

# Package ‘diffuStats’

December 23, 2024

**Type** Package

**Title** Diffusion scores on biological networks

**Version** 1.26.0

**Description** Label propagation approaches are a widely used procedure in computational biology for giving context to molecular entities using network data. Node labels, which can derive from gene expression, genome-wide association studies, protein domains or metabolomics profiling, are propagated to their neighbours in the network, effectively smoothing the scores through prior annotated knowledge and prioritising novel candidates. The R package diffuStats contains a collection of diffusion kernels and scoring approaches that facilitates their computation, characterisation and benchmarking.

**Depends** R (>= 3.4)

**Imports** grDevices, stats, methods, Matrix, MASS, checkmate, expm, igraph, Rcpp, RcppArmadillo, RcppParallel, plyr, precrec

**License** GPL-3

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**RoxygenNote** 7.1.1

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**VignetteBuilder** knitr

**biocViews** Network, GeneExpression, GraphAndNetwork, Metabolomics, Transcriptomics, Proteomics, Genetics, GenomeWideAssociation, Normalization

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| .check_scores | <i>Sanity checks for input</i> |
|---------------|--------------------------------|

---

## Description

.check\_scores ensures that scores are suitable for diffusion  
 .available\_methods is a character vector with the implemented scores  
 .check\_method ensures that 'method' is a valid character  
 .check\_metric ensures that 'metric' is a valid list of metric functions  
 .check\_graph ensures that 'graph' is a valid igraph object  
 .check\_K ensures that 'K' is a formally valid kernel. Does not check for spd

### Usage

```
.check_scores(scores)

.available_methods

.check_method(method)

.check_metric(metric)

.check_graph(graph)

.check_K(K)
```

### Arguments

|        |                 |
|--------|-----------------|
| scores | scores to check |
| method | object to test  |
| metric | object to test  |
| graph  | object to test  |
| K      | object to test  |

### Format

An object of class character of length 7.

### Value

Functions return invisible() but throw warnings and errors as side effect

### Examples

```
data(graph_toy)
diffuStats:::check_scores(diffuStats:::to_list(graph_toy$input_mat))
diffuStats:::check_method("raw")
diffuStats:::check_metric(list(auc = metric_fun(curve = "ROC")))
data(graph_toy)
diffuStats:::check_graph(graph_toy)
data(graph_toy)
diffuStats:::check_K(regularisedLaplacianKernel(graph_toy))
```

---

.connect\_undirected\_graph

*Function to connect a non connected graph*

---

### Description

Function to connect a non connected graph

### Usage

```
.connect_undirected_graph(g)
```

**Arguments**

`g` an igraph object

**Value**

a connected igraph object

**Examples**

```
library(igraph)
g <- diffuStats:::connect_undirected_graph(
  graph.empty(10, directed = FALSE))
g
```

---

`.default_graph_param` *Generate data.frame with default vertex attributes*

---

**Description**

Generate data.frame with default vertex attributes  
 Default proportions for randomly generated graphs

**Usage**

```
.default_graph_param()
.default_prop
```

**Format**

An object of class `numeric` of length 3.

**Value**

data.frame with default node class attributes  
 named numeric with default class proportions

---

`convertSparse` *S4 sparse matrix to arma::sp\_mat*

---

**Description**

Convert an S4 sparse matrix from the [Matrix](#) package to an arma `sp_mat`.

**Usage**

```
convertSparse(mat)
```

**Arguments**

mat S4 sparse matrix from the [Matrix](#)

**Value**

an arma::sp\_mat object

**Source**

<http://gallery.rcpp.org/articles/armadillo-sparse-matrix/>

---

diffuse

*Diffuse scores on a network*

---

**Description**

Function `diffuse` takes a network in **igraph** format (or a graph kernel matrix stemming from a graph) and an initial state to score all the nodes in the network. The seven diffusion scores hereby provided differ on (a) how they distinguish positives, negatives and unlabelled examples, and (b) their statistical normalisation. The argument `method` offers the following options:

Methods without statistical normalisation:

- `raw`: positive nodes introduce unitary flow ( $y_{raw}[i] = 1$ ) to the network, whereas neither negative nor unlabelled nodes introduce anything ( $y_{raw}[j] = 0$ ) [Vandin, 2011]. They are computed as:

$$f_{raw} = K \cdot y_{raw}$$

where  $K$  is a graph kernel, see `?kernels`. These scores treat negative and unlabelled nodes equivalently.

- `m1`: same as `raw`, but negative nodes introduce a negative unit of flow [Zoidi, 2015] and are therefore not equivalent to unlabelled nodes.
- `gm`: same as `m1`, but the unlabelled nodes are assigned a (generally non-null) bias term based on the total number of positives, negatives and unlabelled nodes [Mostafavi, 2008].
- `ber_s`: this is a quantification of the relative change in the node score before and after the network smoothing. The score for a particular node  $i$  can be written as

$$f_{ber_s,i} = \frac{f_{raw,i}}{y_{raw,i} + \epsilon}$$

where  $\epsilon$  is a parameter controlling the importance of the relative change.

Methods with statistical normalisation: the `raw` diffusion score of every node  $i$  is computed and compared to its own diffusion scores stemming from a permuted input.

- `mc`: the score of node  $i$  is based in its empirical p-value, computed by permuting the input `n.perm` times:

$$p_i = \frac{r_i + 1}{n.perm + 1}$$

$p[i]$  is roughly the proportion of input permutations that led to a diffusion score as high or higher than the original diffusion score (a total of  $r[i]$  for node  $i$ , in absolute terms). This assesses how likely a high diffusion score is to arise from chance, in absence of signal. To be consistent with the direction, `mc` is defined as:

$$f_{mc,i} = 1 - p_i$$

- `ber_p`: as used in [Bersanelli, 2016], this score combines `raw` and `mc`, in order to take into account both the magnitude of the `raw` scores and the effect of the network topology:

$$f_{ber_p,i} = -\log_{10}(p_i) \cdot f_{raw,i}$$

- `z`: this is a parametric alternative to `mc`. The `raw` score of node `i` is subtracted its mean value and divided by its standard deviation. The statistical moments have a closed analytical form, see the main vignette, and are inspired in [Harchaoui, 2013]. Unlike `mc` and `ber_p`, the `z` scores do not require actual permutations, giving them an advantage in terms of speed.

