

Package ‘diffudist’

February 27, 2023

Title Diffusion Distance for Complex Networks

Version 1.0.1

URL <https://gbertagnolli.github.io/diffudist/>

BugReports [https://github.com/gbertagnolli/diffudist/issues/](https://github.com/gbertagnolli/diffudist/issues)

Description Enables the evaluation of diffusion distances for complex single-layer networks.

Given a network one can define different types of Laplacian (or transition) matrices corresponding to different continuous-time random walks dynamics on the network. This package enables the evaluation of Laplacians, stochastic matrices, and the corresponding diffusion distance matrices. The metric structure induced by the network-driven process is richer and more robust than the one given by shortest-paths and allows to study the geometry induced by different types of diffusion-like communication mechanisms taking place on complex networks.

For more details see: De Domenico, M. (2017) <[doi:10.1103/physrevlett.118.168301](https://doi.org/10.1103/physrevlett.118.168301)> and Bertagnolli, G. and De Domenico, M. (2021) <[doi:10.1103/PhysRevE.103.042301](https://doi.org/10.1103/PhysRevE.103.042301)>.

Depends R (>= 3.5.0)

Imports expm, ggdendro, ggplot2, grid, igraph, Matrix, stats, RColorBrewer, Rcpp (>= 1.0.10), reshape2, rlang, viridis

LinkingTo Rcpp, RcppEigen

Suggests knitr, cowplot, parallelDist, strex, tidyverse, rmarkdown

License GPL (>= 2)

Encoding UTF-8

RoxygenNote 7.2.3

VignetteBuilder knitr

NeedsCompilation yes

Author Giulia Bertagnolli [aut, cre] (<<https://orcid.org/0000-0001-8637-0632>>), Manlio De Domenico [aut] (<<https://orcid.org/0000-0001-5158-8594>>)

Maintainer Giulia Bertagnolli <giulia.bertagnolli@gmail.com>

Repository CRAN

Date/Publication 2023-02-27 19:42:40 UTC

R topics documented:

eigenMapMatMult	2
eigenMatMult	3
get_ddm_from_eigendec	3
get_diffusion_probability_matrix	4
get_diffusion_probability_matrix_from_T	6
get_distance_matrix	7
get_distance_matrix_from_T	9
get_laplacian	10
get_mean_distance_matrix	11
get_spectral_decomp	12
plotHeatmap	13
plot_distance_matrix	13

Index	15
--------------	-----------

eigenMapMatMult *Matrix Multiplication using RcppEigen*

Description

Matrix multiplication of the two matrices in input, without copy.

Usage

```
eigenMapMatMult(A, B)
```

Arguments

- A numeric matrix of dimension $m \times n$
- B numeric matrix of dimension $n \times l$

Value

C matrix of dimension $m \times p$ of the row-column product of A and B and C

<code>eigenMatMult</code>	<i>Matrix Multiplication using RcppEigen</i>
---------------------------	--

Description

Matrix multiplication of the two matrices in input.

Usage

```
eigenMatMult(A, B)
```

Arguments

- A numeric matrix of dimension $m \times n$
- B numeric matrix of dimension $n \times l$

Value

C matrix of dimension $m \times p$ of the row-column product of A and B and C

<code>get_ddm_from_eigendec</code>	<i>Distance Matrix from Laplacian spectral decomposition</i>
------------------------------------	--

Description

Returns the diffusion distance matrix when the spectrum (more precisely, the eigendecomposition) of the Laplacian is provided as input (useful to speed up batch calculations).

For instance, the random walk normalised Laplacian $I - D^{-1}A$, which generates the classical continuous-time random walk over a network, can be easily and obtained from the spectral decomposition of the symmetric normalised Laplacian $\mathcal{L} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = D^{-\frac{1}{2}}(D - A)D^{-\frac{1}{2}}$. More specifically, $\bar{L} = I - D^{-1}A = D^{-\frac{1}{2}}\mathcal{L}D^{\frac{1}{2}}$ and, since \mathcal{L} is symmetric it can be decomposed into $\mathcal{L} = \sum_{l=1}^N \lambda_l u_l u_l^T$, hence

$$\bar{L} = \sum_{l=1}^N \lambda_l u_l^R u_l^L$$

where $u_l^L = u_l^T D^{\frac{1}{2}}$ and $u_l^R = u_l D^{-\frac{1}{2}}$.

