

Matthias E. Futschik ([http://itb.biologie.hu-berlin.de/~futschik](http://itb.biologie.hu-berlin.de/~futschik)) and Lokesh Kumar

Examples

```r
if (interactive()){
  data(yeast) # data set includes 17 measurements
  yeastF <- filter.NA(yeast)
  yeastF <- fill.NA(yeastF)
}
```

filter.NA Filtering of genes based on number of non-available expression values.

Description

This function can be used to exclude genes with a large number of expression values not available.

Usage

```r
filter.NA(eset, thres=0.25)
```

Arguments

- `eset` object of the class “ExpressionSet”.
- `thres` threshold for excluding genes. If the percentage of missing values (indicated by NA in the expression matrix) is larger than `thres`, the corresponding gene will be excluded.

Value

The function produces an object of the ExpressionSet class. It is the same as the input eset object, except for the genes excluded.

Author(s)

Matthias E. Futschik ([http://itb.biologie.hu-berlin.de/~futschik](http://itb.biologie.hu-berlin.de/~futschik))

Examples

```r
if (interactive()){
  data(yeast) # data set includes 17 measurements
  yeastF <- filter.NA(yeast) # genes are excluded if more than 4 measurements are missing
}
```
filter.std

Filtering of genes based on their standard deviation.

Description

This function can be used to exclude genes with low standard deviation.

Usage

filter.std(eset, min.std, visu=TRUE)

Arguments

- `eset`: object of the class `ExpressionSet`.
- `min.std`: threshold for minimum standard deviation. If the standard deviation of a gene’s expression is smaller than `min.std` the corresponding gene will be excluded.
- `visu`: If `visu` is set to `TRUE`, the ordered standard deviations of genes’ expression values will be plotted.

Value

The function produces an object of the `ExpressionSet` class. It is the same as the input `eset` object, except for the genes excluded.

Note

As soft clustering is noise robust, pre-filtering can usually be avoided. However, if the number of genes with small expression changes is large, such pre-filtering may be necessary to reduce noise.

Author(s)

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

Examples

```r
data(yeast)  # data set includes 17 measurements
yeastF <- filter.NA(yeast)  # filtering of genes based on missing values
yeastF <- filter.std(yeastF, min.std=0.3)  # filtering of genes based on standard deviation
```

kmeans2

K-means clustering for gene expression data

Description

This function is a wrapper function for `kmeans` of the `e1071` package. It performs hard clustering of genes based on their expression values using the k-means algorithm.

Usage

kmeans2(eset, k, iter.max=100)
**Arguments**

- `eset`: object of the class `ExpressionSet`.
- `k`: number of clusters.
- `iter.max`: maximal number of iterations.

**Value**

An list of clustering components (see `kmeans`).

**Author(s)**

Matthias E. Futschik ([http://itb.biologie.hu-berlin.de/~futschik](http://itb.biologie.hu-berlin.de/~futschik))

**See Also**

- `kmeans`

**Examples**

```r
if (interactive()){
  data(yeast)
  # Data pre-processing
  yeastF <- filter.NA(yeast)
  yeastF <- fill.NA(yeastF)
  yeastF <- standardise(yeastF)

  # K-means clustering and visualisation
  kl <- kmeans2(yeastF,k=20)
  kmeans2.plot(yeastF,kl=kl,mfrow=c(2,2))
}
```

---

**kmeans2.plot**  
Plotting results for k-means clustering

**Description**

This function visualises the clusters produced by `kmeans2`.

**Usage**

```r
kmeans2.plot(eset, kl, mfrow=c(1,1))
```

**Arguments**

- `eset`: object of the class "ExpressionSet".
- `kl`: list produced by `kmeans2`.
- `mfrow`: determines splitting of graphic window.

**Value**

The function displays the temporal profiles of clusters detected by k-means.
mfuzz

Author(s)

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

Examples

if (interactive()){
  data(yeast)
  # Data pre-processing
  yeastF <- filter.NA(yeast)
  yeastF <- fill.NA(yeastF)
  yeastF <- standardise(yeastF)

  # K-means clustering and visualisation
  kl <- kmeans2(yeastF,k=20)
  kmeans2.plot(yeastF,kl=kl,mfrow=c(2,2))
}

mfuzz

Function for soft clustering based on fuzzy c-means.