If the input labels are not quantitative, i.e. `positive(1)`, `negative(0)` and possibly unlabelled, all the scores (`raw`, `gm`, `m1`, `z`, `mc`, `ber_s`, `ber_p`) can be used. Quantitative inputs are naturally defined on `raw`, `z`, `mc`, `ber_s` and `ber_p` by extending the definitions above, and are readily available in `diffuStats`. Further details on the scores can be found in the main vignette.

### Usage

```
diffuse(graph, scores, method, ...)
```

```
diffuse_grid(scores, grid_param, ...)
```

### Arguments

|                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|-------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>graph</code>      | <b>igraph</b> object for the diffusion. Alternatively, a kernel matrix can be provided through the argument <code>K</code> instead of the <code>igraph</code> object.                                                                                                                                                                                                                                                                                                                                                                  |
| <code>scores</code>     | scores to be smoothed; either a named numeric vector, a column-wise matrix whose rownames are nodes and colnames are different scores, or a named list of such matrices.                                                                                                                                                                                                                                                                                                                                                               |
| <code>method</code>     | character, one of <code>raw</code> , <code>gm</code> , <code>m1</code> , <code>z</code> , <code>mc</code> , <code>ber_s</code> , <code>ber_p</code> . For batch analysis of several methods, see <code>?diffuse_grid</code> .                                                                                                                                                                                                                                                                                                          |
| <code>...</code>        | additional arguments for the diffusion method. <code>mc</code> and <code>ber_p</code> accept <code>n.perm</code> (number of permutations), <code>seed</code> (for reproducibility, defaults to 1) and <code>sample.prob</code> , a list of named vectors -one per background- with sampling probabilities for the null model, uniform by default. More details available in <code>?diffuse_mc</code> . On the other hand, <code>ber_s</code> accepts <code>eps</code> , a parameter controlling the importance of the relative change. |
| <code>grid_param</code> | data frame containing parameter combinations to explore. The column names should be the names of the parameters. Parameters that have a fixed value can be specified in the <code>grid</code> or through the additional arguments ( <code>...</code> )                                                                                                                                                                                                                                                                                 |

### Details

Input scores can be specified in three formats. A single set of scores to smooth can be represented as (1) a named numeric vector, whereas if several of these vectors that share the node names need to be smoothed, they can be provided as (2) a column-wise matrix. However, if the unlabelled entities are not the same from one case to another, (3) a named list of such score matrices can be passed to this function. The input format will be kept in the output.

The implementation of `mc` and `ber_p` is optimized for sparse inputs. Dense inputs might take a longer time to compute. Another relevant note: `z` can give `NaN` for a particular node when the observed nodes are disconnected from the node being scored. This is because these nodes are neither annotated with experimental nor network (topology) data.

**Value**

`diffuse` returns the diffusion scores, with the same format as `scores`

`diffuse_grid` returns a data frame containing the diffusion scores for the specified combinations of parameters

**References**

Scores "raw": Vandin, F., Upfal, E., & Raphael, B. J. (2011). Algorithms for detecting significantly mutated pathways in cancer. *Journal of Computational Biology*, 18(3), 507-522.

Scores "ml": Zoidi, O., Fotiadou, E., Nikolaidis, N., & Pitas, I. (2015). Graph-based label propagation in digital media: A review. *ACM Computing Surveys (CSUR)*, 47(3), 48.

Scores "gm": Mostafavi, S., Ray, D., Warde-Farley, D., Grouios, C., & Morris, Q. (2008). GeneMANIA: a real-time multiple association network integration algorithm for predicting gene function. *Genome biology*, 9(1), S4.

Scores "mc", "ber\_s", "ber\_p": Bersanelli, M., Mosca, E., Remondini, D., Castellani, G., & Milanese, L. (2016). Network diffusion-based analysis of high-throughput data for the detection of differentially enriched modules. *Scientific reports*, 6.

Scores "z": Harchaoui, Z., Bach, F., Cappe, O., & Moulines, E. (2013). Kernel-based methods for hypothesis testing: A unified view. *IEEE Signal Processing Magazine*, 30(4), 87-97.

