Package 'snifter'

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```
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Description Provides an R wrapper for the implementation of FI-tSNE from the python pack-
     age openTNSE. See Poličar et al. (2019) <doi:10.1101/731877> and the algorithm de-
     scribed by Linderman et al. (2018) <doi:10.1038/s41592-018-0308-4>.
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Project new data into an existing t-SNE embedding object.

Description

project

Project new data into an existing t-SNE embedding object.

Usage

```
project(
 Х,
  new,
 old,
 perplexity = 5,
  initialization = c("median", "weighted", "random"),
 k = 25L
  learning_rate = 0.1,
  early_exaggeration = 4,
  early_exaggeration_iter = 0L,
  exaggeration = 1.5,
  n_{iter} = 250L,
  initial_momentum = 0.5,
  final_momentum = 0.8,
 max\_grad\_norm = 0.25,
  tolerance = 1e-04
)
```

Arguments

X	t-SNE embedding created with fitsne.
new	New data to project into existing embedding
old	Data used to create the original embedding.
perplexity	Numeric scalar. Perplexity can be thought of as the continuous number of nearest neighbors, for which t-SNE will attempt to preserve distances. However, when projecting, we only consider neighbors in the existing embedding i.e. each data point is placed into the embedding, independently of other new data points.
initialization	Character scalar specifying the method used to compute the initial point positions to be used in the embedding space. Can be "median", "weighted" or "random". In all cases, "median" or "weighted" should be preferred.

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k Integer scalar specifying the number of nearest neighbors to consider when ini-

tially placing the point onto the embedding. This is different from "perplexity" because perplexity affects optimization while this only affects the initial point

positions.

learning_rate The learning rate for t-SNE optimization. When learning_rate="auto" the

appropriate learning rate is selected according to max(200, N / 12), as deter-

mined in Belkina et al. Otherwise, a numeric scalar.

early_exaggeration

Numeric scalar; the exaggeration factor to use during the *early exaggeration*

phase. Typical values range from 12 to 32.

early_exaggeration_iter

The number of iterations to run in the *early exaggeration* phase.

exaggeration The exaggeration factor to use during the normal optimization phase. This can

be used to form more densely packed clusters and is useful for large data sets.

n_iter The number of iterations to run in the normal optimization regime.

initial_momentum

The momentum to use during the *early exaggeration* phase.

 $\label{lem:final_momentum} \begin{picture}(200,0) \put(0,0){\line(1,0){100}} \put(0,0){\line(1,0){$

max_grad_norm Maximum gradient norm. If the norm exceeds this value, it will be clipped.

When adding points into an existing embedding, and the new points overlap with the reference points, this may lead to large gradients. This can make points "shoot off" from the embedding, causing the interpolation method to compute a

very large grid, and leads to worse results.

tolerance Numeric scalar specifying the numeric tolerance used to ensure the affinities

calculated on the old data match those of the original embedding.

Value

Numeric matrix of t-SNE co-ordinates resulting from embedding new into the t-SNE embedding x.

References

Automated optimized parameters for T-distributed stochastic neighbor embedding improve visualization and analysis of large datasets. Belkina, A.C., Ciccolella, C.O., Anno, R. et al. Nature Communications 10, 5415 (2019). doi: https://doi.org/10.1038/s41467-019-13055-y

Examples

snifter

snifter: fast interpolated t-SNE in R

Description

An R package for running openTSNE's implementation of fast interpolated t-SNE.

See the openTSNE documentation for further details on these arguments and the general usage of this algorithm.

Usage

```
fitsne(
  simplified = FALSE,
  n_{components} = 2L,
  n_{jobs} = 1L,
  perplexity = 30,
  n_{iter} = 500L,
  initialization = c("pca", "spectral", "random"),
  pca = FALSE,
  pca_dims = 50L,
  partial_pca = FALSE,
  pca_center = TRUE,
  pca_scale = TRUE,
  neighbors = c("auto", "exact", "annoy", "pynndescent", "approx"),
  negative_gradient_method = c("fft", "bh"),
  learning_rate = "auto",
  early_exaggeration = 12,
  early_exaggeration_iter = 250L,
  exaggeration = NULL,
  dof = 1,
  theta = 0.5,
  n_interpolation_points = 3L,
 min_num_intervals = 50L,
  ints_in_interval = 1,
  metric = "euclidean",
 metric_params = NULL,
  initial\_momentum = 0.5,
  final_momentum = 0.8,
 max_grad_norm = NULL,
  random_state = NULL,
  verbose = FALSE
)
```

Arguments

x Input data matrix.

simplified Logical scalar. When FALSE, the function returns an object of class snifter.

