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# DiffuPy Documentation

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DiffuPy is a generalizable Python implementation of the numerous label propagation algorithms inspired by the dif-fuStats R package<sup>1</sup>. DiffuPy supports generic graph formats such as JSON, CSV, GraphML, or GML.

Installation is as easy as getting the code from [PyPI](#) with `python3 -m pip install diffupy`. See the *installation* documentation.

**See also:**

- Documented on [Read the Docs](#)
- Versioned on [GitHub](#)
- Tested on [Travis CI](#)
- Distributed by [PyPI](#)

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<sup>1</sup> Picart-Armada, S., *et al.* (2017). Null diffusion-based enrichment for metabolomics data. *PloS one* 12.12.



## INSTALLATION

The latest stable code can be installed from [PyPI](#) with:

```
$ python3 -m pip install diffupy
```

The most recent code can be installed from the source on [GitHub](#) with:

```
$ python3 -m pip install git+https://github.com/multipaths/DiffuPy.git
```

For developers, the repository can be cloned from [GitHub](#) and installed in editable mode with:

```
$ git clone https://github.com/multipaths/DiffuPy.git
$ cd diffupy
$ python3 -m pip install -e .
```

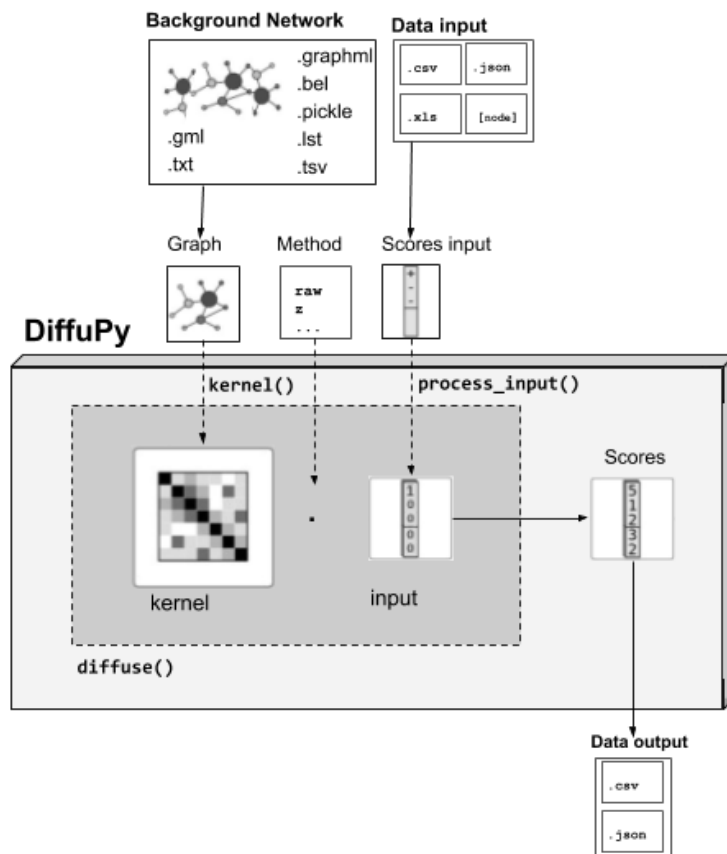




## BASIC USAGE

The two required input elements to run diffusion using DiffuPy are:

- 1) A **network/graph**. (see Network-Input Formatting below)
- 2) A **dataset of scores**. (see Scores-Input Formatting below)



For its usability, you can either:

- Use the [Command Line Interface](#) (see cli).
- Use *pythonically* the **functions** provided in `diffupy.diffuse`:

```
from diffupy.diffuse import run_diffusion
```

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```
# DATA INPUT and GRAPH as PATHs -> returned as *PandasDataFrame*
diffusion_scores = run_diffusion(~/data/input_scores.csv, ~/data/network.csv).as_pd_
↳dataframe()

# DATA INPUT and GRAPH as Python OBJECTS -> exported *as_csv*
diffusion_scores = run_diffusion(input_scores, network).as_csv('~/output/diffusion_
↳results.csv')
```

## 2.1 Methods

The diffusion method by default is `z`, which statistical normalization has previously shown to outperform. Further parameters to adapt the propagation procedure are also provided, such as choosing from the available diffusion methods or providing a custom method function. See [diffusion Methods and/or Method modularity](#).