**Examples**

```
#####

library(igraph)
library(ggplot2)
data(graph_toy)
input_vec <- graph_toy$input_vec
n <- vcount(graph_toy)

#####

# Examples for 'diffuse':

# Using a binary vector as input
diff_scores <- diffuse(
  graph = graph_toy,
  scores = input_vec,
  method = "raw")

# Using a matrix as input
diff_scores <- diffuse(
  graph = graph_toy,
  scores = graph_toy$input_mat,
  method = "raw")

# Using a list of matrices as input
diff_scores <- diffuse(
  graph = graph_toy,
  scores = list(myScores1 = graph_toy$input_mat,
               myScores2 = head(graph_toy$input_mat, n/2)),
  method = "raw")
```

```
#####

# Examples for 'diffuse_grid':

# Using a single vector of scores and comparing the methods
# "raw", "ml", and "z"
df_diff <- diffuse_grid(
  graph = graph_toy,
  scores = graph_toy$input_vec,
  grid_param = expand.grid(method = c("raw", "ml", "z")))
head(df_diff)

# Same settings, but comparing several choices of the
# parameter epsilon ("eps") in the scores "ber_s"
df_diff <- diffuse_grid(
  graph = graph_toy,
  scores = graph_toy$input_vec,
  grid_param = expand.grid(method = "ber_s", eps = 1:5/5))
ggplot(df_diff, aes(x = factor(eps), fill = eps, y = node_score)) +
  geom_boxplot()

# Using a matrix with four set of scores
# called Single, Row, Small_sample, Large_sample
# See the 'quickstart' vignette for more details on these toy scores
# We compute scores for methods "ber_p" and "mc" and
# permute both 1e3 and 1e4 times in each run
df_diff <- diffuse_grid(
  graph = graph_toy,
  scores = graph_toy$input_mat,
  grid_param = expand.grid(
    method = c("mc", "ber_p"),
    n.perm = c(1e3, 1e4)))
dim(df_diff)
head(df_diff)

#####

# Differences when using (1) a quantitative input and
# (2) different backgrounds.

# In this example, the
# small background contains binary scores and continuous scores for
# half of the nodes in the 'graph_toy' example graph.

# (1) Continuous scores have been generated by
# changing the positive labels to a random, positive numeric value.
# The user can see the impact of this in the scores 'raw', 'ber_s',
# 'ber_p', 'mc' and 'z'

# (2) The larger background is just the small background
# completed with zeroes, both for binary and continuous scores.
# This illustrates how 'raw' and 'ber_s' treat unlabelled
# and negative labels equally, whereas 'ml', 'gm', 'ber_p',
# 'mc' and 'z' do not.

# Examples:
```



```

# The input:
lapply(graph_toy$input_list, head)

# 'raw' scores treat equally unlabelled and negative nodes,
# and can account for continuous inputs
diff_raw <- diffuse(
  graph = graph_toy,
  scores = graph_toy$input_list,
  method = "raw")
lapply(diff_raw, head)

# 'z' scores distinguish unlabelled and negatives and accepts
# continuous inputs
diff_z <- diffuse(
  graph = graph_toy,
  scores = graph_toy$input_list,
  method = "z")
lapply(diff_z, head)

# 'ml' and 'gm' are the same score if there are no unobserved nodes
diff_compare <- diffuse_grid(
  graph = graph_toy,
  scores = input_vec,
  grid_param = expand_grid(method = c("raw", "ml", "gm"))
)
df_compare <- reshape2::acast(
  diff_compare,
  node_id~method,
  value.var = "node_score")
head(df_compare)

# 'ml' and 'gm' are different in presence of unobserved nodes
diff_compare <- diffuse_grid(
  graph = graph_toy,
  scores = head(input_vec, n/2),
  grid_param = expand_grid(method = c("raw", "ml", "gm"))
)
df_compare <- reshape2::acast(
  diff_compare,
  node_id~method,
  value.var = "node_score")
head(df_compare)

```

---

diffuse\_mc

---

*Compute the heatrank using permutations*


---

## Description

Function `diffuse_mc` has an implemented parallelisation of the Monte Carlo trials for diffusion in a network. The input scores are assumed to be sparse and are internally sparsified, so very dense scores might take time with current implementation.

**Usage**

```
diffuse_mc(
  graph,
  scores,
  n.perm = 10000,
  sample.prob = NULL,
  seed = 1,
  oneminusHeatRank = TRUE,
  K = NULL,
  ...
)
```

**Arguments**

|                  |                                                                                                                                                                                                                                                                                                        |
|------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| graph            | igraph object                                                                                                                                                                                                                                                                                          |
| scores           | Recursive list, can have either binary or quantitative scores                                                                                                                                                                                                                                          |
| n.perm           | Numeric, number of permutations                                                                                                                                                                                                                                                                        |
| sample.prob      | Numeric, probabilities (needn't be scaled) to permute the input. This is passed to <code>sample</code> 's prob argument. If NULL, sampling is uniform. It has to be in a list format, with the same names as scores, and each element of the list must be the sampling probability of each background. |
| seed             | Numeric, seed for random number generator                                                                                                                                                                                                                                                              |
| oneminusHeatRank | Logical, should 1 - heatrank be returned instead of heatrank?                                                                                                                                                                                                                                          |
| K                | Kernel matrix (if precomputed). If K is not supplied, the regularised Laplacian will be computed on the fly and used.                                                                                                                                                                                  |
| ...              | currently ignored arguments                                                                                                                                                                                                                                                                            |

**Value**

A list containing matrices of heatrank scores

**Examples**

```
# Using a list as input (needed)
data(graph_toy)
list_input <- list(myInput1 = graph_toy$input_mat)
diff_mc <- diffuse_mc(
  graph = graph_toy,
  scores = list_input)
```

---

diffuse\_raw

*Diffuse scores on a network*


---

**Description**

Function `diffuse` takes a network in **igraph** format and an initial state to score all the nodes in the network.

**Usage**

```
diffuse_raw(graph, scores, z = FALSE, K = NULL, ...)
```

**Arguments**

|        |                                                                                                         |
|--------|---------------------------------------------------------------------------------------------------------|
| graph  | <b>igraph</b> object for the diffusion                                                                  |
| scores | list of score matrices. For a single input with a single background, supply a list with a vector column |
| z      | logical, should z-scores be computed instead of raw scores?                                             |
| K      | optional matrix, precomputed diffusion kernel                                                           |
| ...    | currently ignored arguments                                                                             |

**Value**

A list of scores, with the same length and dimensions as scores

**Examples**

```
# Using a list as input (needed)
data(graph_toy)
list_input <- list(myInput1 = graph_toy$input_mat)
diff_raw <- diffuse_raw(
  graph = graph_toy,
  scores = list_input)
diff_z <- diffuse_raw(
  graph = graph_toy,
  scores = list_input,
  z = TRUE)
```

---

diffuStats

*diffuStats: an R package to compute and benchmark diffusion scores*

---

**Description**

The diffuStats package consists of (i) functions to compute graph kernels, see [kernels](#), (ii) the function `diffuse` to compute the diffusion scores and (iii) the function `perf_eval` and its wrapper `perf` to compute performance measures. The user can find two vignettes in `browseVignettes("diffuStats")`: (1) a quick start with concise examples and (2) a detailed explanation of the implemented methods with a practical case study using a yeast protein dataset.

