Package ‘treefit’

October 14, 2022

Title  The First Software for Quantitative Trajectory Inference

Version  1.0.2

Description  Perform two types of analysis: 1) checking the goodness-of-fit of tree models to your single-cell gene expression data; and 2) deciding which tree best fits your data.

License  GPL (>= 3)


BugReports  https://github.com/hayamizu-lab/treefit-r/issues

Encoding  UTF-8

RoxygenNote  7.1.1

Imports  ggplot2, igraph, patchwork, pracma

Suggests  Seurat, gridExtra, knitr, plotly, qpdf, rmarkdown, testthat

VignetteBuilder  knitr

Language  en-US

NeedsCompilation  no

Author  Momoko Hayamizu [aut] (<https://orcid.org/0000-0001-8825-6331>), Kouhei Sutou [aut, cre] (<https://orcid.org/0000-0002-5528-5109>), Ryohei Suzuki [aut] (<https://orcid.org/0000-0002-1528-665X>), Hiromi Ishii [aut] (<https://orcid.org/0000-0002-7752-1782>)

Maintainer  Kouhei Sutou <kou@clear-code.com>

Repository  CRAN

Date/Publication  2022-01-18 07:50:02 UTC

R topics documented:

  generate_2d_n_arms_linked_star_data ........................................ 2
  generate_2d_n_arms_star_data .................................................. 3
  generate_n_arms_star_data ....................................................... 4
generate_2d_n_arms.LinkedStarData

Generate a 2-dimensional linked star tree data

Description
Generate a 2-dimensional linked star tree data. Each star tree data contain n_samples_vector[i] data points and fit a star tree with n_arms_vector[i] arms.

Usage
generate_2d_n_arms.LinkedStarData(n_samples_vector, n_arms_vector, fatness)

Arguments
n_samples_vector The vector of the number of samples to be generated. For example, c(200, 100, 300) means that the first tree has 200 samples, the second tree has 100 samples and the third tree has 300 samples.
n_arms_vector The vector of the number of arms to be generated. For example, c(3, 2, 5) means the first tree fits a star tree with 3 arms, the second tree fits a star tree with 2 arms and the third tree fits a star tree with 5 arms. The size of n_arms_vector must equal to the size of n_samples_vector.
fatness How fat from the based tree. [0.0, 1.0] is available value range.

Value
A generated matrix. The rows and columns correspond to samples and features.

Examples
# Generate a 2-dimensional linked star tree data that contain # 200-400-300 data points and fit a linked star tree with 3-5-4 # arms. The generated data are a bit noisy but tree-like.
linked_star.tree_like <-
  treefit::generate_2d_n_arms.LinkedStarData(c(200, 400, 300),
                                           c(3, 5, 4),
                                           0.1)
plot(linked_star.tree_like)

# Generate a 2-dimensional linked star tree data that contain # 300-200 data points and fit a linked star tree with 4-3 arms.
# The generated data are very noisy and less tree-like.
linked_star.less_tree_like <-
treefit::generate_2d_n_arms_linked_star_data(c(300, 200),
    c(4, 3),
    0.9)
plot(linked_star.less_tree_like)

---

generate_2d_n_arms_star_data

*Generate a 2-dimensional star tree data*

**Description**

Generate a 2-dimensional star tree data that contain \( n_{\text{samples}} \) data points and fit a star tree with \( n_{\text{arms}} \) arms.

**Usage**

```r
generate_2d_n_arms_star_data(n_samples, n_arms, fatness)
```

**Arguments**

- `n_samples` The number of samples to be generated.
- `n_arms` The number of arms to be generated.
- `fatness` How fat from the based star tree. \([0.0, 1.0]\) is available value range.

**Value**

A generated matrix. The rows and columns correspond to samples and features.

**Examples**

```r
# Generate a 2-dimensional star tree data that contain 500 data points
# and fit a star tree with 3 arms. The generated data are a bit noisy but
# tree-like.
star.tree_like <- treefit::generate_2d_n_arms_star_data(500, 3, 0.1)
plot(star.tree_like)

# Generate a 2-dimensional star tree data that contain 600 data points
# and fit a star tree with 5 arms. The generated data are very noisy and
# less tree-like.
star.less_tree_like <- treefit::generate_2d_n_arms_star_data(600, 5, 0.9)
plot(star.less_tree_like)
```
generate_n_arms_star_data

Generate a multi-dimensional star tree data

Description

Generate a multi-dimensional star tree data that contain \texttt{n\_samples} data points and fit a star tree with \texttt{n\_arms} arms.

Usage

generate_n_arms_star_data(n\_features, n\_samples, n\_arms, fatness)

Arguments

- \texttt{n\_features} The number of features (dimensions) to be generated.
- \texttt{n\_samples} The number of samples to be generated.
- \texttt{n\_arms} The number of arms to be generated.
- \texttt{fatness} How fat from the based star tree. \([0.0, 1.0]\) is available value range.

Value

A generated matrix. The rows and columns correspond to samples and features.