Usage

```
get_ddm_from_eigendec(tau, Q, Q_inv, lambdas, verbose = FALSE)
```

Arguments

<code>tau</code>	diffusion time (scalar)
<code>Q</code>	eigenvector matrix
<code>Q_inv</code>	inverse of the eigenvector matrix
<code>lambdas</code>	eigenvalues (vector)
<code>verbose</code>	whether warnings have to be printed or not

Value

The diffusion distance matrix D_t , a square numeric matrix of the Euclidean distances between the rows of the stochastic matrix $P(t) = e^{-\tau L}$, where $-L$ is the Laplacian generating a continuous-time random walk (Markov chain) over the network. The matrix exponential is here computed using the given eigendecomposition of the Laplacian matrix $e^{-\tau L} = Qe^{-\tau \Lambda}Q^{-1}$.

References

Bertagnolli, G., & De Domenico, M. (2021). Diffusion geometry of multiplex and interdependent systems. *Physical Review E*, 103(4), 042301. doi:10.1103/PhysRevE.103.042301 arXiv: 2006.13032

See Also

get_spectral_decomp

get_diff

Diffusion Probability Matrix

Description

Returns a matrix where each entry encodes the diffusion probability between two nodes

Usage

```

g,
tau,
type = "Normalized Laplacian",
weights = NULL,
verbose = TRUE
)

```

Arguments

<code>g</code>	a single-layer network
<code>tau</code>	diffusion time
<code>type</code>	default "Normalized Laplacian". The type of Laplacian (i.e. of dynamics) to consider. Other types available are: Laplacian for the classical combinatorial Laplacian matrix; it governs the diffusion dynamics on the network Normalized Laplacian for the Laplacian matrix normalized by degree matrix, the so-called classical random walk normalized Laplacian; it governs stochastic walks on the network Quantum Laplacian for the Laplacian matrix normalized to be symmetric; it governs quantum walks on the network MERW normalized Laplacian the maximal-entropy random walk (RW) normalized Laplacian; it governs stochastic walks on the network, in which the random walker moves according to a maximal-entropy RW [1].
<code>weights</code>	Note that you can type abbreviations, e.g. "L", "N", "Q", "M" for the respective types (case is ignored). The argument match is done through <code>match_arg</code> . edge weights, representing the strength/intensity (not the cost!) of each link. if weights is NULL (the default) and g has an edge attribute called weight, then it will be used automatically. If this is NA then no weights are used (even if the graph has a weight attribute).
<code>verbose</code>	default TRUE. If information on the type of Laplacian or on edge weights should be printed.

Value

The matrix $\exp^{-\tau L}$, exponential of a Laplacian matrix.

Functions

- `getDiffusionProbabilityMatrix()`: Old deprecated function

References

- De Domenico, M. (2017). Diffusion Geometry Unravels the Emergence of Functional Clusters in Collective Phenomena. *Physical Review Letters*. doi:10.1103/PhysRevLett.118.168301
- Bertagnolli, G., & De Domenico, M. (2021). Diffusion geometry of multiplex and interdependent systems. *Physical Review E*, 103(4), 042301. doi:10.1103/PhysRevE.103.042301 arXiv: 2006.13032

See Also

[get_laplacian](#), [get_distance_matrix](#)

`get_diffusion_probability_matrix_from_T`

Diffusion probability matrix from transition matrix

Description

Description here

Usage

```
get_diffusion_probability_matrix_from_T(Pi, tau)

get_diffu_Pt_from_T(Pi, tau)

get_diffu_Pt_from_Pi(Pi, tau)

get_diffusion_probability_matrix_from_Pi(Pi, tau)
```

Arguments

Pi	Transition matrix. We do not use T to avoid conflicts with the abbreviation for TRUE), instead we indicated the transition matrix with the capital greek letter Π in the equations and Pi in the code.
tau	diffusion time

Value

$\exp^{-\tau(I-\Pi)}$, exponential of the normalized Laplacian matrix corresponding to the given transition rate matrix (or transition probability matrix of a discrete-time Markov chain).

