Package ‘phateR’

May 22, 2020

Title PHATE - Potential of Heat-Diffusion for Affinity-Based Transition Embedding

Version 1.0.4

Description PHATE is a tool for visualizing high dimensional single-cell data with natural progressions or trajectories. PHATE uses a novel conceptual framework for learning and visualizing the manifold inherent to biological systems in which smooth transitions mark the progressions of cells from one state to another. To see how PHATE can be applied to single-cell RNA-seq datasets from hematopoietic stem cells, human embryonic stem cells, and bone marrow samples, check out our publication in Nature Biotechnology at <doi:10.1038/s41587-019-0336-3>.

License GPL-2 | file LICENSE

Encoding UTF-8

LazyData true

Depends R (>= 3.3), Matrix (>= 1.2-0)

Imports methods, stats, graphics, reticulate (>= 1.8), ggplot2, memoise

Suggests gridGraphics, cowplot

RoxygenNote 7.0.2

NeedsCompilation no

Author Krishnan Srinivasan [aut], Scott Gigante [cre] (<https://orcid.org/0000-0002-4544-2764>)

Maintainer Scott Gigante <scott.gigante@yale.edu>

Repository CRAN

Date/Publication 2020-05-22 04:40:02 UTC

R topics documented:

as.data.frame.phate .................................................. 2
as.matrix.phate ..................................................... 2
check_pyphate_version ............................................ 3
as.data.frame.phate

Convert a PHATE object to a data.frame

Description

Returns the embedding matrix with column names PHATE1 and PHATE2

Usage

## S3 method for class 'phate'
as.data.frame(x, ...)

Arguments

x A fitted PHATE object
...
Arguments for as.data.frame()

as.matrix.phate

Convert a PHATE object to a matrix

Description

Returns the embedding matrix. All components can be accessed using phate$embedding, phate$diff.op, etc

Usage

## S3 method for class 'phate'
as.matrix(x, ...)

Arguments

x A fitted PHATE object
...
Arguments for as.matrix()
check_pyphate_version

Check that the current PHATE version in Python is up to date.

Description

Check that the current PHATE version in Python is up to date.

Usage

check_pyphate_version()

cluster_phate

KMeans on the PHATE potential Clustering on the PHATE operator as introduced in Moon et al. This is similar to spectral clustering.

Description

KMeans on the PHATE potential Clustering on the PHATE operator as introduced in Moon et al. This is similar to spectral clustering.

Usage

cluster_phate(phate, k = 8, seed = NULL)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>phate</td>
<td>phate() output</td>
</tr>
<tr>
<td>k</td>
<td>Number of clusters (default: 8)</td>
</tr>
<tr>
<td>seed</td>
<td>Random seed for kmeans (default: NULL)</td>
</tr>
</tbody>
</table>

Value

clusters Integer vector of cluster assignments

Examples

```r
if (reticulate::py_module_available("phate")) {

  # Load data
  # data(tree.data)
  # We use a smaller tree to make examples run faster
  data(tree.data.small)

  # Run PHATE
  phate.tree <- phate(tree.data.small$data)
```
# Clustering
cluster_phate(phate.tree)
}

---

### ggplot.phate
Convert a PHATE object to a data.frame for ggplot

**Description**

Passes the embedding matrix to ggplot with column names PHATE1 and PHATE2

**Usage**

```r
## S3 method for class 'phate'
ggplot(data, ...)
```

**Arguments**

- `data`: A fitted PHATE object
- `...`: Arguments for ggplot()

**Examples**

```r
if (reticulate::py_module_available("phate") && require(ggplot2)) {

  # data(tree.data)
  # We use a smaller tree to make examples run faster
  data(tree.data.small)
  phate.tree <- phate(tree.data.small$data)
  ggplot(phate.tree, aes(x=PHATE1, y=PHATE2, color=tree.data.small$branches)) +
    geom_point()
}
```

---

### install.phate
Install PHATE Python Package

**Description**

Install PHATE Python package into a virtualenv or conda env.
library.size.normalize

Usage

install.phate(
  envname = "r-reticulate",
  method = "auto",
  conda = "auto",
  pip = TRUE,
...
)

Arguments

envname Name of environment to install packages into
method Installation method. By default, "auto" automatically finds a method that will work in the local environment. Change the default to force a specific installation method. Note that the "virtualenv" method is not available on Windows.
conda Path to conda executable (or "auto" to find conda using the PATH and other conventional install locations).
pip Install from pip, if possible.
... Additional arguments passed to conda_install() or virtualenv_install().

