# data_tools Documentation

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# CONTENTS

Data tools: a collection of Python functions and classes designed to make data scientists' life easier.



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CHAPTER

# ONE

# DISCLAIMER

This package is still under development and will be periodically updated with new features. Contributions are very welcome (fork + pull request). If you find any bug or suggestion for upgrades, please use the issue system.

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CHAPTER

TWO

# DEPENDENCIES

- NumPy
- Matplotlib
- Pandas
- SciPy
- Scikit-learn

CHAPTER

THREE

# INSTALLATION

First download/clone `data_tools` from the GitHub repository. From the terminal:

```
git clone https://github.com/Nic-Nic/data_tools.git
cd data_tools
```

Then you can install it by running `setup.py` as follows:

```
python setup.py sdist
```

Or using `pip`:

```
pip install .
```

Along with `data_tools`, all dependencies will be installed as well as the testing suite. In order to run the tests, type on the terminal:

```
python -m test_data_tools
```

**NOTE:** `data_tools.plots` module does not have any tests implemented.

CHAPTER

# FOUR

# MODULES

## 4.1 data_tools.databases

Databases functions module.

data_tools.databases.**kegg_link**(*query*, *target='pathway'*)

Queries a request to the KEGG database to find related entries using cross-references. A list of available database(s) and query examples can be found in https://www.kegg.jp/kegg/rest/keggapi.html#link.

- **Arguments:**
  - *query* [list]: Or any iterable type containing the identifier(s) to be queried as [str]. These can be either valid database identifiers or databases *per se* (see the link above).
  - *target* [str]: Optional, `'pathway'` by default. Targeted database to which the query should be linked to. You can check other options available in the URL above.
- **Returns:**
  - [pandas.DataFrame]: Two-column table containing both the input query identifiers and their linked ones.
- **Example:**

```
>>> my_query = ['hsa:10458', 'ece:Z5100']
>>> kegg_link(my_query)
   query        pathway
0  hsa:10458  path:hsa04520
1  hsa:10458  path:hsa04810
2  ece:Z5100  path:ece05130
```

data_tools.databases.**kegg_pathway_mapping**(*df*, *mapid*, *filename=None*)

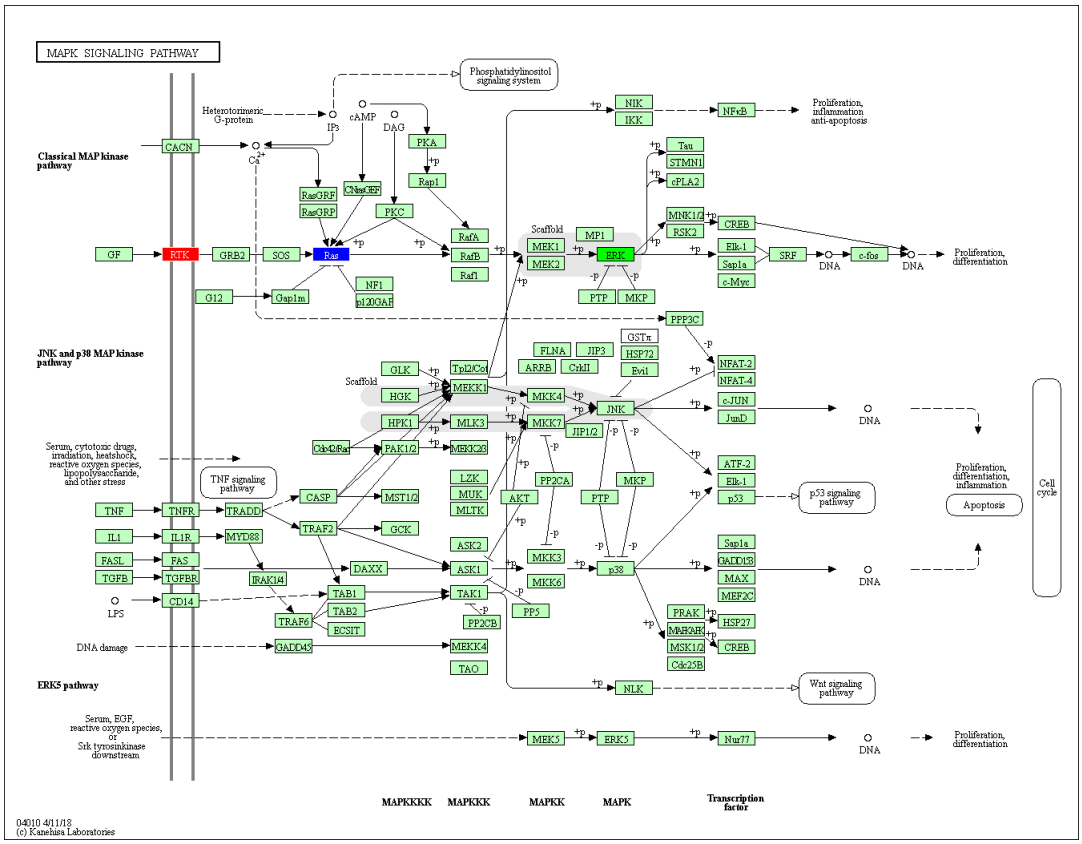
Makes a request to KEGG pathway mapping tool according to a given pathway ID (see https://www.kegg.jp/kegg/tool/map_pathway2.html for more information). The user must provide a query of IDs to be mapped with their corresponding background colors (and optionally also foreground colors). The result is downloaded in the current directory or a user-specified path.