References

De Domenico, M. (2017). Diffusion Geometry Unravels the Emergence of Functional Clusters in Collective Phenomena. *Physical Review Letters*. doi:[10.1103/PhysRevLett.118.168301](https://doi.org/10.1103/PhysRevLett.118.168301)

Bertagnolli, G., & De Domenico, M. (2020). Diffusion Geometry of Multiplex and Interdependent Systems. [arxiv preprint arxiv:2006.13032](#)

See Also

[get_diffusion_probability_matrix](#)

get_distance_matrix	<i>Diffusion Distance Matrix</i>
---------------------	----------------------------------

Description

Returns a matrix where each entry encodes the diffusion distance between two nodes of a network. The diffusion distance at time τ between nodes $i, j \in G$ is defined as

$$D_\tau(i, j) = |\mathbf{p}(t|i) - \mathbf{p}(t|j)|_2$$

with $\mathbf{p}(t|i) = (e^{-\tau L})_{i \cdot} = \mathbf{e}_i e^{-\tau L}$ indicating the i -th row of the stochastic matrix $e^{-\tau L}$ and representing the probability (row) vector of a random walk dynamics corresponding to the initial condition \mathbf{e}_i , i.e. the random walker is in node i at time $\tau = 0$ with probability 1.

Usage

```
get_distance_matrix(
  g,
  tau,
  type = "Normalized Laplacian",
  weights = NULL,
  as_dist = FALSE,
  verbose = TRUE
)

getDistanceMatrix(g, tau, type = "Normalized Laplacian", weights = NULL,
                  verbose = TRUE)

get_DDM(
  g,
  tau,
  type = "Normalized Laplacian",
  weights = NULL,
  as_dist = FALSE,
  verbose = TRUE
)
```

Arguments

<code>g</code>	a (single-layer) network
<code>tau</code>	diffusion time
<code>type</code>	default "Normalized Laplacian". The type of Laplacian (i.e. of dynamics) to consider. Other types available:
	Laplacian for the classical combinatorial Laplacian matrix; it governs the diffusion dynamics on the network

Normalized Laplacian for the Laplacian matrix normalized by degree matrix, the so-called classical random walk normalized Laplacian; it governs stochastic walks on the network

Quantum Laplacian for the Laplacian matrix normalized to be symmetric; it governs quantum walks on the network

MERW normalized Laplacian the maximal-entropy random walk (RW) normalized Laplacian; it governs stochastic walks on the network, in which the random walker moves according to a maximal-entropy RW [1].

Note that you can type abbreviations, e.g. "L", "N", "Q", "M" for the respective types (case is ignored). The argument `match_arg` is done through `match_arg`.

<code>weights</code>	edge weights, representing the strength/intensity (not the cost!) of each link. If <code>weights</code> is NULL (the default) and <code>g</code> has an edge attribute called <code>weight</code> , then it will be used automatically. If this is NA then no weights are used (even if the graph has a <code>weight</code> attribute).
<code>as_dist</code>	If the function should return a matrix or an object of class "dist" as returned from [<code>stats::as.dist</code>]. Default is FALSE if the number of nodes is smaller than 1000.
<code>verbose</code>	default TRUE

Value

The diffusion distance matrix D_t , a square numeric matrix of the L^2 -norm distances between posterior probability vectors, i.e. Euclidean distances between the rows of the stochastic matrix $P(t) = e^{-\tau L}$, where $-L = -(I - T)$ is the generator of the continuous-time random walk (Markov chain) of given type over network `g`.

