Package ‘Rtsne’

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Type Package

Title T-Distributed Stochastic Neighbor Embedding using a Barnes-Hut Implementation

Version 0.16

Description An R wrapper around the fast T-distributed Stochastic Neighbor Embedding implementation by Van der Maaten (see <https://github.com/lvdmaaten/bhtsne/> for more information on the original implementation).

License file LICENSE

URL https://github.com/jkrijthe/Rtsne

Imports Rcpp (>= 0.11.0), stats

LinkingTo Rcpp

Suggests irlba, testthat

RoxygenNote 7.1.2

NeedsCompilation yes

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normalize_input

 Normalize input data matrix

Description
Mean centers each column of an input data matrix so that it has a mean of zero. Scales the entire matrix so that the largest absolute of the centered matrix is equal to unity.

Usage
normalize_input(X)

Arguments
X matrix; Input data matrix with rows as observations and columns as variables/dimensions.

Details
Normalization avoids numerical problems when the coordinates (and thus the distances between observations) are very large. Directly computing distances on this scale may lead to underflow when computing the probabilities in the t-SNE algorithm. Rescaling the input values mitigates these problems to some extent.

Value
A numeric matrix of the same dimensions as X but centred by column and scaled to have a maximum deviation of 1.

Author(s)
Aaron Lun

Examples
iris_unique <- unique(iris) # Remove duplicates
iris_matrix <- as.matrix(iris_unique[,1:4])
X <- normalize_input(iris_matrix)
colMeans(X)
range(X)
Rtsne  

Barnes-Hut implementation of t-Distributed Stochastic Neighbor Embedding

Description

Wrapper for the C++ implementation of Barnes-Hut t-Distributed Stochastic Neighbor Embedding. t-SNE is a method for constructing a low dimensional embedding of high-dimensional data, distances or similarities. Exact t-SNE can be computed by setting theta=0.0.

Usage

Rtsne(X, ...)

## Default S3 method:
Rtsne(
  X,
  dims = 2,
  initial_dims = 50,
  perplexity = 30,
  theta = 0.5,
  check_duplicates = TRUE,
  pca = TRUE,
  partial_pca = FALSE,
  max_iter = 1000,
  verbose = getOption("verbose", FALSE),
  is_distance = FALSE,
  Y_init = NULL,
  pca_center = TRUE,
  pca_scale = FALSE,
  normalize = TRUE,
  stop_lying_iter = ifelse(is.null(Y_init), 250L, 0L),
  mom_switch_iter = ifelse(is.null(Y_init), 250L, 0L),
  momentum = 0.5,
  final_momentum = 0.8,
  eta = 200,
  exaggeration_factor = 12,
  num_threads = 1,
  ...
)

## S3 method for class 'dist'
Rtsne(X, ..., is_distance = TRUE)

## S3 method for class 'data.frame'
Rtsne(X, ...)

Rtsne_neighbors(
  index,
  distance,
  dims = 2,
  perplexity = 30,
  theta = 0.5,
  max_iter = 1000,
  verbose = getOption("verbose", FALSE),
  Y_init = NULL,
  stop_lying_iter = ifelse(is.null(Y_init), 250L, 0L),
  mom_switch_iter = ifelse(is.null(Y_init), 250L, 0L),
  momentum = 0.5,
  final_momentum = 0.8,
  eta = 200,
  exaggeration_factor = 12,
  num_threads = 1,
  ...
)

Arguments

X               matrix; Data matrix (each row is an observation, each column is a variable)
...             Other arguments that can be passed to Rtsne
dims           integer; Output dimensionality (default: 2)
initial_dims   integer; the number of dimensions that should be retained in the initial PCA step (default: 50)
perplexity     numeric; Perplexity parameter (should not be bigger than 3 * perplexity < nrow(X) - 1, see details for interpretation)
theta          numeric; Speed/accuracy trade-off (increase for less accuracy), set to 0.0 for exact TSNE (default: 0.5)
check_duplicates logical; Checks whether duplicates are present. It is best to make sure there are no duplicates present and set this option to FALSE, especially for large datasets (default: TRUE)
pca            logical; Whether an initial PCA step should be performed (default: TRUE)
partial_pca    logical; Whether truncated PCA should be used to calculate principal components (requires the irlba package). This is faster for large input matrices (default: FALSE)
max_iter       integer; Number of iterations (default: 1000)
verbose        logical; Whether progress updates should be printed (default: global "verbose" option, or FALSE if that is not set)
is_distance    logical; Indicate whether X is a distance matrix (default: FALSE)
Y_init         matrix; Initial locations of the objects. If NULL, random initialization will be used (default: NULL). Note that when using this, the initial stage with exaggerated perplexity values and a larger momentum term will be skipped.
**Rtsne**