Details

On Linux and OS X the "virtualenv" method will be used by default ("conda" will be used if virtualenv isn’t available). On Windows, the "conda" method is always used.

library.size.normalize

Performs L1 normalization on input data such that the sum of expression values for each cell sums to 1, then returns normalized matrix to the metric space using median UMI count per cell effectively scaling all cells as if they were sampled evenly.

Description

Performs L1 normalization on input data such that the sum of expression values for each cell sums to 1, then returns normalized matrix to the metric space using median UMI count per cell effectively scaling all cells as if they were sampled evenly.

Usage

library.size.normalize(data, verbose = FALSE)

Arguments

data matrix (n_samples, n_dimensions) 2 dimensional input data array with n cells and p dimensions
verbose boolean, default=FALSE. If true, print verbose output
Run PHATE on an input data matrix

**Description**

PHATE is a data reduction method specifically designed for visualizing **high** dimensional data in **low** dimensional spaces.

**Usage**

```r
phate(
  data,
  ndim = 2,
  knn = 5,
  decay = 40,
  n.landmark = 2000,
  gamma = 1,
  t = "auto",
  mds.solver = "sgd",
  knn.dist.method = "euclidean",
  init = NULL,
  mds.method = "metric",
  mds.dist.method = "euclidean",
  t.max = 100,
  npca = 100,
  plot.optimal.t = FALSE,
  verbose = 1,
  n.jobs = 1,
  seed = NULL,
  potential.method = NULL,
  k = NULL,
  alpha = NULL,
  use.alpha = NULL,
  ...
)
```

**Arguments**

- `data` (matrix) 2 dimensional input data array with `n_samples` samples and `n_dimensions` dimensions. If `knn.dist.method` is `"precomputed"`, `data` is treated as a (n_samples, n_samples) distance or affinity matrix.
- `ndim` (int) Optional, default: 2 number of dimensions in which the data will be embedded.

**Value**

data_norm matrix (n_samples, n_dimensions) 2 dimensional array with normalized gene expression values
phate

knn int, optional, default: 5 number of nearest neighbors on which to build kernel
decay int, optional, default: 40 sets decay rate of kernel tails. If NULL, alpha decaying
kernel is not used
n.landmark int, optional, default: 2000 number of landmarks to use in fast PHATE
gamma float, optional, default: 1 Informational distance constant between -1 and 1. gamma=1 gives the PHATE log potential, gamma=0 gives a square root potential.
t int, optional, default: 'auto' power to which the diffusion operator is powered
sets the level of diffusion
mds.solver 'sgd', 'smacof', optional, default: 'sgd' which solver to use for metric MDS. SGD is substantially faster, but produces slightly less optimal results. Note that SMACOF was used for all figures in the PHATE paper.

knn.dist.method string, optional, default: 'euclidean'. recommended values: 'euclidean', 'cosine', 'precomputed' Any metric from scipy.spatial.distance can be used distance metric for building kNN graph. If 'precomputed', data should be an n_samples x n_samples distance or affinity matrix. Distance matrices are assumed to have zeros down the diagonal, while affinity matrices are assumed to have non-zero values down the diagonal. This is detected automatically using data[0,0]. You can override this detection with knn.dist.method='precomputed_distance' or knn.dist.method='precomputed_affinity'.

init phate object, optional object to use for initialization. Avoids recomputing intermediate steps if parameters are the same.
mds.method string, optional, default: 'metric' choose from 'classic', 'metric', and 'non-metric' which MDS algorithm is used for dimensionality reduction
mds.dist.method string, optional, default: 'euclidean' recommended values: 'euclidean' and 'cosine'

plot.optimal.t boolean, optional, default: FALSE If TRUE, produce a plot showing the Von Neumann Entropy curve for automatic t selection.
verbose int or boolean, optional (default : 1) If TRUE or > 0, print verbose updates.
n.jobs int, optional (default : 1) The number of jobs to use for the computation. If -1 all CPUs are used. If 1 is given, no parallel computing code is used at all, which is useful for debugging. For n.jobs below -1, (n.cpus + 1 + n.jobs) are used. Thus for n.jobs = -2, all CPUs but one are used
seed int or NULL, random state (default: NULL)
potential.method

k deprecated. Use knn.
alpha deprecated. Use decay.
use.alpha deprecated To disable alpha decay, use alpha=NULL