**Author(s)**

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## References

General references:

Most of the graph kernels can be found in: Smola, A. J., & Kondor, R. (2003, August). Kernels and regularization on graphs. In COLT (Vol. 2777, pp. 144-158).

The statistical normalisation of the diffusion scores, which has interest per se, has been introduced in: Bersanelli, M., Mosca, E., Remondini, D., Castellani, G., & Milanesi, L. (2016). Network diffusion-based analysis of high-throughput data for the detection of differentially enriched modules. Scientific reports, 6.

---

|                |                                |
|----------------|--------------------------------|
| generate_graph | <i>Generate a random graph</i> |
|----------------|--------------------------------|

---

## Description

Function `generate_graph` generates a random network using **igraph** graph generators. Several models are available, and

## Usage

```
generate_graph(
  fun_gen,
  param_gen,
  class_label = NULL,
  class_attr = .default_graph_param(),
  fun_curate = .connect_undirected_graph,
  seed = NULL
)
```

## Arguments

|                          |                                                                                                                                                                                                                                                                |
|--------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>fun_gen</code>     | function to generate the graphs. Typically from <b>igraph</b> , like <code>barabasi.game</code> , <code>watts.strogatz.game</code> , <code>erdos.renyi.game</code> , <code>make_lattice</code> , etc.                                                          |
| <code>param_gen</code>   | list with parameters to pass to <code>fun_gen</code>                                                                                                                                                                                                           |
| <code>class_label</code> | character vector with length equal to the number of nodes in the graph to generate. If left to <code>NULL</code> , the default classes are <code>c("source", "filler", "end")</code> with proportions of <code>c(0.05, 0.45, 0.5)</code> .                     |
| <code>class_attr</code>  | data.frame with vertex classes as rownames and a column for each vertex attribute. The name of the column will be used as the attribute name.                                                                                                                  |
| <code>fun_curate</code>  | function to apply to the graph before returning it. Can be set to <code>identity</code> or <code>NULL</code> to skip this step. By default, the graph is connected: nodes not belonging to the largest connected component are randomly wired to a node in it. |
| <code>seed</code>        | numeric, seed for random number generator                                                                                                                                                                                                                      |

## Value

An **igraph** object

**Examples**

```
g <- generate_graph(
  fun_gen = igraph::barabasi.game,
  param_gen = list(n = 100, m = 3, directed = FALSE),
  seed = 1)
g
```

---

|                |                                                    |
|----------------|----------------------------------------------------|
| generate_input | <i>Generate a random input for graph diffusion</i> |
|----------------|----------------------------------------------------|

---

**Description**

Function `generate_input` generates a random list of nodes from an **igraph** object. It also specifies the true solution generating the list. The graph object needs to have some attributes (automatically added through `generate_graph`)

**Usage**

```
generate_input(graph, order, length_inputs, return_matrix = TRUE, seed = NULL)
```

**Arguments**

|               |                                                                        |
|---------------|------------------------------------------------------------------------|
| graph         | an <b>igraph</b> object, typically from <a href="#">generate_input</a> |
| order         | numeric or vector, order of the neighbourhoods that generate the list  |
| length_inputs | numeric, number of nodes in the generated inputs                       |
| return_matrix | logical, should inputs be returned as a matrix?                        |
| seed          | numeric, seed for random number generator                              |

**Value**

A list whose elements are lists with three slots: `pos` for the true signal generators, `neg` for the nodes that did not generate signal and `input` for the signal itself

**Examples**

```
g <- generate_graph(
  fun_gen = igraph::barabasi.game,
  param_gen = list(n = 200, m = 3, directed = FALSE),
  seed = 1)
synth_input <- generate_input(
  g,
  order = 2,
  length_inputs = 3, return_matrix = TRUE)
str(synth_input)
```

---

|           |                                         |
|-----------|-----------------------------------------|
| graph_toy | <i>Toy graph to play with diffusion</i> |
|-----------|-----------------------------------------|

---

**Description**

Small graph that can easily be plotted and experimented with. It has graphical parameters included, such as the vertex colour and the layout. It also includes an example input. Has graph attributes with example inputs and outputs, see `input_*` and `output_*` from `list.graph.attributes(graph_toy)`

**Usage**

```
graph_toy
```

**Format**

An object of class `igraph` of length 10.

**Value**

An **igraph** object

---

|           |                                            |
|-----------|--------------------------------------------|
| is_kernel | <i>Check if a matrix is a valid kernel</i> |
|-----------|--------------------------------------------|

---

**Description**

This function checks whether the eigenvalues are non-negative

**Usage**

```
is_kernel(x, tol = 1e-08)
```

**Arguments**

|                  |                                         |
|------------------|-----------------------------------------|
| <code>x</code>   | numeric, symmetric matrix to be checked |
| <code>tol</code> | numeric, tolerance for zero eigenvalues |

**Value**

scores in desired format

**Examples**

```
data(graph_toy)
K <- regularisedLaplacianKernel(graph_toy)
is_kernel(K)
is_kernel(K - 1)
```

## Description

Function `commuteTimeKernel` computes the commute-time kernel, which is the expected time of going back and forth between a couple of nodes. If the network is connected, then the commute time kernel will be totally dense, therefore reflecting global properties of the network. For further details, see [Yen, 2007]. This kernel can be computed using both the unnormalised and normalised graph Laplacian.