Functions

- `getDistanceMatrix()`: Old deprecated function

References

De Domenico, M. (2017). Diffusion Geometry Unravels the Emergence of Functional Clusters in Collective Phenomena. *Physical Review Letters*. doi:[10.1103/PhysRevLett.118.168301](https://doi.org/10.1103/PhysRevLett.118.168301)

Bertagnolli, G., & De Domenico, M. (2021). Diffusion geometry of multiplex and interdependent systems. *Physical Review E*, 103(4), 042301. doi:[10.1103/PhysRevE.103.042301](https://doi.org/10.1103/PhysRevE.103.042301) arXiv: [2006.13032](https://arxiv.org/abs/2006.13032)

See Also

[get_diffusion_probability_matrix](#)

Examples

```
g <- igraph::sample_pa(10, directed = FALSE)
dm_crw <- get_distance_matrix(g, tau = 1)
dm_merw <- get_distance_matrix(g, tau = 1, type = "MERW")
```

get_distance_matrix_from_T*Diffusion distance matrix from a custom transition matrix*

Description

Returns a matrix where each entry encodes the diffusion distance between two nodes of a network, given a transition matrix on the network and a diffusion time.

The diffusion distance at time τ between nodes $i, j \in G$ is defined as

$$D_\tau(i, j) = |\mathbf{p}(t|i) - \mathbf{p}(t|j)|_2$$

with $\mathbf{p}(t|i) = (e^{-\tau L})_{i \cdot} = \mathbf{e}_i e^{-\tau L}$ indicating the i -th row of the stochastic matrix $e^{-\tau L}$ and representing the probability (row) vector of a random walk dynamics corresponding to the initial condition \mathbf{e}_i , i.e. the random walker is in node i at time $\tau = 0$ with probability 1.

The Laplacian L is the normalised laplacian corresponding to the given transition matrix, i.e. $L = I - P_i$.

Usage

```
get_distance_matrix_from_T(Pi, tau, verbose = TRUE)

get_DDM_from_T(Pi, tau, verbose = TRUE)

get_distance_matrix_from_Pi(Pi, tau, verbose = TRUE)

get_DDM_from_Pi(Pi, tau, verbose = TRUE)
```

Arguments

Pi	a transition matrix (it should be a stochastic matrix)
tau	diffusion time
verbose	default TRUE

Value

The diffusion distance matrix D_t , a square numeric matrix of the L^2 -norm distances between posterior probability vectors, i.e. Euclidean distances between the rows of the stochastic matrix $P(t) = e^{-\tau L}$, where $-L = -(I - T)$ is the generator of the continuous-time random walk (Markov chain) corresponding to the discrete-time transition matrix $T = \text{Pi}$.

References

De Domenico, M. (2017). Diffusion Geometry Unravels the Emergence of Functional Clusters in Collective Phenomena. *Physical Review Letters*. doi:10.1103/PhysRevLett.118.168301

Bertagnolli, G., & De Domenico, M. (2021). Diffusion geometry of multiplex and interdependent systems. *Physical Review E*, 103(4), 042301. doi:10.1103/PhysRevE.103.042301 arXiv: 2006.13032

See Also

[get_distance_matrix](#) [get_diffusion_probability_matrix](#), [get_diffusion_probability_matrix_from_T](#)

Examples

```
g <- igraph::sample_pa(10, directed = FALSE)
dm <- get_distance_matrix(g, tau = 1)
```

<code>get_laplacian</code>	<i>Evaluate a Laplacian Matrix</i>
----------------------------	------------------------------------

Description

Returns a specific Laplacian matrix corresponding to the chosen dynamics type and network. The available types are:

Laplacian for the classical combinatorial Laplacian matrix; it governs the diffusion dynamics on the network

Normalized Laplacian for the Laplacian matrix normalized by degree matrix, the so-called classical random walk normalized Laplacian; it governs stochastic walks on the network

Quantum Laplacian for the Laplacian matrix normalized to be symmetric; it governs quantum walks on the network

MERW normalized Laplacian the maximal-entropy random walk (RW) normalized Laplacian; it governs stochastic walks on the network, in which the random walker moves according to a maximal-entropy RW [1].

