Package ‘lle’

February 20, 2015

Type Package

Title Locally linear embedding

Version 1.1

Date 2012-03-21

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Depends scatterplot3d, MASS, snowfall

Suggests rgl

Description LLE is a non-linear algorithm for mapping high-dimensional data into a lower dimensional (intrinsic) space. This package provides the main functions to performs the LLE alogrithm including some enhancements like subset selection, calculation of the intrinsic dimension etc.

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LazyLoad yes

Repository CRAN

Date/Publication 2012-03-21 12:52:58

NeedsCompilation no

R topics documented:

`calc_k` *Calculation of the optimal number of neighbours.*

Description

Calculates of optimal number of neighbours by using the algorithm proposed by Kayo (see Ref.). Therefore the LLE alorithm is performed for every k-neighbourhood size.

Usage

```
calc_k(X, m, kmin=1, kmax=20, plotres=TRUE,
                 parallel=FALSE, cpus=2, iLLE=FALSE)
```

Arguments

`X`	matrix object containing the input data.
`m`	intrinsic dimension of the data.
`kmin`	minimal value of k.
`kmax`	maximal value of k.
`plotres`	a logical values indicating wheather to plot the result.
`parallel`	a logical values indicating wheather to use parallel computation on multiple cpu cores. See **snowfall**.
`cpus`	number of cpus cores used for parallel computation.
`iLLE`	a logical values indicating wheater to use improved LLE (very CPU intensive). See `lle`.

Details

Since the calculation of the optimal number of neighbours m is a step that is normally applied before the execution of LLE itself, the intrinsic dimension may be unknown. In this case, a good guess is sufficient. If no good estimation can be made the largest plausible value should be chosen.

Value

`res`	dataframe containing the number of neighbours and the calculated parameter ρ. The number of neighbours belonging to the smallest value of ρ should be chosen.

References

Locally linear embedding algorithm - extensions and applications / Olga Kayo / Universitatis Ouluensis, Oulu, Finland / 2006

Examples

```
   ## Not run:
data( lle_scurve_data )
X <- lle_scurve_data
calc_k( X, 2, 1, 15 )

data( lle_scurve_data )
X <- lle_scurve_data
calc_k( X, 2, 1, 15, FALSE, TRUE, 4 )

## End(Not run)
```

`find_coords` *Calculate embedded data.*

Description

Calculates the embedded data of dimension m using the weight matrix.

Usage

```
find_coords(wgts, nns, N, n, m)
```

Arguments

`wgts`	weight matrix calculated by `find_weights`.
`nns`	matrix of neighbours calculated by `find_nn_k` or `find_nn_eps`.
`N`	number of samples.
`n`	dimension of the original data.
`m`	intrinsic dimension of the data.

Value

`Y`	matrix containing the embedded data.

Examples

```
data( lle_scurve_data )
X <- lle_scurve_data
nns <- find_nn_k(X,5)
wgts <- find_weights(nns,X,2)
Y <- find_coords( wgts$wgts, nns, dim(X)[1], 3, 2 )
```

find_nn_eps *Find nearest neighbours in epsilon environment.*

Description

Finds the nearest points for every point in an environment with radius eps.

Usage

```
find_nn_eps(X, eps)
```

Arguments

X	matrix object containing the input data.
eps	size of epsilon environment around x_i.

Details

A good value for eps strongly depends on the scaling of the data. Therefore we recommend to use the R function scale.

Value

neighbours	matrix with N rows and columns. If distance between x_i and x_i is smaller than eps, $neighbours[i, j]$ is one, else zero.

See Also

find_nn_k

Examples

```
data( lle_scurve_data )
X <- lle_scurve_data
neighbours <- find_nn_eps( X, 0.5 )
table( rowSums(neighbours) )
```

find_nn_k — *Find k nearest neighbours.*

Description

Finds the nearest k points for every point of the input data.

Usage

```
find_nn_k(X, k, iLLE = FALSE)
```

Arguments

`X`	matrix object containing the input data.
`k`	number of neighbours.
`iLLE`	a logical values indicating wheater to use improved LLE. See `lle`.

Value

`neighbours`	matrix with N rows and columns. If x_j is a neighbour of x_i then $neighbours[i, j]$ is one, else zero.