Function `diffusionKernel` computes the classical diffusion kernel that involves matrix exponentiation. It has a "bandwidth" parameter  $\sigma^2$  that controls the extent of the spreading. Quoting [Smola, 2003]:  $K(x_1, x_2)$  can be visualized as the quantity of some substance that would accumulate at vertex  $x_2$  after a given amount of time if we injected the substance at vertex  $x_1$  and let it diffuse through the graph along the edges. This kernel can be computed using both the unnormalised and normalised graph Laplacian.

Function `inverseCosineKernel` computes the inverse cosine kernel, which is based on a cosine transform on the spectrum of the normalized Laplacian matrix. Quoting [Smola, 2003]: the inverse cosine kernel treats lower complexity functions almost equally, with a significant reduction in the upper end of the spectrum. This kernel is computed using the normalised graph Laplacian.

Function `pStepKernel` computes the  $p$ -step random walk kernel. This kernel is more focused on local properties of the nodes, because random walks are limited in terms of length. Therefore, if  $p$  is small, only a fraction of the values  $K(x_1, x_2)$  will be non-null if the network is sparse [Smola, 2003]. The parameter  $a$  is a regularising term that is summed to the spectrum of the normalised Laplacian matrix, and has to be 2 or greater. The  $p$ -step kernels can be cheaper to compute and have been successful in biological tasks, see the benchmark in [Valentini, 2014].

Function `regularisedLaplacianKernel` computes the regularised Laplacian kernel, which is a standard in biological networks. The regularised Laplacian kernel arises in numerous situations, such as the finite difference formulation of the diffusion equation and in Gaussian process estimation. Sticking to the heat diffusion model, this function allows to control the constant terms summed to the diagonal through `add_diag`, i.e. the strength of the leaking in each node. If a node has diagonal term of 0, it is not allowed to disperse heat. The larger the diagonal term of a node, the stronger the first order heat dispersion in it, provided that it is positive. Every connected component in the graph should be able to disperse heat, i.e. have at least a node  $i$  with `add_diag[i] > 0`. If this is not the case, the result diverges. More details on the parameters can be found in [Smola, 2003]. This kernel can be computed using both the unnormalised and normalised graph Laplacian.

## Usage

```
commuteTimeKernel(graph, normalized = FALSE)
```

```
diffusionKernel(graph, sigma2 = 1, normalized = TRUE)
```

```
inverseCosineKernel(graph)
```

```
pStepKernel(graph, a = 2, p = 5L)
```

```
regularisedLaplacianKernel(graph, sigma2 = 1, add_diag = 1, normalized = FALSE)
```

**Arguments**

|            |                                                                                                                        |
|------------|------------------------------------------------------------------------------------------------------------------------|
| graph      | undirected igraph object. If the edges have weights, those should typically be non-negative.                           |
| normalized | logical, should the normalised (TRUE) or unnormalised (FALSE) graph Laplacian matrix be used?                          |
| sigma2     | numeric value, parameter $\sigma^2$ of the kernel - higher values force more spreading in the network                  |
| a          | numeric value greater or equal to 2, which acts as a regularisation term. Can also be a vector of length vcount(graph) |
| p          | integer greater than 0, the number of steps for the random walk                                                        |
| add_diag   | numeric value or vector of length vcount(graph), term to regularise the spectrum of the Laplacian                      |

**Details**

Please be aware that the kernel computation can be rather slow and memory demanding. This is a reference table of the peak memory usage and computing time for the regularised Laplacian kernel given the order of the network:

5k: 900MB & 250s

10k: 3,200MB & 2,200s

15k: 8,000MB & 8,000s

20k: 13,000MB & 21,000s

However, given a network to study, this step is a one-time task than can be stored and reused.

**Value**

A kernel matrix with adequate dimnames

**References**

The regularised Laplacian, diffusion, p-step and inverse cosine kernels: Smola, A. J., & Kondor, R. (2003, August). Kernels and regularization on graphs. In COLT (Vol. 2777, pp. 144-158).

The commute time kernel: Yen, L., Fouss, F., Decaestecker, C., Francq, P., & Saerens, M. (2007). Graph nodes clustering based on the commute-time kernel. *Advances in Knowledge Discovery and Data Mining*, 1037-1045.

Benchmark on kernels: Valentini, G., Paccanaro, A., Caniza, H., Romero, A. E., & Re, M. (2014). An extensive analysis of disease-gene associations using network integration and fast kernel-based gene prioritization methods. *Artificial Intelligence in Medicine*, 61(2), 63–78.

**Examples**

```
data(graph_toy)
K_lap <- regularisedLaplacianKernel(graph_toy)
K_diff <- diffusionKernel(graph_toy)
K_pstep <- pStepKernel(graph_toy)
K_ct <- commuteTimeKernel(graph_toy)
K_ic <- inverseCosineKernel(graph_toy)
is_kernel(K_lap)
```



---

|            |                                    |
|------------|------------------------------------|
| largest_cc | <i>Largest connected component</i> |
|------------|------------------------------------|

---

**Description**

Obtain the largest connected component of an igraph object

**Usage**

```
largest_cc(g)
```

**Arguments**

`g` igraph object

**Value**

A connected igraph object

**Examples**

```
library(igraph)
set.seed(1)
g <- erdos.renyi.game(30, p.or.m = .05)
largest_cc(g)
```

---

|            |                                                     |
|------------|-----------------------------------------------------|
| metric_auc | <i>Compute the area under the curves (ROC, PRC)</i> |
|------------|-----------------------------------------------------|

---

**Description**

Function `metric_auc` computes the AUROC (Area Under the Receiver Operating Characteristic Curve) and the AUPRC (Area Under the Precision Recall Curve), measures of goodness of a ranking in a binary classification problem. Partial areas are also supported. Important: the higher ranked classes are assumed to ideally target positives (label = 1) whereas lower ranks correspond to negatives (label = 0).

Function `metric_fun` is a wrapper on `metric_auc` that returns a function for performance evaluation. This function takes as input actual and predicted values and outputs a performance metric. This is needed for functions such as `perf` and `perf_eval`, which iterate over a list of such metric functions and return the performance measured through each of them.