The maximum entropy random walk (MERW) chooses the stochastic matrix which maximizes $H(S)$, so that the walker can explore every walk of the same length with equal probability. Let λ_N, ϕ be the leading eigenvalue and corresponding right eigenvector of the adjacency matrix A . Then the transition matrix corresponding to the discrete-time random walk is $\Pi_{ij} = \frac{A_{ij}}{\lambda_N} \frac{\phi_j}{\phi_i}$. The MERW (normalized) Laplacian is then given by $I - \Pi$. Note that we use the notation Π and P_i to avoid confusion with the abbreviation T for the logical TRUE.

Usage

```
get_laplacian(g, type = "Laplacian", weights = NULL, verbose = TRUE)

getLaplacianMatrix(g, type = "Laplacian", weights = NULL, verbose = TRUE)
```

Arguments

<code>g</code>	a network
<code>type</code>	the type of Laplacian matrix. default "Laplacian", the combinatorial Laplacian. Other types: c("Normalized Laplacian", "Quantum Laplacian", "MERW Normalized Laplacian"). Note that you can type abbreviations, e.g. "L", "N", "Q", "M" for the respective types (case is ignored). The argument <code>match_arg</code> is done through match_arg .

weights	edge weights, representing the strength/intensity (not the cost!) of each link. if weights is NULL (the default) and g has an edge attribute called weight, then it will be used automatically. If this is NA then no weights are used (even if the graph has a weight attribute).
verbose	default TRUE. If information on the type of Laplacian or on edge weights should be printed.

Value

the ('type') Laplacian matrix of network 'g'

References

[1] Burda, Z., et al. (2009). Phys Rev. Lett. 102 160602(April), 1–4. doi:[10.1103/PhysRevLett.102.160602](https://doi.org/10.1103/PhysRevLett.102.160602)

get_mean_distance_matrix
Mean distance matrix

Description

Given a sequence of distance matrices, expected to correspond to sequential increasing values of time, calculate the average distance between any pairs of nodes shortest-path (or geodesic) distance

Usage

```
get_mean_distance_matrix(DM_list)
getMeanDistanceMatrix(DM_list)
```

Arguments

DM_list list of distance matrices

Value

mean-distance matrix

Functions

- `getMeanDistanceMatrix()`: Old deprecated function

References

De Domenico, M. (2017). Diffusion Geometry Unravels the Emergence of Functional Clusters in Collective Phenomena. Physical Review Letters. doi:[10.1103/PhysRevLett.118.168301](https://doi.org/10.1103/PhysRevLett.118.168301)

Bertagnolli, G., & De Domenico, M. (2020). Diffusion Geometry of Multiplex and Interdependent Systems. arxiv preprint arxiv:[2006.13032](https://arxiv.org/abs/2006.13032)

See Also

[get_diffusion_probability_matrix](#), [get_distance_matrix](#)

`get_spectral_decomp` *Laplacian Spectral Decomposition*

Description

Returns the eigenvalue spectrum together with eigenvectors of a Laplacian corresponding to a network. This involves computing the eigendecomposition of a (symmetric) matrix, so it is computationally intense and may take some time. The decomposition of the normalized Laplacian $L = I - D^{-1}A$ takes is computed through the decomposition of its symmetric version $L = D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$. See the package vignette for details.

Usage

```
get_spectral_decomp(g, type = "Normalized Laplacian", verbose = FALSE)
```

Arguments

<code>g</code>	the network in the [igraph] format
<code>type</code>	the Laplacian type, default "Normalized Laplacian". At the moment this is the only available option. For other types of Laplacians one should get autonomously the eigendecomposition, e.g. using eigen . See the package vignette for an example.
<code>verbose</code>	whether warnings have to be printed or not

Value

lambda the eigenvalues of the Laplacian
 ‘u_L’ the matrix of left eigenvectors (rows)
 ‘u_R’ the matrix of right eigenvectors (columns)

References

Bertagnolli, G., & De Domenico, M. (2021). Diffusion geometry of multiplex and interdependent systems. Physical Review E, 103(4), 042301. doi:10.1103/PhysRevE.103.042301 arXiv: [2006.13032](https://arxiv.org/abs/2006.13032)