See Also

`find_nn_eps`

Examples

```
data( lle_scurve_data )
X <- lle_scurve_data
neighbours <- find_nn_k( X, 5 )
table( rowSums( neighbours ) )
```

find_weights — *Calculate weight matrix.*

Description

Calculates the weights for every neighbour of x_i.

Usage

```
find_weights(nns, X, m, reg = 2, ss = FALSE, p = 0.5, id = FALSE, v = 0.99)
```

Arguments

`nns`	matrix of nearest neighbours using `find_nn_k` or `find_nn_eps`.
`X`	matrix object containing the input data.
`m`	intrinsic dimension of the data. See `lle`.
`reg`	regularisation method. See `lle`.
`ss`	a logical values indicating wheather to perform subset selection. See `lle`.
`p`	amount of data remaining after subset selection. See `lle`.
`id`	a logical values indicating wheather to calculate the intrinsic dimension. See `lle`.
`v`	threshold parameter for intrinsic dimension. See details.

Value

A list containing the following variables:

`X`	input data, can change if subset selection is applied
`weights`	weight matrix. If x_i is neighbour of x_j then $-1 < weights[i,j] < 1$, else zero.
`choise`	index vector of kept data while subset selection
`id`	additionally to the (optional) printed intrinsic dimension, the vector of intrinsic dimension for every data point is returned by the function, so that the vector can easily be ploted manually.

Examples

```
data( lle_scurve_data )
X <- lle_scurve_data
nns <- find_nn_k( X, 5 )
weights <- find_weights( nns, X, 2, 2 )
```

`lle` *Locally linear embedding main function.*

Description

Performs all steps of LLE algorithm by calling the functions of the package.

Usage

```
lle(X, m, k, reg = 2, ss = FALSE, p = 0.5, id = FALSE,
   nnk = TRUE, eps = 1, iLLE = FALSE, v = 0.99)
```

Arguments

`X`	matrix object containing the input data.
`m`	intrinsic dimension of the data. This parameter mainly influences the visualisation of the results. The real intrinsic dimension will be calculated automaticly.
`k`	number of neighbours. Optimal number can be calculated using the `calc_k`.
`reg`	regularisation method. Choise between 1, 2 and 3, by default 2. See details.
`ss`	a logical values indicating wheather to perform subset selection. See details.
`p`	amount of data remaining after subset selection. Values between 0 and 1.
`id`	a logical values indicating wheather to calculate the intrinsic dimension.
`nnk`	a logical values indicating wheather to use k nearest neighbours method. If false, epsilon environment neighbourhood will be used.
`eps`	epsilon radius if parameter nnk is FALSE.
`iLLE`	a logical values indicating wheater to use improved LLE after Wang. See details.
`v`	threshold parameter for intrinsic dimension. See details.

Details

This is the main function to execute the LLE alogrithm. Given a data matrix with N rows (samples) and n columns (dimensions), the embedded data of dimension m will be calculated.
As described above, the parameter m influences the visualisation of the embedded data. Therefore see `plot_lle`.
If `id` is true, the intrinsic dimension of the data is automatically calculated during the execution of the function. Since the intrinsic dimension is calculated for every data point x_i the result of this calculation consists of a vector with length N. The used approach is to calculate the mean and the mode of this vector as represention of the overall intrinsic dimension of the data.
The `reg` parameter allows the decision between different regularisation methods. As one step of the LLE algorithm, the inverse of the Gram-matrix $G \in R^{kxk}$ has to be calculated. The rank of G equals m which is mostly smaller than k - this is why a regularisation $G^{(i)} + r \cdot I$ should be performed. The calculation of regularisation parameter r can be done using different methods:

- `reg=1`: standardized sum of eigenvalues of G, see Ref. 1), Ch. 3.2
- `reg=2`: trace of Gram-matrix divided by k, see Ref. 2), Ch. 5.2
- `reg=3`: constant value 3*10e-3

There is no theoretical evidence which method is best to use but several empirical analyses have shown that method #2 works the most reliable.
The most time-consuming step of LLE consists in the calculation of the eigenvalues and -vectors of matrix $M \in R^{NxN}$ in the `find_coords` function. To reduce the dimension of matrix M, which means to reduce the number of samples N in a reliable way, Ref. 1 proposes a subset selection algorithm, which is integrated in the `lle` function. The amount of data that is kept is represented by parameter `p`.
Improved LLE (`iLLE`) is an extension of the LLE algorithm described in Ref. 3. It raises the required amount of memory and time, but makes the algoritm less dependent on the number of neighbours.
Calculating the intrinsic dimension strongly depends on a threshold value v. The best value for this

parameter depends on the origin of the data. For very accurate data a value beyond 0.99 is propose, for very raw data a value of 0.9 is proposed. This parameter should be varied if a specific intrinsic dimension is expected and other results are calculated. Higher values of v lead to a higher number of calculate intrinsic dimensions.