**Usage**

```
metric_auc(
  actual,
  predicted,
  curve = "ROC",
  partial = c(0, 1),
  standardized = FALSE
)

metric_fun(...)
```

**Arguments**

|              |                                                                                                                                                                                                                                   |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| actual       | numeric, binary labels of the negatives (0) and positives (1)                                                                                                                                                                     |
| predicted    | numeric, prediction used to rank the entities - this will typically be the diffusion scores                                                                                                                                       |
| curve        | character, either "ROC" for computing the AUROC or "PRC" for the AUPRC                                                                                                                                                            |
| partial      | vector with two numeric values for computing partial areas. The numeric values are the limits in the x axis of the curve, as implemented in the "xlim" argument in <a href="#">part</a> . Defaults to c(0,1), i.e. the whole area |
| standardized | logical, should partial areas be standardised to range in [0, 1]? Defaults to FALSE and only affects partial areas.                                                                                                               |
| ...          | parameters to pass to <a href="#">metric_auc</a>                                                                                                                                                                                  |

**Details**

The AUROC is a scalar value: the probability of a randomly chosen positive having a higher rank than a randomly chosen negative. AUROC is cutoff-free and an informative of the performance of a ranker. Likewise, AUPRC is the area under the Precision-Recall curve and is also a standard metric for binary classification. Both measures can be found in [Saito, 2017].

AUROC and AUPRC have their partial counterparts, in which only the area enclosed up to a certain false positive rate (AUROC) or recall (AUPRC) is accounted for. This can be useful when assessing the goodness of the ranking, focused on the top entities.

The user can, however, define his or her custom performance metric. AUROC and AUPRC are common choices, but other problem-specific metrics might be of interest. For example, number of hits in the top k nodes. Machine learning metrics can be found in packages such as `Metrics` and `MLmetrics` from the CRAN repository (<http://cran.r-project.org/>).

**Value**

`metric_auc` returns a numeric value, the area under the specified curve  
`metric_fun` returns a function (performance metric)

**References**

Saito, T., & Rehmsmeier, M. (2017). Precrec: fast and accurate precision–recall and ROC curve calculations in R. *Bioinformatics*, 33(1), 145-147.

**Examples**

```

# generate class and numeric ranking
set.seed(1)
n <- 50
actual <- rep(0:1, each = n/2)
predicted <- ifelse(
  actual == 1,
  runif(n, min = 0.2, max = 1),
  runif(n, min = 0, max = 0.8))

# AUROC
metric_auc(actual, predicted, curve = "ROC")

# partial AUC (up until false positive rate of 10%)
metric_auc(
  actual, predicted, curve = "ROC",
  partial = c(0, 0.1))

# The same are, but standardised in (0, 1)
metric_auc(
  actual, predicted, curve = "ROC",
  partial = c(0, 0.1), standardized = TRUE)

# AUPRC
metric_auc(actual, predicted, curve = "PRC")

# Generate performance functions for perf and perf_eval
f_roc <- metric_fun(
  curve = "ROC", partial = c(0, 0.5),
  standardized = TRUE)
f_roc
f_roc(actual = actual, predicted = predicted)

```

---

moments

---

*Compute exact statistical moments*


---

**Description**

Function `get_mu()` computes the exact expected values of the null distributions

Function `get_covar()` computes the exact covariance matrix of the null distributions (square matrix, same size as kernel matrix); the variances are the values in the matrix diagonal

Function `get_mu_reference()` computes the reference expected values (one scalar value for each node/entity)

Function `get_var_reference()` computes the reference variances (one scalar value for each node/entity), log10-transformed

**Usage**

```
get_mu(K, id_labelled = colnames(K), mu_y)
```

```
get_covar(K, id_labelled = colnames(K), var_y)
```

```
get_mu_reference(K, id_labelled = colnames(K))
```

```
get_var_reference(K, id_labelled = colnames(K))
```

### Arguments

|             |                                                                                |
|-------------|--------------------------------------------------------------------------------|
| K           | square matrix, precomputed diffusion graph kernel, see ?kernels                |
| id_labelled | character, names of the labelled nodes (must be a subset of the colnames of K) |
| mu_y, var_y | (scalar) mean and variance of the input, see details                           |

### Details

These functions enable exploring the properties of the null distributions of diffusion scores. They provide the exact statistical moments mentioned in:

Sergio Picart-Armada, Wesley K Thompson, Alfonso Buil, Alexandre Perera-Lluna. The effect of statistical normalisation on network propagation scores. *Bioinformatics*, 2020, btaa896. <https://doi.org/10.1093/bioinform>

Specifically, `get_mu_reference()` and `get_var_reference()` provide the so-called 'Reference expected values' and 'Reference variances', which are input-independent (one only needs the kernel and the ids of the labelled nodes). Getting the actual expected values and variances requires providing the input expected value and variance, and can be achieved with `get_mu()` and `get_covar()`.

### Value

`get_mu_reference()`, `get_var_reference()` and `get_mu()` return a vector, whereas `get_covar()` returns a square matrix.