- **Arguments:**
  - *df* [pandas.DataFrame]: Dataframe containing KEGG valid IDs in the first column and corresponding background colors (e.g.: red, blue, ...). Optionally, a third column with the foreground (font) colors can also be provided (black by default). **NOTE:** hexadecimal codes for colors is also supported. Index and column names of dataframe are ignored.
  - *mapid* [str]: A valid KEGG pathway ID. It can be a general (e.g.: "mapXXXXX") or organism-specific ID (e.g.: "hsaXXXXX").

  - *filename* [str]: Optional, `None` by default. This is, the image will be stored in the current directory with the *mapid* provided as file name. If provided, the image will be stored within the specified path/file name.

- **Example:**

```
>>> my_query = pandas.DataFrame([['1956', 'red', '#f1f1f1'],
...                              ['3845', 'blue', '#f1f1f1'],
...                              ['5594', 'green', 'black']])
>>> kegg_pathway_mapping(my_query, 'hsa04010')
```




`data_tools.databases.`**`op_kinase_substrate`**(*organism='9606'*)

`data_tools.databases.`**`up_map`**(*query*, *source='ACC'*, *target='GENENAME'*)

Queries a request to UniProt.org in order to map a given list of identifiers. You can check the options available of input/output identifiers at https://www.uniprot.org/help/api_idmapping.

- **Arguments:**

  - *query* [list]: Or any iterable type containing the identifiers to be queried as [str].

  - *source* [str]: Optional, `'ACC'` by default. This is, UniProt accesion number. You can check other options available in the URL above.

  - *target* [str]: Optional, `'GENENAME'` by default. You can check other options available in the URL above.

- **Returns:**

  - [pandas.DataFrame]: Two-column table containing both the inputed identifiers and the mapping result of these.

- **Examples:**

```
>>> my_query = ['P00533', 'P31749', 'P16220']
>>> up_map(my_query)
      ACC GENENAME
0  P00533     EGFR
1  P31749     AKT1
2  P16220    CREB1
>>> up_map(my_query, target='KEGG_ID')
      ACC   KEGG_ID
0  P00533  hsa:1956
2  P16220  hsa:1385
1  P31749   hsa:207
```

## 4.2 data_tools.diffusion

Diffusion solvers module.

`data_tools.diffusion.`**`euler_explicit1D`**(*x0*, *dt*, *dx2*, *d=1*, *bcs='periodic'*)

Computes diffusion on a 1D space over a time-step using Euler explicit method.