Value

A list containing the following variables:

`X`	input data, can change if subset selection is applied
`Y`	embedded data
`choise`	(only if `ss==TRUE`) index vector of kept data while subset selection
`id`	(only if `id==TRUE`) vector of intrinsic dimension for every data point.

References

1) Locally linear embedding / Dick de Ridder and Robert P.W. Duin / Delft University of Technology, Delft, Netherlands / 2002
2) Automated Local Linear Embedding with an application to microarray data / Elisa Grilli / Universita di Bologna, Italy / 2005
3) Improved Locally Linear Embedding Through New Distance Computing / Heyong Wang et al / Sun Yat-sen University, China / 2010

Examples

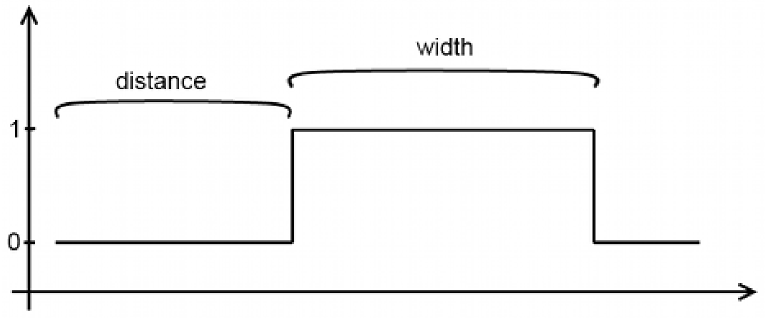
```
# perform LLE
data( lle_scurve_data )
X <- lle_scurve_data
results <- lle( X=X, m=2, k=12, reg=2, ss=FALSE, id=TRUE, v=0.9 )
str( results )

# plot results and intrinsic dimension (manually)
split.screen( c(2,1) )
screen(1)
plot( results$Y, main="embedded data", xlab=expression(y[1]), ylab=expression(y[2]) )
screen(2)
plot( results$id, main="intrinsic dimension", type="l", xlab=expression(x[i]), ylab="id", lwd=2 )
```

`lle_rectangular` *Example on a rectangular signal.*

Description

A rectangular signal with variable width and distance is generated and analysed (see figure). Every sample has dimension $n = 500$. In the example N samples are generated, that only differ by the two parameters width and distance. As a result it can be seen that the data can be embedded from a 500- into a 2-dimensional space which's limits are specified by the limits of the two parameters.



Usage

```
lle_rectangular(N = 40, k = 5, v = 0.9)
```

Arguments

N	number of samples.
k	number of neighbours. See lle.
v	threshold parameter for intrinsic dimension. See lle.

Examples

```
    ## Not run:
lle_rectangular()
lle_rectangular( 30, 10, 0.8 ) \

## End(Not run)
```

`lle_scurve` *Example application on a three-dimensional S-curve dataset.*

Description

Performs the LLE alogrithm on a three dimensional S-curve, which is a standard example for data embedding algorithms.

Usage

```
lle_scurve(N = 800, k = 12, ss = FALSE, p = 0.5, reg = 2,
                    iLLE = FALSE, v = 0.8)
```

Arguments

N	number of samples. See lle.
k	number of neighbours. See lle.
ss	a logical values indicating wheather to perform subset selection. See lle.
p	amount of data remaining after subset selection. See lle.
reg	regularisation method. See lle.
iLLE	a logical values indicating wheater to use iLLE. See lle.
v	threshold parameter for intrinsic dimension. See lle.

Examples

```
lle_scurve()
lle_scurve( N=1800, k=11, ss=TRUE )
```

---

lle_scurve_data *S-curve data*

Description

Syntheticly generated empiric data of a three-dimensional S-curve.