### References

Article: <https://doi.org/10.1093/bioinformatics/btaa896> Functions: <https://github.com/b2slab/diffuBench/blob/master/he>

### Examples

```
data(graph_toy)
## Kernel
K_pstep <- pStepKernel(graph_toy)
## Labelled nodes
ids <- head(rownames(K_pstep), ncol(K_pstep)/3)
## Reference values
get_mu_reference(K_pstep, ids)
get_var_reference(K_pstep, ids)
## Actual moments with an input y
y <- graph_toy$input_vec[ids]
mu_y <- mean(y)
var_y <- var(y)
mu <- get_mu(K_pstep, ids, mu_y = mu_y)
covar <- get_covar(K_pstep, ids, var_y = var_y)
## mean values
mu
## variances
diag(covar)
## covariances
covar[1:6, 1:6]
```

---

|            |                            |
|------------|----------------------------|
| named.list | <i>Create a named list</i> |
|------------|----------------------------|

---

**Description**

Create a list with variables and name the slots using the variables names

**Usage**

```
named.list(...)
```

**Arguments**

... Variables to pack in a list

**Value**

A list of variables

**Examples**

```
diffuStats:::named.list(LETTERS, mean)
```

---

|                  |                                     |
|------------------|-------------------------------------|
| ParallelHeatrank | <i>Compute heatrank in parallel</i> |
|------------------|-------------------------------------|

---

**Description**

ParallelHeatrank is a wrapper that computes heatranks for (possibly) different backgrounds and for multiple inputs at once. It will reuse the permutations, which have to be passed to the function. The input must be binary for this implementation, so numeric values for each node are not supported.

**Usage**

```
ParallelHeatrank(R, perm, G)
```

**Arguments**

|      |                                                                                                                                                                                             |
|------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| R    | dense matrix with the diffusion kernel                                                                                                                                                      |
| perm | dense matrix with the permutations (indices in columns). This has to ensure that enough indices are sampled, i.e. at least as great as the largest list in the input (largest colSums in G) |
| G    | S4 sparse matrix with the heat sources                                                                                                                                                      |

**Value**

a matrix with the same amount of rows that R and columns in G, containing the heatrank scores. These scores are corrected using  $(r + 1)/(p + 1)$  instead of  $r/p$ . The smaller the score, the warmer the node.

---

 perf

---

*Compare diffusions to a target score on a grid of parameters*


---

### Description

Function `perf` computes diffusion scores on a grid of parameters and evaluates them using the gold standard scores provided by the user.

### Usage

```
perf(
  scores,
  validation,
  grid_param,
  metric = list(auc = metric_fun(curve = "ROC")),
  ...
)
```

### Arguments

|                         |                                                                                                                                                                                                                |
|-------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>scores</code>     | scores to be smoothed; either a named numeric vector, a column-wise matrix whose rownames are nodes and colnames are different scores, or a named list of such matrices.                                       |
| <code>validation</code> | target scores to which the smoothed scores will be compared to. Must have the same format as the input scores, although the number of rows may vary and only the matching rows will give a performance measure |
| <code>grid_param</code> | data frame containing parameter combinations to explore. The column names should be the names of the parameters.                                                                                               |
| <code>metric</code>     | named list of metrics to apply. Each metric should accept the form <code>f(actual, predicted)</code>                                                                                                           |
| <code>...</code>        | additional named arguments for the diffusion method. It's important to input at least an <code>igraph</code> object or, alternative, a kernel matrix <code>K</code>                                            |

### Details

Function `perf` takes a network in **igraph** format, an initial state to score all the nodes in the network, a target score set. To explore the parameter combinations, it needs a grid and a list of metrics to apply. The validation scores might be only a subset of the network nodes, in which case the metric will be restricted to this set as well.

### Value

A data frame containing the performance of each diffusion score

### Examples

```
# Using a single vector of scores
data(graph_toy)
df_perf <- perf(
  graph = graph_toy,
  scores = graph_toy$input_vec,
```

```

validation = graph_toy$input_vec,
grid_param = expand.grid(method = c("raw", "ml"))
df_perf
# Using a matrix with four set of scores
# called Single, Row, Small_sample, Large_sample
df_perf <- perf(
  graph = graph_toy,
  scores = graph_toy$input_mat,
  validation = graph_toy$input_mat,
  grid_param = expand.grid(method = c("raw", "ml"))
df_perf

```

---

perf\_eval

---

*Compute performance of diffusion scores on a single case*


---

### Description

Function `perf_eval` directly compares a desired output with the scores from diffusion. It handles the possible shapes of the scores (vector, matrix, list of matrices) and gives the desired metrics.

### Usage

```

perf_eval(
  prediction,
  validation,
  metric = list(auc = metric_fun(curve = "ROC"))
)

```

### Arguments

|                         |                                                                                                                                                                                                                 |
|-------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>prediction</code> | smoothed scores; either a named numeric vector, a column-wise matrix whose rownames are nodes and colnames are different scores, or a named list of such matrices.                                              |
| <code>validation</code> | target scores to which the smoothed scores will be compared to. Must have the same format as the input scores, although the number of rows may vary and only the matching rows will give a performance measure. |
| <code>metric</code>     | named list of metrics to apply. Each metric should accept the form <code>f(actual, predicted)</code>                                                                                                            |

### Value

A data frame containing the metrics for each comparable pair of output-validation.

### Examples

```

# Using a matrix with four set of scores
# called Single, Row, Small_sample, Large_sample
data(graph_toy)
diff <- diffuse(
  graph = graph_toy,
  scores = graph_toy$input_mat,

```

```

    method = "raw")
df_perf <- perf_eval(
  prediction = diff,
  validation = graph_toy$input_mat)
df_perf

```

---

perf\_wilcox

---

*Compute column-wise statistics in a performance matrix*


---

## Description

Function `perf_wilcox` compares all the columns of a matrix through a `wilcox.test`. The columns are assumed to be performance measures (e.g. AUROC) whereas the rows are instances.

