

Package ‘mmtsne’

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Type Package

Title Multiple Maps t-SNE

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Description An implementation of multiple maps t-distributed stochastic neighbor embedding (t-SNE). Multiple maps t-SNE is a method for projecting high-dimensional data into several low-dimensional maps such that non-metric space properties are better preserved than they would be by a single map. Multiple maps t-SNE with only one map is equivalent to standard t-SNE. When projecting onto more than one map, multiple maps t-SNE estimates a set of latent weights that allow each point to contribute to one or more maps depending on similarity relationships in the original data. This implementation is a port of the original 'Matlab' library by Laurens van der Maaten.
See Van der Maaten and Hinton (2012) <[doi:10.1007/s10994-011-5273-4](https://doi.org/10.1007/s10994-011-5273-4)>.
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hbeta	<i>Estimate perplexity and probability values</i>
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Description

hbeta returns the perplexity and probability values for a row of data D.

Usage

hbeta(D, beta = 1)

Arguments

- | | |
|------|--------------------|
| D | A distance vector. |
| beta | A constant scalar. |

mmtsne	<i>Multiple maps t-SNE</i>
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Description

mmtsne estimates a multiple maps t-distributed stochastic neighbor embedding (multiple maps t-SNE) model.

Usage

```
mmtsne(X, no_maps = 1, no_dims = 2, perplexity = 30, max_iter = 500,  
       momentum = 0.5, final_momentum = 0.8, mom_switch_iter = 250,  
       eps = 1e-07)
```

Arguments

- | | |
|------------|---|
| X | A dataframe or matrix of N rows and D columns. |
| no_maps | The number of maps (positive whole number) to be estimated. |
| no_dims | The number of dimensions per map. Typical values are 2 or 3. |
| perplexity | The target perplexity for probability matrix construction. Commonly recommended values range from 5 to 30. Perplexity roughly corresponds to the expected number of neighbors per data point. |

<code>max_iter</code>	The number of iterations to run.
<code>momentum</code>	Constant scaling factor for update momentum in gradient descent algorithm.
<code>final_momentum</code>	Constant scaling factor for update momentum in gradient descent algorithm after the momentum switch point.
<code>mom_switch_iter</code>	The iteration at which momentum switches from <code>momentum</code> to <code>final_momentum</code> .
<code>eps</code>	A small positive value near zero.

Details

`mmtsne` is a wrapper that performs multiple maps t-SNE on an input dataset, X . The function will pre-process X , an N by D matrix or dataframe, then call `mmtsneP`. The pre-processing steps include calls to `x2p` and `p2sp` to convert X into an N by N symmetrical joint probability matrix.

The `mmtsneP` code is an almost direct port of the original multiple maps t-SNE Matlab code by van der Maaten and Hinton (2012). `mmtsne` estimates a multidimensional array of $N \times \text{no_dims} \times \text{no_maps}$. Each map is an $N \times \text{no_dims}$ matrix of estimated t-SNE coordinates. When `no_maps=1`, multiple maps t-SNE reduces to standard t-SNE.

Value

A list that includes the following objects:

Y An $N \times \text{no_dims} \times \text{no_maps}$ array of predicted coordinates.

weights An $N \times \text{no_maps}$ matrix of unscaled weights. A high weight on entry i, j indicates a greater contribution of point i on map j .

proportions An $N \times \text{no_maps}$ matrix of scaled weights. A high weight on entry i, j indicates a greater contribution of point i on map j .

References

L.J.P. van der Maaten and G.E. Hinton. "Visualizing Non-Metric Similarities in Multiple Maps." *Machine Learning* 87(1):33-55, 2012. [PDF](#).

Examples

```
# Load the iris dataset
data("iris")

# Estimate a mmtsne model with 2 maps, 2 dimensions each
model <- mmtsne(iris[,1:4], no_maps=2, max_iter=100)

# Plot the results side-by-side for inspection
# Points scaled by map proportion weights plus constant factor
par(mfrow=c(1,2))
plot(model$Y[,1], col=iris$Species, cex=model$proportions[,1] + .2)
plot(model$Y[,2], col=iris$Species, cex=model$proportions[,2] + .2)
par(mfrow=c(1,1))
```

mmtsneP

*Multiple maps t-SNE with symmetric probability matrix***Description**

mmtsneP estimates a multiple maps t-distributed stochastic neighbor embedding (multiple maps t-SNE) model.