Examples

\begin{verbatim}
# Generate a 100-dimensional star tree data that contain 500 data points
# and fit a star tree with 3 arms. The generated data are a bit noisy but
# tree-like.
star100.tree_like <- treefit::generate_n_arms_star_data(100, 500, 3, 0.1)
# Reduce dimension to visualize.
star3.tree_like = prcomp(star100.tree_like, rank.=3)$x
plotly::plot_ly(data.frame(star3.tree_like),
  x=PC1, y=PC2, z=PC3,
  type="scatter3d",
  mode="markers",
  marker=list(size=1))
\end{verbatim}
perturbate_knn

Generate perturbated expression by k-NN data

Description
Generate perturbated expression from the original expression based on k-NN (k-nearest neighbor) data.

Usage
perturbate_knn(expression, strength = 1)

Arguments
- expression: The original expression. The rows and columns correspond to samples and features. The expression is normalized count of features.
- strength: How much perturbated. 0.0 is weak. 1.0 is strong.

Value
A perturbated expression as a matrix. The matrix's expression values are perturbated from the original expression values. The shape of the matrix is the same as the original expression. The dimension names of the matrix are also the same as the original expression.

Note
This is an API for advanced users. This API may be changed.

perturbate_poisson

Generate perturbated counts by the Poisson distribution

Description
Generate perturbated counts from the original counts by the Poisson distribution.

Usage
perturbate_poisson(counts, strength = 1)

Arguments
- counts: The original counts. The rows and columns correspond to samples and features. The values are count of features.
- strength: How much perturbated. 0.0 is weak. 1.0 is strong.
Value

A perturbated counts as a matrix. The matrix’s counts are perturbated from the original counts. The shape of the matrix is the same as the original counts. The dimension names of the matrix are also the same as the original counts.

Note

This is an API for advanced users. This API may be changed.

plot.treefit

Plot estimated results

Description

Plot estimate results to get insight.

Usage

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

Arguments

- `x` The estimated result by treefit() to be visualized.
- `...` The more estimated results to be visualized together or other graphical parameters.

Value

A plot object as a ggplot object. It plots the given one or more estimated results to get insights from one or more treefit() results.

Examples

```r
## Not run:
# Generate a tree data.
tree <- treefit::generate_2d_n_arms_star_data(200, 3, 0.1)
# Estimate the goodness-of-fit between tree models and the tree data.
fit <- treefit::treefit(list(expression=tree), "tree")
# Visualize the estimated result.
plot(fit)

# You can mix multiple estimated results by adding "name" column.
tree2 <- treefit::generate_2d_n_arms_star_data(200, 3, 0.9)
fit2 <- treefit::treefit(list(expression=tree2), "tree2")
plot(fit, fit2)
```

## End(Not run)
**treefit**

Estimate the goodness-of-fit between tree models and data

**Description**

Estimate the goodness-of-fit between tree models and data.

**Usage**

```r
treefit(
    target,
    name = NULL,
    perturbations = NULL,
    normalize = NULL,
    reduce_dimension = NULL,
    build_tree = NULL,
    max_p = 20,
    n_perturbations = 20
)
```

**Arguments**

`target`  
The target data to be estimated. It must be one of them:

- `list(counts=COUNTS, expression=EXPRESSION)`: You must specify at least one of `COUNTS` and `EXPRESSION`. They are matrix. The rows and columns correspond to samples such as cells and features such as genes. `COUNTS`'s value is count data such as the number of genes expressed. `EXPRESSION`'s value is normalized count data.
- Seurat object

`name`  
The name of `target` as string.

`perturbations`  
How to perturbate the target data.

- If this is `NULL`, all available perturbation methods are used.
- You can specify used perturbation methods as a list. Here are available methods:

`normalize`  
How to normalize counts data.

- If this is `NULL`, the default normalization is applied.
- You can specify a function that normalizes counts data.

`reduce_dimension`  
How to reduce dimension of expression data.

- If this is `NULL`, the default dimensionality reduction is applied.
- You can specify a function that reduces dimension of expression data.

`build_tree`  
How to build a tree of expression data.

- If this is `NULL`, MST is built.
- You can specify a function that builds tree of expression data.
max_p
How many low dimension Laplacian eigenvectors are used.
The default is 20.

n_perturbations
How many times to perturb.
The default is 20.

Value
An estimated result as a treefit object. It has the following attributes:

- `max_cca_distance`: The result of max canonical correlation analysis distance as `data.frame`.
- `rms_cca_distance`: The result of root mean square canonical correlation analysis distance as `data.frame`.
- `n_principal_paths_candidates`: The candidates of the number of principal paths.

data.frame of `max_cca_distance` and `rms_cca_distance` has the same structure. They have the following columns:

- `p`: Dimensionality of the feature space of tree structures.
- `mean`: The mean of the target distance values.
- `standard_deviation`: The standard deviation of the target distance values.

Examples
```
## Not run:
# Generate a star tree data that have normalized expression values
# not count data.
star <- treefit::generate_2d_n_arms_star_data(300, 3, 0.1)
# Estimate tree-likeness of the tree data.
fit <- treefit::treefit(list(expression=star))
## End(Not run)
```
Index

generate_{2d}_n_arms_linked_star_data, 2
generate_{2d}_n_arms_star_data, 3
generate_n_arms_star_data, 4

perturbate_knn, 5
perturbate_poisson, 5
plot.treefit, 6

treefit, 7