This contains all information necessary to project new data into the embedding using project If TRUE, all extra attributes will be omitted, and the return value

is a base matrix.

n_components Number of t-SNE components to be produced.

n_jobs Integer scalar specifying the number of cores to be used.

perplexity Numeric scalar controlling the neighborhood used when estimating the embed-

ding.

n_iter Integer scalar specifying the number of iterations to complete.

initialization Character scalar specifying the initialization to use. "pca" may preserve global

distance better than other options.

pca Logical scalar specifying whether PCA should be run on the data before creating

the embedding.

pca_dims Integer scalar specifying the number of principal components to be calculated

in the initial PCA step if pca=TRUE.

partial_pca Logical scalar specifying whether prcomp_irlba should be used if pca=TRUE.

This is useful for very large data matrices.

pca_center, pca_scale

Logical scalars specifying whether centering and scaling should be performed

before running PCA, if pca=TRUE.

neighbors Character scalar specifying the nearest neighbour algorithm to use.

 ${\tt negative_gradient_method}$

Character scalar specifying the negative gradient approximation to use. "bh", referring to Barnes-Hut, is more appropriate for smaller data sets, while "fft" referring to fast Fourier transform, is more appropriate for larger datasets.

referring to fast rounce transform, is more appropriate for larger data

learning_rate Numeric scalar specifying the learning rate, or the string "auto", which uses

max(200, N / 12), where N is the number of observations.

early_exaggeration

Numeric scalar specifying the exaggeration factor to use during the early exag-

geration phase. Typical values range from 12 to 32.

early_exaggeration_iter

Integer scalar specifying the number of iterations to run in the early exaggeration

phase.

exaggeration Numeric scalar specifying the exaggeration factor to use during the normal op-

timization phase. This can be used to form more densely packed clusters and is

useful for large data sets.

dof Numeric scalar specifying the degrees of freedom, as described in Kobak et al.

(2019).

theta Numeric scalar, only used when negative_gradient_method="bh". This is the

trade-off parameter between speed and accuracy of the tree approximation method. Typical values range from 0.2 to 0.8. The value 0 indicates that no approximation is to be made and produces exact results also producing longer runtime.

n_interpolation_points

Integer scalar, only used when negative_gradient_method="fft". The number of interpolation points to use within each grid cell for interpolation based t-SNE. It is highly recommended leaving this value at the default 3.

min_num_intervals

Integer scalar, only used when negative_gradient_method="fft". The minimum number of grid cells to use, regardless of the ints_in_interval parameter. Higher values provide more accurate gradient estimations.

ints_in_interval

Numeric scalar, only used when negative_gradient_method="fft". Indicates how large a grid cell should be e.g. a value of 3 indicates a grid side length of 3. Lower values provide more accurate gradient estimations.

metric Character scalar specifying the metric to be used to compute affinities between

points in the original space.

metric_params Named list of additional keyword arguments for the metric function.

initial_momentum

Numeric scalar specifying the momentum to use during the early exaggeration

phase.

final_momentum Numeric scalar specifying the momentum to use during the normal optimization

phase.

max_grad_norm Numeric scalar specifying the maximum gradient norm. If the norm exceeds

this value, it will be clipped.

random_state Integer scalar specifying the seed used by the random number generator.

verbose Logical scalar controlling verbosity.

Value

A matrix of t-SNE embeddings.

References

openTSNE: a modular Python library for t-SNE dimensionality reduction and embedding Pavlin G. Poličar, Martin Stražar, Blaž Zupan bioRxiv (2019) 731877; doi: https://doi.org/10.1101/731877

Fast interpolation-based t-SNE for improved visualization of single-cell RNA-seq data George C. Linderman, Manas Rachh, Jeremy G. Hoskins, Stefan Steinerberger, and Yuval Kluger Nature Methods 16, 243–245 (2019) doi: https://doi.org/10.1038/s41592-018-0308-4

Accelerating t-SNE using Tree-Based Algorithms Laurens van der Maaten Journal of Machine Learning Research (2014) http://jmlr.org/papers/v15/vandermaaten14a.html

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Heavy-tailed kernels reveal a finer cluster structure in t-SNE visualisations Dmitry Kobak, George Linderman, Stefan Steinerberger, Yuval Kluger and Philipp Berens arXiv (2019) doi: https://doi.org/10.1007/978-3-030-46150-8_8.

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