```
diffusion_scores_select_method = run_diffusion(input_scores, network, method = 'raw')

from networkx import page_rank # Custom method function

diffusion_scores_custom_method = run_diffusion(input_scores, network, method = page_
↳rank)
```

You can also provide your own kernel method or select among the ones provided in the `kernels.py` function which you can provide as a `kernel_method` argument. By default `regularised_laplacian_kernel` is used.

```
from diffupath.kernels import p_step_kernel # Custom kernel calculation function

diffusion_scores_custom_kernel_method = run(input_scores, method = 'raw', kernel_method_
↳= p_step_kernel)
```

So `method` stands for the **diffusion process** method, and `kernel_method` for the **kernel calculation** method.

## 2.2 Formatting

Before running diffusion algorithms on your network using DiffuPy, take into account the **graph and input data/scores formats**. You can find specified here samples of supported input scores and networks.

## INPUT FORMAT

The input is preprocessed and further mapped before the diffusion. See [input mapping](#) or [see process\\_input docs](#) for further details. Here we outline the input formats covered for its preprocessing.

### 3.1 Scores

You can submit your dataset in any of the following formats:

- CSV (*.csv*)
- TSV (*.tsv*)
- *pandas.DataFrame*
- *List*
- *Dictionary*

(check Input dataset examples)

So you can **either** provide a **path** to a *.csv* or *.tsv* file:

```
from diffupy.diffuse import run_diffusion

diffusion_scores_from_file = run_diffusion('~data/diffusion_scores.csv', network)
```

or **Pythonically** as a data structure as the *input\_scores* parameter:

```
data = {'Node': ['A', 'B', ...],
        'Node Type': ['Metabolite', 'Gene', ...],
        ....
        }
df = pd.DataFrame (data, columns = ['Node', 'Node Type', ...])

diffusion_scores_from_dict = run_diffusion(df, network)
```

Please ensure that the dataset minimally has a column 'Node' containing node IDs. You can also optionally add the following columns to your dataset:

- NodeType
- LogFC\*<sup>0</sup>
- p-value

---

<sup>0</sup> Log<sub>2</sub> fold change

## 3.2 Networks

If you would like to submit your own networks, please ensure they are in one of the following formats:

- BEL (.bel)
- CSV (.csv)
- Edge list (.lst)
- GML (.gml or .xml)
- GraphML (.graphml or .xml)
- Pickle (.pickle). BELGraph object from [PyBEL 0.13.2](#)
- TSV (.tsv)
- TXT (.txt)

Minimally, please ensure each of the following columns are included in the network file you submit:

- Source
- Target

Optionally, you can choose to add a third column, “Relation” in your network (as in the example below). If the relation between the **Source** and **Target** nodes is omitted, and/or if the directionality is ambiguous, either node can be assigned as the **Source** or **Target**.

## 3.3 Kernel

If you dispose of a precalculated kernel, you can provide directly the kernel object without needing to also provide a graph object. As mentioned above, if you wish to use your kernel method function you can provide it as *kernel\_method* argument on the previous described function.

## INPUT DATASET EXAMPLES

DiffuPath accepts several input formats which can be codified in different ways. See the [diffusion scores](#) summary for more details on how the labels input are treated according each available method.

1. You can provide a dataset with a column 'Node' containing node IDs.

Node
A
B
C
D

```
from diffupy.diffuse import run_diffusion
diffusion_scores = run_diffusion(dataframe_nodes, network)
```

Also as a list of nodes:

```
['A', 'B', 'C', 'D']
```

```
diffusion_scores = run_diffusion(['A', 'B', 'C', 'D'], network)
```

2. You can also provide a dataset with a column 'Node' containing node IDs as well as a column 'NodeType', indicating the entity type of the node to run diffusion by entity type.

Node	NodeType
A	Gene
B	Gene
C	Metabolite
D	Gene

Also as a dictionary of type:list of nodes :