Usage

```
mmtsneP(P, no_maps, no_dims = 2, max_iter = 500, momentum = 0.5,
        final_momentum = 0.8, mom_switch_iter = 250, eps = 1e-07)
```

Arguments

P	An $N \times N$ symmetric joint probability distribution matrix. These can be constructed from an N by D matrix with <code>x2p</code> and <code>p2sp</code> . Alternatively, the wrapper function <code>mmtsne</code> will wrap the matrix construction and multiple maps t-SNE model estimation into a single step.
no_maps	The number of maps (positive whole number) to be estimated.
no_dims	The number of dimensions per map. Typical values are 2 or 3.
max_iter	The number of iterations to run.
momentum	Constant scaling factor for update momentum in gradient descent algorithm.
final_momentum	Constant scaling factor for update momentum in gradient descent algorithm after the momentum switch point.
mom_switch_iter	The iteration at which momentum switches from momentum to final_momentum.
eps	A small positive value near zero.

Details

This code is an almost direct port of the original multiple maps t-SNE Matlab code by van der Maaten and Hinton (2012). mmtsne estimates a multidimensional array of $N \times \text{no_dims} \times \text{no_maps}$. Each map is an $N \times \text{no_dims}$ matrix of estimated t-SNE coordinates. When `no_maps=1`, multiple maps t-SNE reduces to standard t-SNE.

Value

A list that includes the following objects:

Y An $N \times \text{no_dims} \times \text{no_maps}$ array of predicted coordinates.

weights An $N \times \text{no_maps}$ matrix of unscaled weights. A high weight on entry i, j indicates a greater contribution of point i on map j .

proportions An $N \times \text{no_maps}$ matrix of scaled weights. A high weight on entry i, j indicates a greater contribution of point i on map j .

References

L.J.P. van der Maaten and G.E. Hinton. “Visualizing Non-Metric Similarities in Multiple Maps.” *Machine Learning* 87(1):33-55, 2012. [PDF](#).

Examples

```
# Load the iris dataset
data("iris")

# Produce a symmetric joint probability matrix
prob_matrix <- p2sp(x2p(as.matrix(iris[,1:4])))

# Estimate a mmtsne model with 2 maps, 2 dimensions each
model <- mmtsneP(prob_matrix, no_maps=2, max_iter=100)

# Plot the results side-by-side for inspection
# Points scaled by map proportion weights plus constant factor
par(mfrow=c(1,2))
plot(model$Y[,1], col=iris$Species, cex=model$proportions[,1] + 0.2)
plot(model$Y[,2], col=iris$Species, cex=model$proportions[,2] + 0.2)
par(mfrow=c(1,1))
```

p2sp

Probability matrix to symmetric probability matrix

Description

p2sp returns a symmetrical pair-wise joint probability matrix given an input probability matrix P .

Usage

```
p2sp(P)
```

Arguments

P An $N \times N$ probability matrix, like those produced by [x2p](#)

Value

An $N \times N$ symmetrical matrix of pair-wise probabilities.

x2p

Data to probability matrix

Description

x2p returns a pair-wise conditional probability matrix given an input matrix X .

Usage

```
x2p(X, perplexity = 30, tol = 1e-05)
```

Arguments

<code>X</code>	A data matrix with N rows.
<code>perplexity</code>	The target perplexity. Values between 5 and 50 are generally considered appropriate. Loosely translates into the expected number of neighbors per point.
<code>tol</code>	A small positive value.

Details

This function is an almost direct port of the original Python implementation by van der Maaten and Hinton (2008). It uses a binary search to estimate probability values for all pairwise-elements of X . The conditional Gaussian distributions should all be of equal perplexity.

Value

An $N \times N$ matrix of pair-wise probabilities.

References

L.J.P. van der Maaten and G.E. Hinton. “Visualizing High-Dimensional Data Using t-SNE.” *Journal of Machine Learning Research* 9(Nov):2579-2605, 2008. [PDF](#).

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