
data_tools Documentation

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

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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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DEPENDENCIES

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

INSTALLATION

First download/clone `data_tools` from the [GitHub repository](https://github.com/Nic-Nic/data_tools). 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.

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', incl_phosphatases=False)`
 Queries OmniPath to retrieve the kinase-substrate interactions for a given organism.

- **Arguments:**

- *organism* [str]: Optional, '9606' by default (Homo sapiens). NCBI taxonomic identifier for the organism of interest.
- *incl_phosphatases* [bool]: Optional `False` by default. Determines whether to include dephosphorylation interactions or not.

- **Returns:**

- [pandas.DataFrame]: Table containing the enzyme-substrate (kinase/phosphatase-target) network of each phospho-site.

`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 accession 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. **NOTE:** The returned table may not have the same order as in *query*. Also, if some ID could not be mapped, the size of the returned table will differ from the length of *query*.

- **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 diffusion 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'. Note that Dirichlet BCs do not hold mass conservation.

- **Returns:**

- [numpy.ndarray]: Computed state array (1D) after one time-step according to the parameters and conditions selected.

`data_tools.diffusion.euler_explicit2D(x0, dt, dx2, d=1, bcs='periodic')`

Computes diffusion on a 2D space over a time-step using Euler explicit method.

- **Arguments:**

- *x0* [numpy.ndarray]: Initial state of a 2D array from which the diffusion is to be computed.
- *dt* [float]: Discretization time-step.

- `dx2` [float]: Discretization spatial-step (squared). It is assumed that is the same in both dimensions ($dx = dy$).
- `d` [float]: Diffusion coefficient.
- `bcs` [str]: Optional, 'periodic' by default. Determines the boundary conditions. Available options are 'periodic', 'dirichlet' or 'neumann'. Note that Dirichlet BCs do not hold mass conservation.

- **Returns:**

- [numpy.ndarray]: Computed state array (2D) after one time-step according to the parameters and conditions selected.

4.3 data_tools.iterables

Iterable-type operations module.

`data_tools.iterables.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.iterables.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 defined 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.iterables.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.iterables.in_all(x, N)`

Checks if a element `x` is present in all collections contained in a list `N`.

- **Arguments:**
 - `x [object]`: Any type of object, it is assumed to be the same type as the objects contained in the elements of `N`.
 - `N [list]`: Or any iterable type containing a collection of other iterables containing the objects.
- **Returns:**
 - `[bool]`: True if `x` is found in all elements 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
>>> N = [['Hello', 'world', '!'],
...      ['Hello', 'user']]
>>> x = 'Hello'
>>> in_all(x, N)
True
```

`data_tools.iterables.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}]
```

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

`data_tools.iterables.unzip_dicts(*dicts)`

Unzips the keys and values for any number of dictionaries passed as arguments (see below for examples).

- **Arguments:**

- **dicts* [dict]: Dictionaries from which key/value pairs are to be unzipped.

- **Returns:**

- [list]: Two-element list containing all keys and all values respectively from the dictionaries in **dicts*.

- **Example:**

```
>>> a = dict([('x_a', 2), ('y_a', 3)])
>>> b = dict([('x_b', 1), ('y_b', -1)])
>>> unzip(a, b)
[('y_a', 'x_a', 'x_b', 'y_b'), (3, 2, 1, -1)]
```

4.4 data_tools.models

Model classes module.

class `data_tools.models.DoseResponse` (*d_data, r_data, x0=None, x_scale=None, 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, `None` 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 . If `None` (default), the initial guess is inferred from *r_data*.
- *x_scale* [list]: Optional, `None` 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. If `None` (default), the scale is inferred from *x0*.
- *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:**

- `x0` [list]: 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]: Scale of each parameter.
- `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 found 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.

4.5 data_tools.plots

Plotting functions module.

`data_tools.plots.density` (*df*, *cvf=0.25*, *sample_col=False*, *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 unless otherwise stated by keyword argument *sample_col*.