```
{'Gene': ['A', 'B', 'D'], 'Metabolite': ['C']}
```

```
diffusion_scores = run_diffusion({'Genes': ['A', 'B', 'D'], 'Metabolites': ['C']}, ↵
↵network)
```

3. You can also choose to provide a dataset with a column 'Node' containing node IDs as well as a column 'logFC' with their logFC. You may also add a 'NodeType' column to run diffusion by entity type.

Node	LogFC
A	4
B	-1
C	1.5
D	3

Also as a dictionary of node:score\_value :

```
{'A':-1, 'B':-1, 'C':1.5, 'D':4}
```

```
diffusion_scores = run_diffusion({'A':-1, 'B':-1, 'C':1.5, 'D':4})
```

Combining point 2., you can also indicating the node type:

Node	LogFC	NodeType
A	4	Gene
B	-1	Gene
C	1.5	Metabolite
D	3	Gene

Also as a dictionary of type:node:score\_value :

```
{Gene: {A:-1, B:-1, D:4}, Metabolite: {C:1.5}}
```

```
diffusion_scores = run_diffusion({Gene: {A:-1, B:-1, D:4}, Metabolite: {C:1.5}}, network)
```

4. Finally, you can provide a dataset with a column 'Node' containing node IDs, a column 'logFC' with their logFC and a column 'p-value' with adjusted p-values. You may also add a 'NodeType' column to run diffusion by entity type.

Node	LogFC	p-value
A	4	0.03
B	-1	0.05
C	1.5	0.001
D	3	0.07

This only accepted pythonicaly in dataframe format.

See the [sample datasets](#) directory for example files.

## CUSTOM-NETWORK EXAMPLE

Source	Target	Relation
A	B	Increase
B	C	Association
A	D	Association

You can also take a look at our [sample networks](#) folder for some examples.





## INPUT MAPPING/COVERAGE

Even though it is not relevant for the input user usage, taking into account the input mapped entities over the background network is relevant for the diffusion process assessment, since the coverage of the input implies the actual entities-scores that are being diffused. In other words, only the entities whose labels match an entity in the network will be further processed for diffusion.

Running diffusion will report the mapping as follows:

### Mapping descriptive statistics

#### wikipathways:

```
gene_nodes (474 mapped entities, 15.38% input coverage)
mirna_nodes (2 mapped entities, 4.65% input coverage)
metabolite_nodes (12 mapped entities, 75.0% input coverage)
bp_nodes (1 mapped entities, 0.45% input coverage)
total (489 mapped entities, 14.54% input coverage)
```

#### kegg:

```
gene_nodes (1041 mapped entities, 33.80% input coverage)
mirna_nodes (3 mapped entities, 6.98% input coverage)
metabolite_nodes (6 mapped entities, 0.375% input coverage)
bp_nodes (12 mapped entities, 5.36% input coverage)
total (1062 mapped entities, 31.58% input coverage)
```

#### reactome:

```
gene_nodes (709 mapped entities, 23.02% input coverage)
mirna_nodes (1 mapped entities, 2.33% input coverage)
metabolite_nodes (6 mapped entities, 37.5% input coverage)
total (716 mapped entities, 22.8% input coverage)
```

#### total:

```
gene_nodes (1461 mapped entities, 43.44% input coverage)
mirna_nodes (4 mapped entities, 0.12% input coverage)
metabolite_nodes (13 mapped entities, 0.38% input coverage)
bp_nodes (13 mapped entities, 0.39% input coverage)
total (1491 mapped entities, 44.34% input coverage)
```

To graphically see the mapping coverage, you can also plot a [heatmap view of the mapping](#) (see views). To see how the mapping is performed over an input pipeline preprocessing, take a look at this [Jupyter Notebook](#) or see [process\\_input docs](#) in DiffuPy.



## OUTPUT FORMAT

The returned format is a custom *Matrix* type, with node labels as rows and a column with the diffusion score, which can be exported into the following formats:

```
diffusion_scores.to_dict()
diffusion_scores.as_pd_dataframe()
diffusion_scores.as_csv()
diffusion_scores.to_nx_graph()
```



## COMMAND LINE INTERFACE

DiffuPy Command Line Interface

### 8.1 diffupy

DiffuPy