See Also

[get_laplacian](#) [get_ddm_from_eigendec](#)

plotHeatmap *Plot distance matrix as heatmap*

Description

‘r lifecycle::badge("deprecated")‘

Usage

```
plotHeatmap(  
  DM,  
  colPalette = NULL,  
  log.scale = FALSE,  
  cex = 1,  
  showDendrogram = TRUE,  
  title = ""  
)
```

Arguments

DM	a distance matrix
colPalette	‘r lifecycle::badge("deprecated")‘ in the new function plot_distance_matrix it is called <code>col_palette</code>
log.scale	‘r lifecycle::badge("deprecated")‘ in the new function plot_distance_matrix it is called <code>log_scale</code>
cex	numerical value by which text should be magnified (default font size in [ggplot2:theme] is 11)
showDendrogram	‘r lifecycle::badge("deprecated")‘ in the new function plot_distance_matrix it is called <code>show_dendro</code>
title	Title of the plot passed to labs . No title by default

Value

a [ggplot](#)

plot_distance_matrix *Plot distance matrix*

Description

Plot a heatmap of the distance matrix using [geom_tile](#).

Usage

```
plot_distance_matrix(
  DM,
  col_palette = viridis(n = 11),
  log_scale = FALSE,
  cex = 1,
  show_dendro = TRUE,
  title = ""
)
```

Arguments

DM	a distance matrix
col_palette	a colour palette, previously it was set to the ‘spectral’ palette of brewer.pal but now it is, by default, to the color-blind friendly viridis .
log_scale	logical. Default FALSE
cex	numerical value by which text should be magnified (default font size in theme is 11)
show_dendro	If the dendrogram resulting from hclust should be shown. Default TRUE
title	Title of the plot passed to labs . No title by default.

Value

plot [ggplot](#)

Index

```
* Markov-chain
    get_diffusion_probability_matrix,
        4
    get_diffusion_probability_matrix_from_T,
        6
* diffusion
    get_distance_matrix, 7
    get_distance_matrix_from_T, 9
* distance
    get_distance_matrix, 7
    get_distance_matrix_from_T, 9
    get_mean_distance_matrix, 11
    plot_distance_matrix, 13
* heatmap
    plot_distance_matrix, 13
* matrix;
    plot_distance_matrix, 13
* plot;
    plot_distance_matrix, 13
* probabilities
    get_diffusion_probability_matrix,
        4
    get_diffusion_probability_matrix_from_T,
        6
* transition
    get_diffusion_probability_matrix,
        4
    get_diffusion_probability_matrix_from_T,
        6
brewer.pal, 14
eigen, 12
eigenMapMatMult, 2
eigenMatMult, 3
geom_tile, 13
get_DDM(get_distance_matrix), 7
get_ddm_from_eigendec, 3, 12
get_DDM_from_Pi
    (get_distance_matrix_from_T), 9
get_DDM_from_T
    (get_distance_matrix_from_T), 9
get_diffu_Pt
    (get_diffusion_probability_matrix),
        4
get_diffu_Pt_from_Pi
    (get_diffusion_probability_matrix_from_T),
        6
get_diffu_Pt_from_T
    (get_diffusion_probability_matrix_from_T),
        6
get_diffusion_probability_matrix, 4, 6,
    8, 10, 12
get_diffusion_probability_matrix_from_Pi
    (get_diffusion_probability_matrix_from_T),
        6
get_diffusion_probability_matrix_from_T,
    6, 10
get_distance_matrix, 6, 7, 10, 12
get_distance_matrix_from_Pi
    (get_distance_matrix_from_T), 9
get_distance_matrix_from_T, 9
get_laplacian, 6, 10, 12
get_mean_distance_matrix, 11
get_spectral_decomp, 4, 12
getDiffusionProbabilityMatrix
    (get_diffusion_probability_matrix),
        4
getDistanceMatrix
    (get_distance_matrix), 7
getLaplacianMatrix (get_laplacian), 10
getMeanDistanceMatrix
    (get_mean_distance_matrix), 11
ggplot, 13, 14
hclust, 14
labs, 13, 14
```

match_arg, [5](#), [8](#), [10](#)

plot_distance_matrix, [13](#), [13](#)
plotHeatmap, [13](#)

theme, [14](#)

viridis, [14](#)