- **Arguments:**
  - *x0* [numpy.ndarray]: Initial state of a 1D array from which the difusion is to be computed.
  - *dt* [float]: Discretization time-step.
  - *dx2* [float]: Discretization spatial-step (squared).
  - *d* [float]: Diffusion coefficient.
  - *bcs* [str]: Optional, `'periodic'` by default. Determines the boundary conditions. Available options are `'periodic'`, `'dirichlet''` or `'neumann'`.
- **Returns:**
  - [numpy.ndarray]: Computed state array (1D) after one time-step according to the parameters and conditions selected.

## 4.3 data_tools.models

Model classes module.

**`class`** `data_tools.models.`**`DoseResponse`**(*d_data*, *r_data*, *x0=[1, 1, 1]*, *x_scale=[1, 1, 1]*, *bounds=([0, 0, -inf], [inf, inf, inf])*)

Wrapper class for `scipy.optimize.least_squares` to fit dose-response curves on a pre-defined Hill function with the following form:

$$R = \frac{mD^n}{k^n + D^n}$$

Where $D$ is the dose, $k$, $m$ and $n$ are the parameters to be fitted.

- **Arguments:**
  - *d_data* [numpy.ndarray]: Or any iterable (1D). Contains the training data corresponding to the dose.

- *r_data* [numpy.ndarray]: Or any iterable (1D). Contains the training data corresponding to the response.
- *x0* [list]: Optional, `[1, 1, 1]` by default. Or any iterable of three elements. Contains the initial guess for the parameters. Parameters are considered to be in alphabetical order. This is, first element corresponds to $k$, second is $m$ and last is $n$.
- *x_scale* [list]: Optional, `[1, 1, 1]` by default. Or any iterable of three elements. Scale of each parameter. May improve the fitting if the scaled parameters have similar effect on the cost function.
- *bounds* [tuple]: Optional `([0, 0, -inf], [inf, inf, inf])` by default. Two-element tuple containing the lower and upper boundaries for the parameters (elements of the tuple are iterables of three elements each).

- **Attributes:**
  - *model* [scipy.optimize.OptimizeResult]: Contains the result of the optimized model. See SciPy's reference for more information.
  - *params* [numpy.ndarray]: Three-element array containing the fitted parameters $k$, $m$ and $n$.

**ec**(*p=50*)

Computes the effective concentration for the specified percentage of maximal concentration ($EC_p$).

- **Arguments:**
  - *p* [int]: Optional, `50` by default ($EC_{50}$). Defines the percentage of the maximal from which the effective concentration is to be computed.
- **Returns**
  - [float]: Value of the $EC_p$ computed according to the model parameters.

**plot**(*title=None*, *filename=None*, *figsize=None*, *legend=True*)

Plots the data points and the fitted function together.

- **Arguments:**
  - *title* [str]: Optional, `None` by default. Defines the plot title.
  - *filename* [str]: Optional, `None` by default. If passed, indicates the file name or path where to store the figure. Format must be specified (e.g.: .png, .pdf, etc)
  - *figsize* [tuple]: Optional, `None` by default (default matplotlib size). Any iterable containing two values denoting the figure size (in inches) as [width, height].
  - *legend* [bool]: Optional, `True` by default. Indicates whether to show the plot legend or not.
- **Returns:**
  - [matplotlib.figure.Figure]: Figure object showing the data points and the fitted model function.

**class** data_tools.models.**Lasso**(*Cs=500*, *cv=10*, *sampler='skf'*, *solver='liblinear'*, ***kwargs*)

Wrapper class inheriting from `sklearn.linear_model.LogisticRegressionCV` with L1 regularization.

- **Arguments:**
  - *Cs* [int]: Optional, `500` by default. Integer or list of float values of regularization parameters to test. If an integer is passed, it will determine the number of values taken from a logarithmic scale between `1e-4` and `1e4`. Note that the value of the parameter is defined as the inverse of the regularization strength.