```
diffupy [OPTIONS] COMMAND [ARGS]...
```

#### 8.1.1 diffuse

Run a diffusion method for the provided input\_scores over a given network.

**param input** Path to a (miscellaneous format) data input to be processed/formatted.

**param network** Path to the network as a (NetworkX) graph or as a (diffuPy.Matrix) kernel.

**param output** Path (with file name) for the generated scores output file. By default '\$OUTPUT/diffusion\_scores.csv'

**param method** Elected method ["raw", "ml", "gm", "ber\_s", "ber\_p", "mc", "z"] or custom method FUNCTION(network, scores, kargs). By default 'raw'

**param binarize** If logFC provided in dataset, convert logFC to binary. By default False

**param threshold** Codify node labels by applying a threshold to logFC in input. By default None

**param absolute\_value** Codify node labels by applying threshold to |logFC| in input. By default False

**param p\_value** Statistical significance. By default 0.05

**param format\_output** Elected output format ["CSV", "JSON"]. By default 'CSV'

**param kernel\_method** Callable method for kernel computation.

```
diffupy diffuse [OPTIONS]
```

## Options

- i, --input** <input>  
Required Input data
- n, --network** <network>  
Required Path to the network graph or kernel
- o, --output** <output>  
Output file
- m, --method** <method>  
Diffusion method  
**Options** z | gm | ml | ber\_p | raw | mc | ber\_s
- b, --binarize** <binarize>  
If logFC provided in dataset, convert logFC to binary (e.g., up-regulated entities to 1, down-regulated to -1). For scoring methods that accept quantitative values (i.e., raw & z), node labels can also be codified with LogFC (in this case, set binarize==False).
- t, --threshold** <threshold>  
Codify node labels by applying a threshold to logFC in input.
- a, --absolute\_value** <absolute\_value>  
Codify node labels by applying threshold to |logFC| in input. If absolute\_value is set to False, node labels will be signed.
- p, --p\_value** <p\_value>  
Statistical significance (p-value).  
**Default** 0.05
- f, --format\_output** <format\_output>  
Choose CSV or JSON output scores file format.  
**Default** csv

### 8.1.2 kernel

Generate a kernel for a given network.

**param network** Path to the network as a (NetworkX) graph to be transformed to kernel.

**param output** Path (with file name) for the generated scores output file. By default '\$OUT-PUT/diffusion\_scores.csv'

**param log** Logging profiling option.

```
diffupy kernel [OPTIONS]
```

## Options

- g, --graph** <graph>  
    **Required** Input network
- o, --output** <output>  
    Output path to store the generated kernel pickle  
        **Default** /home/docs/.diffupy/output/kernel.json
- l, --log**  
    Activate debug mode





## KERNEL

Compute graph kernels.

`diffupy.kernels.diffusion_kernel`(*graph*: *networkx.classes.graph.Graph*, *sigma2*: *float = 1*, *normalized*:  
*bool = True*) → *diffupy.matrix.Matrix*

Compute 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. :param *graph*: A graph :param *sigma2*: Controls the extent of the spreading. :param *normalized*: Indicates if Laplacian transformation is normalized or not. :return: Laplacian representation of the graph

`diffupy.kernels.compute_time_kernel`(*graph*: *networkx.classes.graph.Graph*, *normalized*: *bool = False*) →  
*diffupy.matrix.Matrix*

Compute 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 commuted 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.

### Parameters

- **graph** – A graph
- **normalized** – Indicates if Laplacian transformation is normalized or not.

**Returns** Laplacian representation of the graph.

`diffupy.kernels.inverse_cosine_kernel`(*graph*: *networkx.classes.graph.Graph*) → *diffupy.matrix.Matrix*

Compute the inverse cosine kernel, which is based on a cosine transform on the spectrum of the normalized LM.

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.

**Parameters** **graph** – A graph

**Returns** Laplacian representation of the graph

`diffupy.kernels.regularised_laplacian_kernel`(*graph*: *networkx.classes.graph.Graph*, *sigma2*: *float = 1*,  
*add\_diag*: *int = 1*, *normalized*: *bool = False*) →  
*diffupy.matrix.Matrix*

Compute 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.

**Parameters**

- **graph** – A graph
- **a** – regularising summed to the spectrum. Spectrum of the normalised Laplacian matrix.
- **p** – p-step kernels can be cheaper to compute and have been successful in biological tasks.

**Returns** Laplacian representation of the graph.

`diffupy.kernels.p_step_kernel` (*graph*: `networkx.classes.graph.Graph`, *a*: `int = 2`, *p*: `int = 5`) → `diffupy.matrix.Matrix`

Compute the inverse cosine kernel, which is based on a cosine transform on the spectrum of the normalized LM.

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].

**Parameters**

- **graph** – A graph
- **a** – regularising summed to the spectrum. Spectrum of the normalised Laplacian matrix.
- **p** – p-step kernels can be cheaper to compute and have been successful in biological tasks.

**Returns** Laplacian representation of the graph.

## DIFFUSION

The methods in this modules manage the treatment of the different score diffusion methods applied to/from a path set of labels/scores of/on a certain network (as a graph format or a graph kernel matrix stemming from a graph).

Diffusion methods procedures provided in this package differ on: (a) How to distinguish positives, negatives and unlabelled examples. (b) Their statistical normalisation.

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

If the path labels are not quantitative, i.e. positive(1), negative(0) and possibly unlabelled, all the scores `raw`, `gm`, `ml`, `z`, `mc`, `ber_s`, `ber_p` can be used.

### 10.1 Methods

The provided methods can be elected for the diffusion computation through the parameter `method`.