Description

This function is a wrapper function for cmeans of the e1071 package. It performs soft clustering of genes based on their expression values using the fuzzy c-means algorithm.

Usage

mfuzz(eset,centers,m,...)

Arguments

eset object of the class “ExpressionSet”.

centers number of clusters.

m fuzzification parameter.

... additional parameters for cmeans.

Details

This function is the core function for soft clustering. It groups genes based on the Euclidean distance and the c-means objective function which is a weighted square error function. Each gene is assigned a membership value between 0 and 1 for each cluster. Hence, genes can be assigned to different clusters in a gradual manner. This contrasts hard clustering where each gene can belong to a single cluster.

Value

An object of class flcust (see cmeans) which is a list with components:

centers the final cluster centers.

size the number of data points in each cluster of the closest hard clustering.
mfuzz.plot

cluster a vector of integers containing the indices of the clusters where the data points are assigned to for the closest hard clustering, as obtained by assigning points to the (first) class with maximal membership.

iter the number of iterations performed.

membership a matrix with the membership values of the data points to the clusters.

withinerror the value of the objective function.

call the call used to create the object.

Author(s)

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

References


See Also

cmeans

Examples

if (interactive()){
  data(yeast)
  # Data pre-processing
  yeastF <- filter.NA(yeast)
  yeastF <- fill.NA(yeastF) # for illustration only; rather use knn method
  yeastF <- standardise(yeastF)

  # Soft clustering and visualisation
  cl <- mfuzz(yeastF,c=20,m=1.25)
  mfuzz.plot(yeastF,cl=cl,mfrow=c(2,2))

  # Plotting center of cluster 1
  X11(); plot(cl[[1]][1,],type="l",ylab="Expression")

  # Getting the membership values for the first 10 genes in cluster 1
  cl[[4]][1:10,1]
}
mfuzz.plot2

Arguments

- eset: object of the class `ExpressionSet`.
- cl: object of class `fcluster`.
- mfrow: determines splitting of graphic window.
- colo: color palette to be used for plotting. If the color argument remains empty, the default palette is used.
- min.mem: Genes with membership values below `min.mem` will not be displayed.
- time.labels: labels can be given for the time axis.
- new.window: should a new window be opened for graphics.

Value

The function generates plots where the membership of genes is color-encoded.

Author(s)

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

Examples

```r
if (interactive()){
  data(yeast)
  # Data pre-processing
  yeastF <- filter.NA(yeast)
  yeastF <- fill.NA(yeastF)
  yeastF <- standardise(yeastF)

  # Soft clustering and visualisation
  cl <- mfuzz(yeastF,c=20,m=1.25)
  mfuzz.plot(yeastF,cl=cl,mfrow=c(2,2))

  # display of cluster cores with alpha = 0.5
  mfuzz.plot(yeastF,cl=cl,mfrow=c(2,2),min.mem=0.5)

  # display of cluster cores with alpha = 0.7
  mfuzz.plot(yeastF,cl=cl,mfrow=c(2,2),min.mem=0.7)
}
```

mfuzz.plot2

Plotting results for soft clustering with additional options

Description

This function visualises the clusters produced by `mfuzz`. It is similar to `mfuzz.plot`, but offers more options for adjusting the plots.