- *cv* [int]: Optional, `10` by default. Denotes the number of cross validation (CV) folds.
- *sampler* [str]: Optional, `'skf'` by default. Determines which sampling method is used to generate the test and training sets for CV. Methods available are K-Fold (`'kf'`), Shuffle Split (`'ss'`) and their stratified variants (`'skf'` and `'sss'` respectively).
- *solver* [str]: Optional, `'liblinear'` by default. Determines which solver algorithm to use. Note that L1 regularization can only be handled by `'liblinear'` and `'saga'`. Additionally if the classification is multinomial, only the latter option is available.
- ***kwargs*: Optional. Any other keyword argument accepted by the `sklearn.linear_model.LogisticRegressionCV` class.

Other keyword arguments and functions available from the parent class `LogisticRegressionCV` can be fount in Scikit-Learn's reference.

**`fit_data`** (*x*, *y*, *silent=False*)

Fits the data to the logistic model.

- **Arguments:**
  - *x* [pandas.DataFrame]: Contains the values/measurements [float] of the features (columns) for each sample/replicate (rows).
  - *y* [pandas.Series]: List or any iterable containing the observed class of each sample (must have the same order as in *x*).
  - *silent* [bool]: Optional, `False` by default. Determines whether messages are printed or not.

**`plot_coef`** (*filename=None*, *figsize=None*)

Plots the non-zero coefficients for the fitted predictor features.

- **Arguments:**
  - *filename* [str]: Optional, `None` by default. If passed, indicates the file name or path where to store the figure. Format must be specified (e.g.: .png, .pdf, etc)
  - *figsize* [tuple]: Optional, `None` by default (default matplotlib size). Any iterable containing two values denoting the figure size (in inches) as [width, height].
- **Returns:**
  - [matplotlib.figure.Figure]: Figure object containing the bar plot of the non-zero coefficients.

**`plot_score`** (*filename=None*, *figsize=None*)

Plots the mean score across all folds obtained during CV. The optimum C parameter chosen and its score are highlighted.

- **Arguments:**
  - *filename* [str]: Optional, `None` by default. If passed, indicates the file name or path where to store the figure. Format must be specified (e.g.: .png, .pdf, etc)
  - *figsize* [tuple]: Optional, `None` by default (default matplotlib size). Any iterable containing two values denoting the figure size (in inches) as [width, height].
- **Returns:**
  - [matplotlib.figure.Figure]: Figure object containing the score plot.

## 4.4 data_tools.plots

Plotting functions module.

data_tools.plots.**density**(*df*, *cvf=0.25*, *title=None*, *filename=None*, *figsize=None*)

Generates a density plot of the values on a data frame (row-wise).

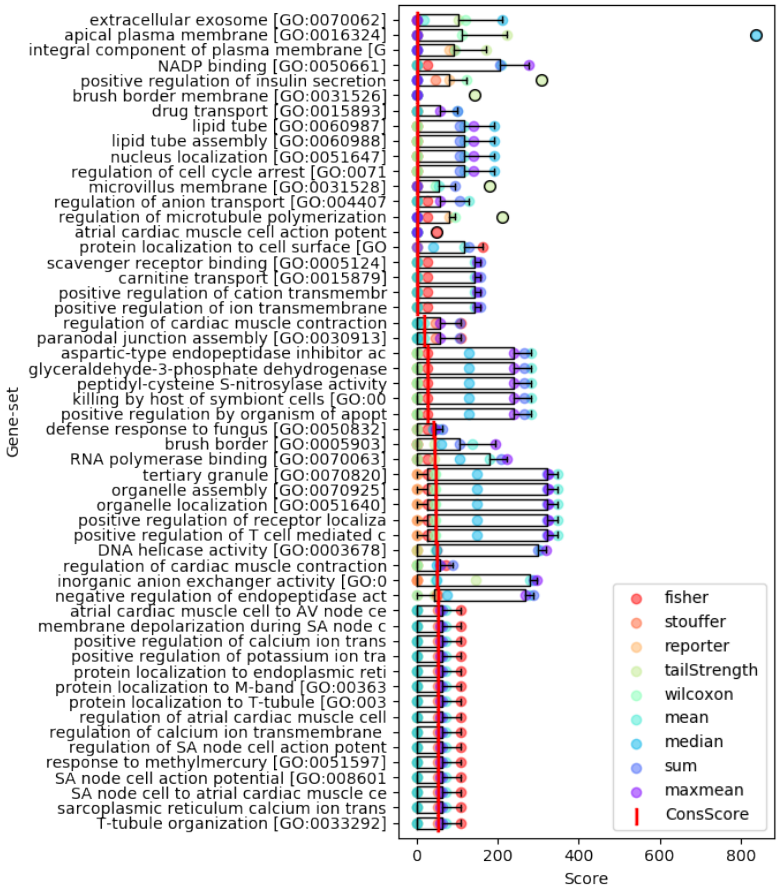
- **Arguments:**
  - *df* [pandas.DataFrame]: Contains the values to generate the plot. Each row is considered as an individual sample while each column contains a measured value.
  - *cvf* [float]: Optional, `0.25` by default. Co-variance factor used in the gaussian kernel estimation. A higher value increases the smoothness.
  - *title* [str]: Optional, `None` by default. Defines the plot title.
  - *filename* [str]: Optional, `None` by default. If passed, indicates the file name or path where to store the figure. Format must be specified (e.g.: .png, .pdf, etc)
  - *figsize* [tuple]: Optional, `None` by default (default matplotlib size). Any iterable containing two values denoting the figure size (in inches) as [width, height].
- **Returns:**
  - [*matplotlib.figure.Figure*]: the figure object containing the density plot.