```
from diffupy.diffuse import run_diffusion

diffusion_scores = run_diffusion(input_scores, network, method = 'raw')
```

#### 10.1.1 Methods without statistical normalisation

- **raw**: positive nodes introduce unitary flow  $\{y_{\text{raw}}[i] = 1\}$  to the network, whereas either negative and unlabelled nodes introduce null diffusion  $\{y_{\text{raw}}[j] = 0\}$ .<sup>1</sup> They are computed as:  $f_{\text{raw}} = K \cdot y_{\text{raw}}$ . Where  $K$  is a graph kernel, see *kernels*. These scores treat negative and unlabelled nodes equivalently.
- **ml**: Same as `raw`, but negative nodes introduce a negative unit of flow. Therefore not equivalent to unlabelled nodes<sup>2</sup>.
- **gl**: Same as `ml`, but the unlabelled nodes are assigned a (generally non-null) bias term based on the total number of positives, negatives and unlabelled nodes<sup>3</sup>.
- **ber\_s**: 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  $f_{\text{ber_s}}[i] = f_{\text{raw}}[i] / (y_{\text{raw}}[i] + \text{eps})$ . Where `eps` is a parameter controlling the importance of the relative change.

---

<sup>1</sup> Vandin, F., *et al.* (2010). Algorithms for detecting significantly mutated pathways in cancer. Lecture Notes in Computer Science. 6044, 506–521.

<sup>2</sup> Zoidi, O., *et al.* (2015). Graph-based label propagation in digital media: A review. ACM Computing Surveys (CSUR), 47(3), 1-35.

<sup>3</sup> Mostafavi, S., *et al.* (2008). Genemania: a real-time multiple association network integration algorithm for predicting gene function. Genome Biology. (9), S4.

## 10.1.2 Methods with statistical normalisation

- **z**: a parametric alternative to the raw score of node is subtracted its mean value and divided by its standard deviation. Differential trait of this package. The statistical moments have a closed analytical form and are inspired in<sup>4</sup>.
- **mc**: the score of node code {i} is based on its empirical p-value, computed by permuting the path {n.perm} times. It is roughly the proportion of path permutations that led to a diffusion score as high or higher than the original diffusion score.
- **ber\_p**: used in<sup>5</sup>, 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: this is a quantification of the relative change in the node score before and after the network smoothing.

## 10.2 Summary tables

### 10.2.1 Methods without statistical normalization

Scores	y+	y-	yn	Normalized	Stochastic	Quantitative	Reference
raw	1	0	0	No	No.	Yes	?
ml	1	-1	0	No	No	No	<sup>6</sup>
gm	1	-1	k	No	No	No	?
ber_s	1	0	0	No	No	Yes	?

### 10.2.2 Methods with statistical normalization

Scores	y+	y-	yn	Normalized	Stochastic	Quantitative	Reference
ber_p	1	0	0*	Yes	Yes	Yes	?
mc	1	0	0*	Yes	Yes	Yes	?
z	1	0	0*	Yes	No	Yes	?

## 10.3 Method modularity

Through the parameter *method* can also be provided a callable function as a custom method.