Usage

```r
mfuzz.plot2(eset,cl,mfrow=c(1,1),colo,min.mem=0,time.labels,x11=TRUE,
ax.col="black",bg = "white",col.axis="black",col.lab="black",
col.main="black",col.sub="black",col="black",cex.main=2,
Xwidth=5,Xheight=5,single=FALSE,...)
```
Arguments

- `eset`: object of the class `ExpressionSet`.
- `cl`: object of class `flclust`.
- `mfrow`: determines splitting of graphic window. Use `mfrow=NA` if layout is used (see example).
- `colo`: color palette to be used for plotting. If the color argument remains empty, the default palette is used. If the `colo = "fancy"`, an alternative (fancier) palette will be used.
- `min.mem`: Genes with membership values below `min.mem` will not be displayed.
- `time.labels`: labels can be given for the time axis.
- `x11`: If TRUE, a new window will be open for plotting.
- `ax.col`: Color of axis line.
- `bg`: Background color.
- `col.axis`: Color for axis annotation.
- `col.lab`: Color for axis labels.
- `col.main`: Color for main titles.
- `col.sub`: Color for sub-titles.
- `col`: Default plotting color.
- `cex.main`: Magnification to be used for main titles.
- `Xwidth`: Width of window.
- `Xheight`: Height of window.
- `single`: Integer if a specific cluster is to be plotted, otherwise it should be set to FALSE.
- `...`: Additional, optional plotting arguments passed to `plot.default` function.

Value

The function generates plots where the membership of genes is color-encoded.

Author(s)

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

Examples

```r
if (interactive()){
  data(yeast)
  # Data pre-processing
  yeastF <- filter.NA(yeast)
  yeastF <- fill.NA(yeastF)
  yeastF <- standardise(yeastF)

  # Soft clustering and visualisation
  cl <- mfuzz(yeastF, c=20, m=1.25)
  mfuzz.plot2(yeastF, cl=cl, mfrow=c(2,2)) # same output as mfuzz.plot

  # More fancy choice of colors
  mfuzz.plot2(yeastF, cl=cl, mfrow=c(2,2), colo="fancy", ax.col="red", bg = "black", col.axis="red", col.lab="white")
```
mfuzzColorBar

Plots a colour bar

Description

This function produces a (separate) colour bar for graphs produced by mfuzz.plot

Usage

mfuzzColorBar(col, horizontal=FALSE,...)

Arguments

col    vector of colours used. If missing, the same vector as the default vector for
        mfuzz.plot is used. If col="fancy", an alternative color palette is used (see
        mfuzz.plot2.
horizontal    If TRUE, a horizontal colour bar is generated, otherwise a vertical one will be
    produced.
...    additional parameter passed to maColorBar (see also example in mfuzz.plot2)

Author(s)

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

See Also

maColorBar

Examples

if (interactive()){
  X11(w=1.5,h=5);
  par(mar=c(1,1,1,5))
  mfuzzColorBar()
  mfuzzColorBar(col="fancy",main="Membership value")
}

### Single cluster with colorbar (cluster # 3)
X11(width=12)
mat <- matrix(1:2,ncol=2,nrow=1,byrow=TRUE)
l <- layout(mat,width=c(5,1))
mfuzz.plot2(yeastF,cl=cl,mfrow=NA,colo="fancy",ax.col="red",bg="black",col.axis="red",
col.main="green",col.sub="blue",col="blue",cex.main=2,single=3,x11=FALSE)

mfuzzColorBar(col="fancy",main="Membership",cex.main=1)
overlap  

Calculation of the overlap of soft clusters

Description

This function calculates the overlap of clusters produced by \texttt{mfuzz}.

Usage

\texttt{overlap(cl)}

Arguments

\begin{description}
\item [\texttt{cl}] \hspace{1cm} object of class \texttt{flclust}
\end{description}

Value

The function generates a matrix of the normalised overlap of soft clusters. The overlap indicates the extent of “shared” genes between clusters. For a mathematical definition of the overlap, see the vignette of the package or the reference below.

Author(s)

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

References


Examples

\begin{verbatim}
if (interactive()){
  data(yeast)
  # Data pre-processing
  yeastF <- filter.NA(yeast)
  yeastF <- fill.NA(yeastF)
  yeastF <- standardise(yeastF)
  # Soft clustering and visualisation
  cl <- mfuzz(yeastF,c=20,m=1.25)
  mfuzz.plot(yeastF,cl=cl,mfrow=c(4,5))
  # Calculation of cluster overlap and visualisation
  O <- overlap(cl)
  X11()
  Ptmp <- overlap.plot(cl,over=O,thres=0.05)
}
\end{verbatim}
Description

This function visualises the cluster overlap produced by `overlap`.