data_tools.plots.**piano_consensus**(*df*, *nchar=40*, *boxes=True*, *title=None*, *filename=None*, *figsize=None*)

Generates a GSEA consensus score plot like R package `piano`'s `consensusScores` function, but prettier. The main input is assumed to be a `pandas.DataFrame` whose data is the same as the `rankMat` from the result of `consensusScores`.

- **Arguments:**
  - *df* [pandas.DataFrame]: Values contained correspond to the scores of the gene-sets (consensus and each individual methods). Index must contain the gene-set labels. Columns are assumed to be `ConsRank` (ignored), `ConsScore` followed by the individual methods (e.g.: `mean`, `median`, `sum`, etc).
  - *nchar* [int]: Optional, `40` by default. Number of string characters of the gene-set labels of the plot.
  - *boxes* [bool]: Optional, `True` by default. Determines whether to show the boxplots of the gene-sets or not.
  - *title* [str]: Optional, `None` by default. Defines the plot title.
  - *filename* [str]: Optional, `None` by default. If passed, indicates the file name or path where to store the figure. Format must be specified (e.g.: .png, .pdf, etc)
  - *figsize* [tuple]: Optional, `None` by default (default matplotlib size). Any iterable containing two values denoting the figure size (in inches) as [width, height].
- **Returns:**
  - [*matplotlib.figure.Figure*]: the figure object containing a combination of box and scatter plots of the gene-set scores.
- **Example:**

```
>>> piano_consensus(df, figsize=[7, 8])
```




`data_tools.plots.`**`venn`**(*N, labels=['A', 'B', 'C', 'D', 'E'], c=['C0', 'C1', 'C2', 'C3', 'C4'], title=None, filename=None, figsize=None*)

Plots a Venn diagram from a list of sets *N*. Number of sets must be between 2 and 5 (inclusive).

- **Arguments:**
  - *N* [list]: Or any iterable type containing [set] objects.
  - *labels* [list]: Optional, `['A', 'B', 'C', 'D', 'E']` by default. Labels for the sets following the same order as provided in *N*.
  - *c* [list]: Optional, `['C0', 'C1' 'C2', 'C3', 'C4']` by default (matplotlib default colors). Any iterable containing color arguments tolerated by matplotlib (e.g.: `['r', 'b']` for red and blue). Must contain at least the same number of elements as *N* (if more are provided, they will be ignored).
  - *title* [str]: Optional, `None` by default. Defines the plot title.
  - *filename* [str]: Optional, `None` by default. If passed, indicates the file name or path where to store the figure. Format must be specified (e.g.: .png, .pdf, etc)
  - *figsize* [tuple]: Optional, `None` by default (default matplotlib size). Any iterable containing two values denoting the figure size (in inches) as [width, height].
- **Returns:**
  - [*matplotlib.figure.Figure*]: the figure object containing a combination of box and scatter plots of the gene-set scores.