... Additional arguments for graphtools.Graph.
Value

"phate" object containing:

- **embedding**: the PHATE embedding
- **operator**: The PHATE operator (python phate.PHATE object)
- **params**: Parameters passed to phate

Examples

```r
if (reticulate::py_module_available("phate")) {
  # Load data
  # data(tree.data)
  # We use a smaller tree to make examples run faster
  data(tree.data.small)

  # Run PHATE
  phate.tree <- phate(tree.data.small$data)
  summary(phate.tree)
  ## PHATE embedding
  ## knn = 5, decay = 40, t = 58
  ## Data: (3000, 100)
  ## Embedding: (3000, 2)

  library(graphics)
  # Plot the result with base graphics
  plot(phate.tree, col=tree.data.small$branches)
  # Plot the result with ggplot2
  if (require(ggplot2)) {
    ggplot(phate.tree) +
    geom_point(aes(x=PHATE1, y=PHATE2, color=tree.data.small$branches))
  }

  # Run PHATE again with different parameters
  # We use the last run as initialization
  phate.tree2 <- phate(tree.data.small$data, t=150, init=phate.tree)
  # Extract the embedding matrix to use in downstream analysis
  embedding <- as.matrix(phate.tree2)
}
```

---

**plot.phate**

Plot a PHATE object in base R

**Description**

Plot a PHATE object in base R
print.phate

Usage

```r
## S3 method for class 'phate'
plot(x, ...)
```

Arguments

- `x`: A fitted PHATE object
- `...`: Arguments for plot()

Examples

```r
if (reticulate::py_module_available("phate")) {
  library(graphics)
  # data(tree.data)
  # We use a smaller tree to make examples run faster
  data(tree.data.small)
  phate.tree <- phate(tree.data.small$data)
  plot(phate.tree, col=tree.data.small$branches)
}
```

Description

This avoids spamming the user's console with a list of many large matrices

print.phate

Print a PHATE object

Usage

```r
## S3 method for class 'phate'
print(x, ...)
```

Arguments

- `x`: A fitted PHATE object
- `...`: Arguments for print()

Examples

```r
if (reticulate::py_module_available("phate")) {
  # data(tree.data)
  # We use a smaller tree to make examples run faster
  data(tree.data.small)
  phate.tree <- phate(tree.data.small$data)
  print(phate.tree)
```
Summary a PHATE object

Description

Summarize a PHATE object

Usage

## S3 method for class 'phate'
summary(object, ...)

Arguments

object A fitted PHATE object
... Arguments for summary()

Examples

if (reticulate::py_module_available("phate")) {

# We use a smaller tree to make examples run faster
phate.tree <- phate(tree.data.small$data)
summary(phate.tree)
## PHATE embedding
## knn = 5, decay = 40, t = 58
## Data: (3000, 100)
## Embedding: (3000, 2)
}
tree.data

Fake branching data for examples

Description
A dataset containing high dimensional data that has 10 unique branches

Usage
tree.data

Format
A list containing data, a matrix with 3000 rows and 100 variables and branches, a factor containing 3000 elements.

Source
The authors

tree.data.small

Fake branching data for running examples fast

Description
A dataset containing high dimensional data that has 10 unique branches

Usage
tree.data.small

Format
A list containing data, a matrix with 250 rows and 50 variables and branches, a factor containing 250 elements.

Source
The authors
Index

*Topic **datasets**
  - tree.data, 11
  - tree.data.small, 11

- as.data.frame.phate, 2
- as.matrix.phate, 2
- check_pyphate_version, 3
- cluster_phate, 3
- ggplot.phate, 4
- install.phate, 4
- library.size.normalize, 5
- phate, 6
- plot.phate, 8
- print.phate, 9
- summary.phate, 10

- tree.data, 11
- tree.data.small, 11