**pca_center** logical; Should data be centered before pca is applied? (default: TRUE)
**pca_scale** logical; Should data be scaled before pca is applied? (default: FALSE)
**normalize** logical; Should data be normalized internally prior to distance calculations with `normalize_input`? (default: TRUE)
**stop_lying_iter** integer; Iteration after which the perplexities are no longer exaggerated (default: 250, except when Y_init is used, then 0)
**mom_switch_iter** integer; Iteration after which the final momentum is used (default: 250, except when Y_init is used, then 0)
**momentum** numeric; Momentum used in the first part of the optimization (default: 0.5)
**final_momentum** numeric; Momentum used in the final part of the optimization (default: 0.8)
**eta** numeric; Learning rate (default: 200.0)
**exaggeration_factor** numeric; Exaggeration factor used to multiply the P matrix in the first part of the optimization (default: 12.0)
**num_threads** integer; Number of threads to use when using OpenMP, default is 1. Setting to 0 corresponds to detecting and using all available cores
**index** integer matrix; Each row contains the identity of the nearest neighbors for each observation
**distance** numeric matrix; Each row contains the distance to the nearest neighbors in index for each observation

**Details**

Given a distance matrix $D$ between input objects (which by default, is the euclidean distances between two objects), we calculate a similarity score in the original space $p_{ij}$.

$$ p_{ij} = \frac{\exp(-\|D_{ij}\|^2/2\sigma^2)}{\sum_{k \neq l} \exp(-\|D_{ij}\|^2/2\sigma^2)} $$

which is then symmetrized using:

$$ p_{ij} = \frac{p_{ji} + p_{ij}}{2n}. $$

The $\sigma$ for each object is chosen in such a way that the perplexity of $p_{ji}$ has a value that is close to the user defined perplexity. This value effectively controls how many nearest neighbours are taken into account when constructing the embedding in the low-dimensional space. For the low-dimensional space we use the Cauchy distribution (t-distribution with one degree of freedom) as the distribution of the distances to neighbouring objects:

$$ q_{ij} = \frac{(1 + \|y_i - y_j\|^2)^{-1}}{\sum_{k \neq l} (1 + \|y_k - y_l\|^2)^{-1}}. $$

By changing the location of the objects $y$ in the embedding to minimize the Kullback-Leibler divergence between these two distributions $q_{ij}$ and $p_{ij}$, we create a map that focusses on small-scale structure, due to the asymmetry of the KL-divergence. The t-distribution is chosen to avoid the
crowding problem: in the original high dimensional space, there are potentially many equidistant objects with moderate distance from a particular object, more than can be accounted for in the low dimensional representation. The t-distribution makes sure that these objects are more spread out in the new representation.

For larger datasets, a problem with a simple gradient descent to minimize the Kullback-Leibler divergence is the computational complexity of each gradient step (which is $O(n^2)$). The Barnes-Hut implementation of the algorithm attempts to mitigate this problem using two tricks: (1) approximating small similarities by 0 in the $p_{ij}$ distribution, where the non-zero entries are computed by finding $3^*perplexity$ nearest neighbours using an efficient tree search. (2) Using the Barnes-Hut algorithm in the computation of the gradient which approximates large distance similarities using a quadtree. This approximation is controlled by the theta parameter, with smaller values leading to more exact approximations. When theta=0.0, the implementation uses a standard t-SNE implementation. The Barnes-Hut approximation leads to a $O(n\log(n))$ computational complexity for each iteration.