- **Example:**

```
>>> N = [{0, 1}, {2, 3}, {1, 3, 4}] # Sets A, B, C
>>> venn(N)
```

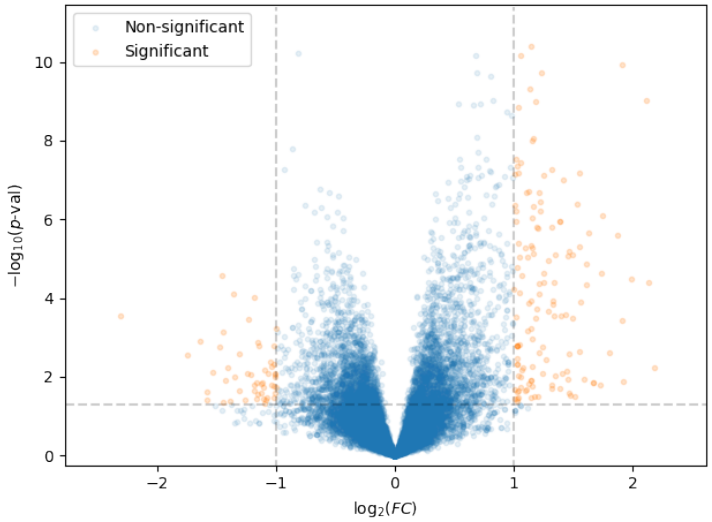

data_tools.plots.**volcano**(*logfc*, *logpval*, *thr_pval=0.05*, *thr_fc=2.0*, *c=('C0', 'C1')*, *legend=True*, *title=None*, *filename=None*, *figsize=None*)

Generates a volcano plot from the differential expression data provided.

- **Arguments:**
  - *logfc* [list]: Or any iterable type. Contains the log (usually base 2) fold-change values. Must have the same length as *logpval*.
  - *logpval* [list]: Or any iterable type. Contains the -log p-values (usually base 10). Must have the same length as *logfc*.
  - *thr_pval* [float]: Optional, `0.05` by default. Specifies the p-value (non log-transformed) threshold to consider a measurement as significantly differentially expressed.
  - *thr_fc* [float]: Optional, `2.` by default. Specifies the FC (non log-transformed) threshold to consider a measurement as significantly differentially expressed.
  - *c* [tuple]: Optional, `('C0', 'C1')` by default (matplotlib default colors). Any iterable containing two color arguments tolerated by matplotlib (e.g.: `['r', 'b']` for red and blue). First one is used for non-significant points, second for the significant ones.
  - *legend* [bool]: Optional, `True` by default. Indicates whether to show the plot legend or not.
  - *title* [str]: Optional, `None` by default. Defines the plot title.
  - *filename* [str]: Optional, `None` by default. If passed, indicates the file name or path where to store the figure. Format must be specified (e.g.: .png, .pdf, etc)
  - *figsize* [tuple]: Optional, `None` by default (default matplotlib size). Any iterable containing two values denoting the figure size (in inches) as [width, height].

- **Returns:**
  - [matplotlib.figure.Figure]: Figure object containing the volcano plot.
- **Example:**

```
>>> volcano(my_log_fc, my_log_pval)
```




## 4.5 data_tools.sets

Set operations module.

data_tools.sets.**bit_or**(*a*, *b*)

Returns the bit operation OR between two bit-strings *a* and *b*. **NOTE:** *a* and *b* must have the same size.

- **Arguments:**
  - *a* [tuple]: Or any iterable type.
  - *b* [tuple]: Or any iterable type.
- **Returns:**
  - [tuple]: OR operation between *a* and *b* element-wise.
- **Examples:**

```
>>> a, b = (0, 0, 1), (1, 0, 1)
>>> bit_or(a, b)
(1, 0, 1)
```

data_tools.sets.**chunk_this**(*L*, *n*)

For a given list *L*, returns another list of *n*-sized chunks from it (in the same order).