```
from diffuPy.diffuse import run_diffusion
from networkx import pagerank

diffusion_scores = run_diffusion(input_scores, network, method = pagerank)
```

<sup>4</sup> Harchaoui, Z., *et al.* (2013). Kernel-based methods for hypothesis testing: a unified view. IEEE Signal Processing Magazine. (30), 87–97.

<sup>5</sup> Bersanelli, M. *et al.* (2016). Network diffusion-based analysis of high-throughput data for the detection of differentially enriched modules. Scientific Reports. (6), 34841.

<sup>6</sup> Tsuda, K., *et al.* (

## 10.4 References



## CONSTANTS

Constants of diffupy.

```
diffupy.constants.DEFAULT_DIFFUPY_DIR = '/home/docs/.diffupy'  
    Default DiffuPy directory
```

```
diffupy.constants.OUTPUT = '/home/docs/.diffupy/output'  
    Default DiffuPy output directory
```

```
diffupy.constants.ensure_output_dirs()  
    Ensure that the output directories exists.
```

```
diffupy.constants.EMOJI = ''  
    Available diffusion methods
```

```
diffupy.constants.RAW = 'raw'  
    raw
```

```
diffupy.constants.ML = 'ml'  
    ml
```

```
diffupy.constants.GM = 'gm'  
    gm
```

```
diffupy.constants.MC = 'mc'  
    mc
```

```
diffupy.constants.Z = 'z'  
    z
```

```
diffupy.constants.BER_S = 'ber_s'  
    ber_s
```

```
diffupy.constants.BER_P = 'ber_p'  
    ber p
```

```
diffupy.constants.METHODS = {'ber_p', 'ber_s', 'gm', 'mc', 'ml', 'raw', 'z'}  
    Available formats
```

```
diffupy.constants.CSV = 'csv'  
    csv
```

```
diffupy.constants.XLS = 'xls'  
    xml
```

```
diffupy.constants.XLSX = 'xlsx'  
    xmls
```

```
diffupy.constants.TSV = 'tsv'  
    tsv
```

`diffupy.constants.GRAPHML = 'graphml'`  
graphML

`diffupy.constants.BEL = 'bel'`  
bel

`diffupy.constants.JSON = 'json'`  
node link json

`diffupy.constants.PICKLE = 'pickle'`  
pickle

`diffupy.constants.GML = 'gml'`  
gml

`diffupy.constants.EDGE_LIST = '.lst'`  
edge list

`diffupy.constants.GRAPH_FORMATS = ('csv', 'tsv', 'graphml', 'bel', 'json', 'pickle', 'gml')`  
Available graph formats

`diffupy.constants.KERNEL_FORMATS = ('csv', 'tsv', 'json', 'pickle')`  
Available kernel formats

`diffupy.constants.FORMAT_SEPARATOR_MAPPING = {'csv': ',', 'tsv': '\t'}`  
Optional parameters

`diffupy.constants.THRESHOLD = 'threshold'`  
Expression value threshold

`diffupy.constants.ABSOLUTE_VALUE_EXP = 'absolute_value'`  
Acceptable column names of user submitted network

`diffupy.constants.SOURCE = 'Source'`  
Column name for source node

`diffupy.constants.TARGET = 'Target'`  
Column name for target node

`diffupy.constants.RELATION = 'Relation '`  
Dataset column names

`diffupy.constants.NODE = 'Node'`  
Node name

`diffupy.constants.NODE_TYPE = 'NodeType'`  
Node type

`diffupy.constants.SCORE = 'Score'`  
Unspecified score type

`diffupy.constants.LOG_FC = 'LogFC'`  
Log2 fold change (logFC)

`diffupy.constants.P_VALUE = 'p-value'`  
Statistical significance (p-value)



## MATRIX

Matrix class

Main Matrix Class.