## Usage

```

perf_wilcox(
  perf_mat,
  adjust = function(p) stats::p.adjust(p, method = "fdr"),
  ci = 0.95,
  digits_ci = 2,
  digits_p = 3,
  ...
)

```

## Arguments

|                        |                                                                                                                              |
|------------------------|------------------------------------------------------------------------------------------------------------------------------|
| <code>perf_mat</code>  | Numeric matrix whose columns contain performance metrics of different methods.                                               |
| <code>adjust</code>    | Function to adjust the p-values for multiple testing. By default, <code>p.adjust</code> with its default parameters is used. |
| <code>ci</code>        | Numeric, confidence interval (defaults to 0.95)                                                                              |
| <code>digits_ci</code> | Integer, digits to display in the confidence interval                                                                        |
| <code>digits_p</code>  | Integer, digits to display in the p-value                                                                                    |
| <code>...</code>       | further arguments for <code>format</code>                                                                                    |

## Details

The statistical comparison of the columns is intended to ease comparisons between methods in a rigorous way. Methods are compared pairwise and a p-value for difference in performance. The function `perf_wilcox` returns a character matrix so that (1) the upper triangular matrix contains confidence intervals on the estimate of the difference between performances, and (2) the lower triangular matrix contains the two-tailed p-value that tests difference in performance, with multiple testing correction. The comparison takes place between row and column in that precise order: a positive difference favours the row and a negative one, the column.

## Value

Character matrix. The upper triangular matrix contains a confidence interval and the estimate of the pairwise difference in performance. The lower triangular matrix shows the associated two-tailed p-value, with multiple testing correction.



**Examples**

```
# Dummy data frame to test
n <- 100
perf_mat <- cbind(
  good = runif(n = n, min = 0.5, max = 1),
  so_so = runif(n = n, min = 0.2, max = 0.7),
  bad = runif(n = n, min = 0, max = 0.5)
)
wilcox_mat <- perf_wilcox(perf_mat)

# See how the methods in the rows compare to those
# in the columns, confidence interval
# (upper) and p-value (lower)
wilcox_mat
```

---

 scores2colours

*Translate values into colours*


---

**Description**

Create a vector of hex colours from numeric values, typically diffusion scores

**Usage**

```
scores2colours(
  x,
  range = c(min(0, min(x)), max(x)),
  n.colors = 10,
  palette = colorRampPalette(c("#3C5488FF", "white", "#F39B7FFF"))
)
```

**Arguments**

|          |                                                                                                                                                                |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| x        | numeric vector to be colorised                                                                                                                                 |
| range    | range of values to filter x (values out of the range will be collapsed to the closest limit)                                                                   |
| n.colors | integer, number of colors in the palette                                                                                                                       |
| palette  | palette function that generates a scale of colours given the number of desired colours. Defaults to a blue-white-red scale by <a href="#">colorRampPalette</a> |

**Value**

Character vector with hex colours

**Examples**

```
set.seed(1)
scores2colours(runif(20))
```

---

scores2shapes                    *Translate values into shapes*

---

**Description**

Translate 0/1 to shapes, by default "circle" and "square"

**Usage**

```
scores2shapes(x, shapes = c("circle", "square"))
```

**Arguments**

x                                numeric vector to generate shapes from  
 shapes                         character vector with two shapes, respectively zeroes and ones

**Value**

Character vector with shapes

**Examples**

```
set.seed(1)
scores2shapes(rbinom(n = 20, size = 1, prob = .5))
```

---

serialHeatrank                    *Compute heatrank for a single case*

---

**Description**

The heatrank incorporates the correction  $(r + 1)/(p + 1)$  instead of  $r/p$

**Usage**

```
serialHeatrank(R, perm, G, ind)
```

**Arguments**

R                                dense matrix with the diffusion kernel  
 perm                            sparse matrix with the permutations  
 G                                sparse matrix with the heat sources  
 ind                              index of the G column for current source

**Value**

an arma::vec with node heatranks

---

|           |                                             |
|-----------|---------------------------------------------|
| sparsify2 | <i>Sparsify arma::mat into arma::sp_mat</i> |
|-----------|---------------------------------------------|

---

**Description**

Return permutations as a numeric sparse matrix (can be binary or continuous)

**Usage**

```
sparsify2(perm, nrow, G)
```

**Arguments**

|      |                                      |
|------|--------------------------------------|
| perm | dense matrix with the permutations   |
| nrow | number of rows for the sparse matrix |
| G    | sparse column matrix                 |

**Value**

an arma::sp\_mat object

---

|         |                                     |
|---------|-------------------------------------|
| to_list | <i>Convert input to list format</i> |
|---------|-------------------------------------|

---

**Description**

Convert any input to list format

**Usage**

```
to_list(scores, dummy_column = "X1", dummy_list = "X1")
```

**Arguments**

|                          |                                              |
|--------------------------|----------------------------------------------|
| scores                   | object to reformat                           |
| dummy_column, dummy_list | character, names for the dummy columns/items |

**Value**

scores in list format

**Examples**

```
data(graph_toy)
x_v <- diffuStats:::to_list(graph_toy$input_vec)
x_m <- diffuStats:::to_list(graph_toy$input_mat)
```

---

|                |                                              |
|----------------|----------------------------------------------|
| to_x_from_list | <i>Convert list format to desired format</i> |
|----------------|----------------------------------------------|

---

**Description**

Convert any list format to the convenient one

**Usage**

```
to_x_from_list(scores, x)
```

**Arguments**

|        |                           |
|--------|---------------------------|
| scores | list to reformat          |
| x      | character, desired format |

**Value**

scores in desired format

**Examples**

```
data(graph_toy)
x_v <- diffuStats:::to_x_from_list(
  diffuStats:::to_list(graph_toy$input_vec), "vector")
x_m <- diffuStats:::to_x_from_list(
  diffuStats:::to_list(graph_toy$input_vec), "matrix")
```

---

|              |                                      |
|--------------|--------------------------------------|
| which_format | <i>In which format is the input?</i> |
|--------------|--------------------------------------|

---

**Description**

Tell apart vector, matrix or list of matrices

**Usage**

```
which_format(x)
```

**Arguments**

|   |                    |
|---|--------------------|
| x | object to evaluate |
|---|--------------------|

**Value**

character: vector, matrix or list.

**Examples**

```
data(graph_toy)
diffuStats:::which_format(graph_toy$input_vec)
diffuStats:::which_format(graph_toy$input_mat)
```

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