During the minimization of the KL-divergence, the implementation uses a trick known as early exaggeration, which multiplies the $p_{ij}$'s by 12 during the first 250 iterations. This leads to tighter clustering and more distance between clusters of objects. This early exaggeration is not used when the user gives an initialization of the objects in the embedding by setting Y_init. During the early exaggeration phase, a momentum term of 0.5 is used while this is changed to 0.8 after the first 250 iterations. All these default parameters can be changed by the user.

After checking the correctness of the input, the Rtsne function (optionally) does an initial reduction of the feature space using prcomp, before calling the C++ TSNE implementation. Since R's random number generator is used, use set.seed before the function call to get reproducible results.

If X is a data.frame, it is transformed into a matrix using model.matrix. If X is a dist object, it is currently first expanded into a full distance matrix.

Value

List with the following elements:

- Y Matrix containing the new representations for the objects
- N Number of objects
- origD Original Dimensionality before TSNE (only when X is a data matrix)
- perplexity See above
- theta See above
- costs The cost for every object after the final iteration
- intercosts The total costs (KL-divergence) for all objects in every 50th + the last iteration
- stop_lying_iter Iteration after which the perplexities are no longer exaggerated
- mom_switch_iter Iteration after which the final momentum is used
- momentum Momentum used in the first part of the optimization
- final_momentum Momentum used in the final part of the optimization
- eta Learning rate
- exaggeration_factor Exaggeration factor used to multiply the P matrix in the first part of the optimization
Methods (by class)

- default: Default Interface
- dist: tsne on given dist object
- data.frame: tsne on data.frame

Supplying precomputed distances

If a distance matrix is already available, this can be directly supplied to Rtsne by setting is_distance=TRUE. This improves efficiency by avoiding recalculation of distances, but requires some work to get the same results as running default Rtsne on a data matrix. Specifically, Euclidean distances should be computed from a normalized data matrix - see normalize_input for details. PCA arguments will also be ignored if is_distance=TRUE.

NN search results can be directly supplied to Rtsne_neighbors to avoid repeating the (possibly time-consuming) search. To achieve the same results as Rtsne on the data matrix, the search should be conducted on the normalized data matrix. The number of nearest neighbors should also be equal to three-fold the perplexity, rounded down to the nearest integer. Note that pre-supplied NN results cannot be used when theta=0 as they are only relevant for the approximate algorithm.

Any kind of distance metric can be used as input. In contrast, running Rtsne on a data matrix will always use Euclidean distances.

References


Examples

iris_unique <- unique(iris) # Remove duplicates
iris_matrix <- as.matrix(iris_unique[,1:4])

# Set a seed if you want reproducible results
set.seed(42)
tsne_out <- Rtsne(iris_matrix,pca=FALSE,perplexity=30,theta=0.0) # Run TSNE

# Show the objects in the 2D tsne representation
plot(tsnr_out$Y,col=iris_unique$Species, asp=1)

# data.frame as input
tsne_out <- Rtsne(iris_unique,pca=FALSE, theta=0.0)

# Using a dist object
set.seed(42)
tsne_out <- Rtsne(dist(normalize_input(iris_matrix)), theta=0.0)
plot(tsnr_out$Y,col=iris_unique$Species, asp=1)

set.seed(42)
tsne_out <- Rtsne(as.matrix(dist(normalize_input(iris_matrix))),theta=0.0)
plot(tsne_out$Y, col=iris_unique$Species, asp=1)

# Supplying starting positions (example: continue from earlier embedding)
set.seed(42)
tsne_part1 <- Rtsne(iris_unique[,1:4], theta=0.0, pca=FALSE, max_iter=350)
tsne_part2 <- Rtsne(iris_unique[,1:4], theta=0.0, pca=FALSE, max_iter=650, Y_init=tsne_part1$Y)
plot(tsne_part2$Y, col=iris_unique$Species, asp=1)

## Not run:
# Fast PCA and multicore

tsne_out <- Rtsne(iris_matrix, theta=0.1, partial_pca = TRUE, initial_dims=3)
tsne_out <- Rtsne(iris_matrix, theta=0.1, num_threads = 2)

## End(Not run)
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