```
class diffupy.matrix.Matrix(mat=None, rows_labels=None, cols_labels=None, graph=None,  
                             quadratic=False, name="", init_value=None)
```

Matrix class.

Initialize matrix.

### Parameters

- **mat** – matrix initialization
- **rows\_labels** –
- **cols\_labels** – column labels
- **graph** – graph
- **quadratic** – quadratic
- **name** – name
- **init\_value** – value to be initialized (int) or list of values from labels

**validate\_labels()**

Sanity function to check the dimensionality of the Matrix.

**update\_ix\_mappings()**

Update the index-label mapping.

**validate\_labels\_and\_update\_ix\_mappings()**

Update function, called when the Matrix mutates, combining the two previous functionalities.

**property cols\_labels**

Return a copy of Matrix Object.

**property rows\_labels\_ix\_mapping**

Set row labels to ix.

**property cols\_labels\_ix\_mapping**

Set column labels to ix.

**property rows\_idx\_scores\_mapping**

Set mapping indexes to scores.

**property cols\_idx\_scores\_mapping**

Set mapping indexes to scores.

**get\_row\_from\_label**(*label*)  
Get row from labels.

**set\_row\_from\_label**(*label*, *x*)  
Set row from label.

**delete\_row\_from\_label**(*label*)  
Set row from label.

**get\_col\_from\_label**(*label*)  
Get col from labels.

**delete\_col\_from\_label**(*label*)  
Set col from label.

**set\_cell\_from\_labels**(*row\_label*, *col\_label*, *x*)  
Set cell from labels.

**get\_cell\_from\_labels**(*row\_label*, *col\_label*)  
Get cell from labels.

**row\_bind**(*rows=None*, *rows\_labels=None*, *matrix=None*)  
Return a copy of Matrix Object.

**col\_bind**(*cols=None*, *cols\_labels=None*, *matrix=None*)  
Return a copy of Matrix Object.

**match\_rows**(*reference\_matrix*)  
Match method to set rows labels as reference matrix.

**match\_cols**(*reference\_matrix*)  
Match method to set cols labels as reference matrix.

**match\_mat**(*reference\_matrix*, *match\_quadratic=None*)  
Match method to set axis labels as reference matrix.

**match\_missing\_rows**(*reference\_labels*, *missing\_fill=0*)  
Match method to set missing rows labels from reference labels with the *missing\_fill* value.

**match\_delete\_rows**(*reference\_labels*)  
Match method to set missing rows labels from reference labels with the *missing\_fill* value.

**match\_missing\_cols**(*reference\_labels*, *missing\_fill*)  
Match method to set missing cols labels from reference labels with the *missing\_fill* value.

**order\_rows**(*reverse=True*, *col\_ref\_idx=None*)  
Order matrix rows by cell values.

**len\_not\_null**()  
Get count of n cells not 0 in matrix.

**binarize**(*null\_value=-1*, *threshold=0*, *positive\_value=1*)  
Get count of n cells not 0 in matrix.

**to\_dict**(*ordered=True*)  
Export/convert matrix as a dictionary data structure.

**as\_pd\_dataframe**(*ordered=True*)  
Export matrix as a data frame using the headers (*row\_labels*, *cols\_labels*) of the Matrix class.

**as\_csv**(*path*, *index=True*, *ordered=True*)  
Export matrix to csv file using the headers (*row\_labels*, *cols\_labels*) of the Matrix class.

**to\_nx\_graph()**

Export matrix as a Graph using the headers (row\_labels, cols\_labels) of the Matrix class.

**class** diffupy.matrix.**LaplacianMatrix**(*graph*, *normalized=False*, *node\_argument='name'*, *name=''*)

Laplacian matrix class.

Initialize laplacian.



---

CHAPTER  
**THIRTEEN**

---

**REFERENCES**



**DISCLAIMER**

DiffuPy is a scientific software that has been developed in an academic capacity, and thus comes with no warranty or guarantee of maintenance, support, or back-up of data.





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