- **Arguments:**
  - *L* [list]: The list to be sliced into sublists of the definded size.
  - *n* [int]: The size of the chunks.
- **Returns:**

  - [list]: List of *n*-sized chunks from *L*. **NOTE:** If the number of items in *L* is not divisible by *n*, the last element returned will have an inferior size.

- **Examples:**

```
>>> L = range(6)
>>> chunk_this(L, 2)
[[0, 1], [2, 3], [4, 5]]
>>> chunk_this(L, 4)
[[0, 1, 2, 3], [4, 5]]
```

data_tools.sets.**find_min**(*A*)

Finds and returns the subset of vectors whose sum is minimum from a given set *A*.

- **Arguments:**

  - *A* [set]: Set of vectors ([tuple] or any iterable).

- **Returns:**

  - [set]: Subset of vectors in *A* whose sum is minimum.

- **Examples:**

```
>>> A = {(0, 1, 1), (0, 1, 0), (1, 0, 0), (1, 1, 1)}
>>> find_min(A)
set([(0, 1, 0), (1, 0, 0)])
```

data_tools.sets.**in_all**(*x*, *N*)

Checks if a vector *x* is present in all sets contained in a list *N*.

- **Arguments:**

  - *x* [tuple]: Or any hashable type as long as is the same contained in the sets of *N*.

  - *N* [list]: Or any iterable type containing [set] objects.

- **Returns:**

  - [bool]: `True` if *x* is found in all sets of *N*, `False` otherwise.

- **Examples:**

```
>>> N = [{(0, 0), (0, 1)}, # <- set A
...      {(0, 0), (1, 1), (1, 0)}] # <- set B
>>> x = (0, 0)
>>> in_all(x, N)
True
>>> y = (0, 1)
>>> in_all(y, N)
False
```

data_tools.sets.**subsets**(*N*)

Function that computes all possible logical relations between all sets on a list *N* and returns all subsets. This is, the subsets that would represent each intersecting area on a Venn diagram.

- **Arguments:**

  - *N* [list]: Or any iterable type containing [set] objects.

- **Returns:**

  - [dict]: Collection of subsets according to the logical relations between the sets in *N*. The keys are binary codes that denote the logical relation (see examples below).

- **Examples:**

```
>>> N = [{0, 1, 2}, {2, 3, 4}]
>>> subsets(N)
{'11': set([2]), '10': set([0, 1]), '01': set([3, 4])}
>>> N = [{0, 1}, {2, 3}, {1, 3, 4}]
>>> subsets(N)
{'010': set([2]), '011': set([3]), '001': set([4]), '111': set([
]), '110': set([]), '100': set([0]), '101': set([1])}
```

## 4.6 data_tools.strings

String operations module.

data_tools.strings.**is_numeric**(*s*)

Determines if a string can be considered a numeric value. NaN is also considered, since it is float type.

- **Arguments:**
  - *s* [str]: String to be evaluated.
- **Returns:**
  - [bool]: `True`/`False` depending if the condition is satisfied.
- **Examples:**

```
>>> is_numeric('4')
True
>>> is_numeric('-3.2')
True
>>> is_numeric('number')
False
>>> is_numeric('NaN')
True
```

data_tools.strings.**join_str_lists**(*a*, *b*, *sep=''*)

Joins element-wise two lists (or any 1D iterable) of strings with a given separator (if provided). Length of the input lists must be equal.

- **Arguments:**
  - *a* [list]: Contains the first elements [str] of the joint strings.
  - *b* [list]: Contains the second elements [str] of the joint strings.
  - *sep* [str]: Optional `''` (non separated) by default. Determines the separator between the joint strings.
- **Returns:**
  - [list]: List of the joint strings.
- **Example:**

```
>>> a = ['a', 'b']
>>> b = ['1', '2']
>>> join_str_lists(a, b, sep='_')
['a_1', 'b_2']
```

# PYTHON MODULE INDEX

## d

# INDEX