- *cvf* [float]: Optional, 0.25 by default. Co-variance factor used in the gaussian kernel estimation. A higher value increases the smoothness.
- *sample_col* [bool]: Optional, False by default. Specifies whether the samples are column-wise 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 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:**

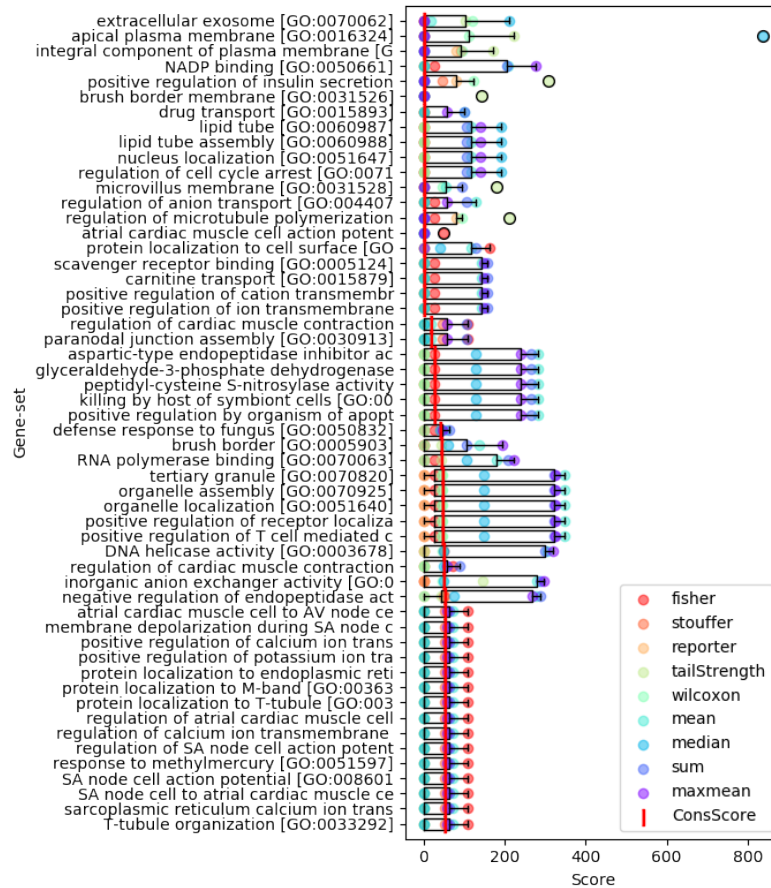
- *df* [`pandas.DataFrame`]: Values contained correspond to the scores of the gene-sets (consensus and each individual methods). Index must contain the gene-set labels. Columns are assumed to be `ConsRank` (ignored), `ConsScore` followed by the individual methods (e.g.: `mean`, `median`, `sum`, etc).
- *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'], pct=False, 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).
- *pct* [bool]: Optional, False by default. Indicates whether to show percentages instead of absolute counts.
- *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)

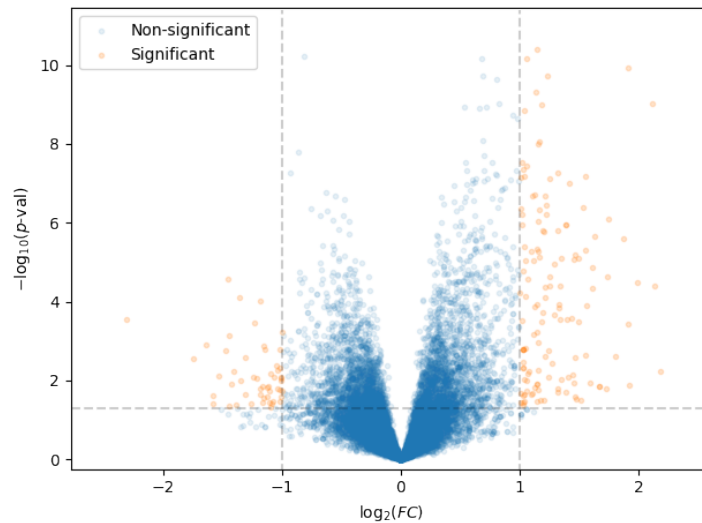
- *figsize* [tuple]: Optional, `None` by default (default matplotlib size). Any iterable containing two values denoting the figure size (in inches) as [width, height].

- **Returns:**

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

- **Example:**

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



4.6 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']
```


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