Usage

```r
overlap.plot(cl, overlap, thres=0.1, scale=TRUE, magni=30, P=NULL)
```

Arguments

- `cl`: object of class “flclust”
- `overlap`: matrix of cluster overlap produced by `overlap`
- `thres`: threshold for visualisation. Cluster overlaps below the threshold will not be visualised.
- `scale`: Scale parameter for principal component analysis by `prcomp`
- `magni`: Factor for increase the line width for cluster overlap.
- `P`: Projection matrix produced by principal component analysis.

Value

A plot is generated based on a principal component analysis of the cluster centers. The overlap is visualised by lines with variable width indicating the strength of the overlap. Additionally, the matrix of principal components is returned. This matrix can be re-used for other projections to compare the overlap and global cluster structure of different clusterings.

Author(s)

Matthias E. Futschik ([http://itb.biologie.hu-berlin.de/~futschik](http://itb.biologie.hu-berlin.de/~futschik))

See Also

- `prcomp`

Examples

```r
if (interactive()){
  data(yeast)
  # Data pre-processing
  yeastF <- filter.NA(yeast)
  yeastF <- fill.NA(yeastF)
  yeastF <- standardise(yeastF)
  # Soft clustering
  cl <- mfuzz(yeastF,c=20,m=1.25)
  X11();mfuzz.plot(yeastF,cl=cl,mfrow=c(4,5))
  O <- overlap(cl)
  X11();Ptmp <- overlap.plot(cl,over=O,thres=0.05)
}
Alternative clustering

\texttt{cl} <- mfuzz(yeastF, c=10, m=1.25)
\texttt{X11();mfuzz.plot(yeastF, cl=cl, mfrow=c(3,4))}
\texttt{O <- overlap(cl)}
\texttt{X11();overlap.plot(cl, over=O, P=Ptmp, thres=0.05)}

# visualisation based on principal components from previous projection

\begin{verbatim}
partcoef
calculation of the partition coefficient matrix for soft clustering
\end{verbatim}

\textbf{Description}

This function calculates partition coefficient for clusters within a range of cluster parameters. It can be used to determine the parameters which lead to uniform clustering.

\textbf{Usage}

\texttt{partcoef(eset, crange=seq(4,32,4), mrange=seq(1.05,2,0.1), \ldots)}

\textbf{Arguments}

- \texttt{eset}: object of class “ExpressionSet”.
- \texttt{crange}: range of number of clusters \texttt{c}.
- \texttt{mrange}: range of clustering parameter \texttt{m}.
- \ldots: additional arguments for underlying \texttt{mfuzz}.

\textbf{Details}

Introduced by Bezdek (1981), the partition coefficient \texttt{F} is defined as the sum of squares of values of the partition matrix divided by the number of values. It is maximal if the partition is hard and reaches a minimum for \texttt{U=1/c} when every gene is equally assigned to every cluster.

It is well-known that the partition coefficient tends to decrease monotonically with increasing \texttt{n}. To reduce this tendency we defined a normalized partition coefficient where the partition for uniform partitions are subtracted from the actual partition coefficients (Futschik and Kasabov, 2002).

\textbf{Value}

The function generates the matrix of partition coefficients for a range of \texttt{c} and \texttt{m} values. It also produces a matrix of normalised partition coefficients as well as a matrix with partition coefficient for uniform partitions.

\textbf{Author(s)}

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

\textbf{References}

1. J.C. Bezdek, Pattern recognition with fuzzy objective function algorithms, Plenum, 1981
randomise

Examples

```r
if (interactive()) {
  data(yeast)
  # Data pre-processing
  yeastF <- filter.NA(yeast)
  yeastF <- fill.NA(yeastF)
  yeastF <- standardise(yeastF)