Usage

```
data(lle_scurve_data)
```

Format

matrix with dimensions $n = 1000, m = 3$

See Also

lle_scurve

`lle_sound` *Example application on a soundfile.*

Description

Performs the LLE alogrithm on a sound(file). As a first step, the sound is scanned piecewice with time windows sized `t`. In every scanning step, the time windows is shifted by `dt`. This generates an overall data set with dimension $n =$`t` and sample size $N \approx$`t/dt`. This dataset can then be embedded using LLE algorithm.

Usage

```
lle_sound(t = 500, dt = 20, k = 25, reg = 2, ss = FALSE,
                  p = 0.5, id = TRUE)
```

Arguments

`t`	time window used to scan.
`dt`	time window shift.
`k`	number of neighbours. See `lle`.
`reg`	regularisation method. See `lle`.
`ss`	a logical values indicating wheather to perform subset selection. See `calc_k`.
`p`	amount of data remaining after subset selection. See `lle`.
`id`	a logical values indicating wheather to calculate the intrinsic dimension. See `lle`.

Examples

```
    ## Not run:
lle_sound()
lle_sound( 200, 20, 20 )

## End(Not run)
```

`lle_spiral` *Example application on a n-dimensional spiral*

Description

In this example nine three-dimensional spirals are generated. Every spiral has a higher number of windings than the previous. The first spiral's intrinsic dimension is determined as $m = 1$. It can be observed that a higher number of windings with constant sampling rate leads to a higher calculated intrinsic dimension. Due to this fact, the last spiral's intrinsic dimension is computed as $m = 2$.

Usage

```
lle_spiral()
```

`lle_swissrole` *Example application on a swissrole.*

Description

Like the S-curve this is a standard example to demonstrate the functioning of LLE.

Usage

```
lle_swissrole(N = 1500, k = 10, ss = FALSE, p = 0.5, reg = 2, iLLE = FALSE, v = 0.8)
```

Arguments

`N`	number of samples.
`k`	number of neighbours. See `lle`.
`ss`	a logical values indicating wheather to perform subset selection. See `lle`.
`p`	amount of data remaining after subset selection. See `lle`.
`reg`	regularisation method. See `lle`.
`iLLE`	a logical values indicating wheater to use iLLE. See `lle`.
`v`	threshold parameter for intrinsic dimension. See `lle`.

Examples

```
    ## Not run:
lle_swissrole()
lle_swissrole( 3000, k=12, ss=TRUE )

## End(Not run)
```

`lle_wave` *wavefile*

Description

syntheticly generated wavefile with 10 modes.

Usage

```
data(lle_wave)
```

Format

numeric vector of length 17640 (0.4 seconds, 44 kHz)

Details

To analyse an acustic signal a wavefile with 10 modes was generated and transformed into text.

`plot_lle` *Plot LLE results*

Description

Function for plotting LLE results either in static or in dynamic way.

Usage

```
plot_lle( Y, X, print = FALSE, col = 3, name = as.numeric(Sys.time()),
               angle = 60, inter = FALSE )
```

Arguments

`Y`	matrix object with calculated embedded data.
`X`	matrix object with original data.
`print`	a logical values indicating wheather to plot the graphical results to a file.
`col`	string or number dtermining the plotting colours.
`name`	(if `print==true`) filename.
`angle`	(if `inter==false`) angle between x- and y-axis in scatterplot3d. See documentation of **scatterplot3d**.
`inter`	a logical values indicating wheather to use interactive 3D-plots. See **rgl**.

Details

`col` determines the way that the points in the plot are coloured. Choosing a string name of a colour leads to a monocoloured plot. Choosing a number between leads to a colour gradient plot build up by N colours (taking only the rainbow colours into account). Choosing a numeric vector with length N leads to points coloured respecting to the values in the vector (for unique colours only values between 0 and 600 should be used).
If `inter==false`, two plots are generated in one window. The left plot is the plot of the original data. These will only be plotted if $n \in \{1, 2, 3\}$. The right plot shows the embedded data. These will only be plotted $m \in \{1, 2, 3\}$.
if `inter==true`, one interactive plot of the embedded data will be shown. This plot can be scrolled and zoomed. It requires OpenGL drivers.

Examples

```
data( lle_scurve_data )
X <- lle_scurve_data
Y <- lle( X, m=2, k=12 )$Y
plot_lle( Y, X, FALSE, col="red", inter=TRUE )
```

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