  #### parameter selection
  yeastFR <- randomise(yeastF)
  cl <- mfuzz(yeastFR, c=20, m=1.1)
  mfuzz.plot(yeastFR, cl=cl, mfrow=c(4,5)) # shows cluster structures (non-uniform partition)

  tmp <- partcoef(yeastFR) # This might take some time.
  F <- tmp[[1]]; F.n <- tmp[[2]]; F.min <- tmp[[3]]

  # Which clustering parameters result in a uniform partition?
  F > 1.01 * F.min

  cl <- mfuzz(yeastFR, c=20, m=1.25) # produces uniform partion
  mfuzz.plot(yeastFR, cl=cl, mfrow=c(4,5))
  # uniform coloring of temporal profiles indicates uniform partition
}
```

data(yeast) # data set includes 17 measurements
yeastR <- randomise(yeast)

randomise Randomisation of data

Description

This function randomise the time order for each gene separately.

Usage

```r
randomise(eset)
```

Arguments

- `eset` object of the class `ExpressionSet`

Value

The function produces an object of the ExpressionSet class with randomised expression data.

Author(s)

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

Examples

```r
data(yeast) # data set includes 17 measurements
yeastR <- randomise(yeast)
```
standardise

Standardization of microarray data for clustering.

Description

Standardisation of the expression values of every gene is performed, so that the average expression value for each gene is zero and the standard deviation is one.

Usage

standardise(eset)

Arguments

eset  object of the classe ExpressionSet.

Value

The function produces an object of the ExpressionSet class with standardised expression values.

Author(s)

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

Examples

if (interactive()){  
data(yeast)  
  # Data pre-processing  
  yeastF <- filter.NA(yeast)  
  yeastF <- fill.NA(yeastF)  
  yeastF <- standardise(yeastF)  

  # Soft clustering and visualisation  
  cl <- mfuzz(yeastF,c=20,m=1.25)  
  mfuzz.plot(yeastF,cl=cl,mfrow=c(4,5))  
}  

standardise2

Standardization in regards to selected time-point

Description

Standardisation of the expression values of every gene is performed, so that the expression values at a chosen time point are zero and the standard deviations are one.

Usage

standardise2(eset,timepoint=1)
Arguments

eset   object of the class ExpressionSet.
timepoint   integer: which time point should have expression values of zero.

Value

The function produces an object of the ExpressionSet class with standardised expression values.

Author(s)

Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)

Examples

if (interactive()){  
data(yeast)  
  # Data pre-processing  
  yeastF <- filter.NA(yeast)  
  yeastF <- fill.NA(yeastF)  
  yeastF <- standardise2(yeastF,timepoint=1)  
  # Soft clustering and visualisation  
  cl <- mfuzz(yeastF,c=20,m=1.25)  
  mfuzz.plot(yeastF,cl=cl,mfrow=c(4,5))  
}

determines the number for which each gene has highest membership value in all cluster

Description

This function calculates the number, for which each gene appears to have the top membership score in the partition matrix of clusters produced by mfuzz.

Usage

top.count(cl)

Arguments

cl   object of class “flclust”

Value

The function generates a vector containing a count for each gene, which is just the number of times that particular gene has acquired the top membership score.

Author(s)

Lokesh Kumar and Matthias E. Futschik (http://itb.biologie.hu-berlin.de/~futschik)
Examples

```r
if (interactive()){
  data(yeast)
  # Data pre-processing
  yeastF <- filter.NA(yeast)
  yeastF <- fill.NA(yeastF)
  yeastF <- standardise(yeastF)
  
  # Soft clustering and visualisation
  cl <- mfuzz(yeastF,c=20,m=1.25)
  top.count(cl)
}
```

---

**yeast**

*Gene expression data of the yeast cell cycle*

**Description**

The data contains gene expression measurements for 3000 randomly chosen genes of the yeast mutant cdc28 as performed and described by Cho et al. For details, see the reference.

**Usage**

```r
data(yeast)
```

**Format**

An object of class “ExpressionSet”.

**Source**

The data was downloaded from Yeast Cell Cycle Analysis Project webside and converted to an ExpressionSet object.

**References**

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