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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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
- UpSetPlot
- adjustText
- certifi

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.

MODULE REFERENCE

4.1 data_tools.databases

Databases functions module.

4.1.1 Contents

`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'*,   *gsymbols=False*, *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.

- *gsymbols* [bool]: Optional, `False` by default. Whether to show the identifiers as gene symbols or not (UniProt AC otherwise).

- *incl_phosphatases* [bool]: Optional `False` by default. Determines wether 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 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. **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.

4.2.1 Introduction

The following functions provide tools to solve the diffusion problem for any number of spatial dimensions with different explicit and implicit methods. The problem is defined as follows:

$$\frac{\partial u}{\partial t} = D\nabla^2 u$$

Where u is the diffusing component, D is the diffusion coefficient and ∇^2 is the Laplace operator (in Euclidean space $\nabla^2 f = \nabla \cdot \nabla f = \sum_{i=1}^{n} \frac{\partial^2 f}{\partial x_i^2}$).

Some numerical methods to solve this probelm will be explained in the following subsections. These are based in approximation of the derivatives by finite-differences. Therefore we define the discretization step sizes as Δt for the time derivative and Δx, Δy and so on for first, second and subsequent spatial dimensions respectively.

From here on we will assume that space is homogeneously discretized (e.g.: $\Delta x = \Delta y$). All second-order partial derivatives in the spatial dimension are discretized using central finite differences. For instance, in one dimension:

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2}$$

4.2.1.1 Euler explicit method

"Classic" method, first-order accurate, uses forward difference over time:

$$\frac{\partial u}{\partial t} \approx \frac{u^{k+1} - u^k}{\Delta t}$$

Where k is the current time-step. Applied to the diffusion problem for one dimension and rearranging terms:

$$u_i^{k+1} = \frac{D\Delta t}{\Delta x^2} \left(u_{i+1}^k + u_{i-1}^k \right) + \left(1 - 2\frac{D\Delta t}{\Delta x^2} \right) u_i^k$$

Let us define from here on $\lambda \equiv \frac{D\Delta t}{\Delta x^2}$ for simplicity. Rewriting the equation above in terms of linear algebra, each time-step the next state of u is:

$$u^{k+1} = \mathbf{A} u^k$$

Where $\mathbf{A}$ is the tri-diagonal coefficient matrix whose central element is $(1 - 2\lambda)$ and its adjacent diagonals are λ. Note that for n-dimensional case, central element will then be $(1 - 2n\lambda)$ and u must be flattened (coerced into one dimension) and $\mathbf{A}$ becomes a block tri-diagonal matrix.

NOTE: Explicit methods are conditionally stable. This means that in order to keep numerical stability of the solution (and obtain an accurate result), these methods need to fulfill the Courant–Friedrichs–Lewy (CFL) condition. For any n-dimensional case:

$$D\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2n}$$

The implicit methods are (theoretically) unconditionally stable, hence are more permissive in terms of discretization step-size.

4.2.1.2 Euler implicit method

Similar to Euler explicit (first-order accurate) but uses backward difference over time (theoretically, unconditionally stable):

$$\frac{\partial u}{\partial t} \approx \frac{u^k - u^{k-1}}{\Delta t}$$

Applied to the diffusion problem in one dimension and taking one step forward over discrete time ($k \rightarrow k+1$):

$$u_i^k = -\lambda \left(u_{i+1}^{k+1} + u_{i-1}^{k+1} \right) + (1 + 2\lambda) u_i^{k+1}$$

Posed as a linear algebra problem:

$$u^k = \mathbf{A} u^{k+1}$$

Where $\mathbf{A}$ is the tri-diagonal coefficient matrix whose central element is $(1 + 2\lambda)$ and its adjacent diagonals are $-\lambda$. For n-dimensional case, central element will then be $(1 + 2n\lambda)$ and u must be flattened (coerced into one dimension) and $\mathbf{A}$ becomes a block tri-diagonal matrix.

4.2.1.3 Crank-Nicolson method

Implicit method, second-order accurate that uses trapezoidal rule for integration time between forward and backward differences. Therefore, assuming $u_t = f(u, t)$ then:

$$\frac{u^{k+1} - u^k}{\Delta t} = \frac{1}{2} \left(f(u^k, t^k) + f(u^{k+1}, t^{k+1}) \right)$$

Applied to the diffusion problem in one dimension:

$$\frac{\lambda}{2} \left(u_{i+1}^k + u_{i-1}^k \right) + (1 - \lambda) u_i^k = -\frac{\lambda}{2} \left(u_{i+1}^{k+1} + u_{i-1}^{k+1} \right) + (1 + \lambda) u_i^{k+1}$$

Posed as a linear algebra problem:

$$\mathbf{A} u^{k+1} = \mathbf{B} u^k$$

Where $\mathbf{A}$ is the tri-diagonal coefficient matrix for $k + 1$ whose central element is $(1 + \lambda)$ and its adjacent diagonals are $-\frac{\lambda}{2}$. Similarly, $\mathbf{B}$ is the tri-diagonal matrix for k whose central element is $(1 - \lambda)$ and its adjacent diagonals are $\frac{\lambda}{2}$. For n-dimensional case, central elements will then be $(1 + n\lambda)$ and $(1 - n\lambda)$ for $\mathbf{A}$ and $\mathbf{B}$ respectively and u must be flattened (coerced into one dimension) as well as that coefficient matrices become block tri-diagonal matrices.

Independently of the numerical method, it is assumed that the problem is posed in terms of linear algebra. This is, the current and next state of the diffusing field u can be expressed with matrix multiplication(s) as shown above.

Currently only the coefficient matrix construction is available. To solve the diffusion problem user can use any of the available linear algebra solvers by providing the current diffusing field state (flattened) and the coefficient matrix on each time-step (or simple matrix multiplication for time explicit methods).

- Simplest options are either `numpy.linalg.solve()` or `scipy.linalg.solve()` (both not very fast).

- If the coefficient matrix is positive-definite (it is most of the times, but can be double-checked, specially if errors arise) and symmetric, a good option is Choleski's factorization. This is already implemented in `scipy.linalg.cholesky()` which factorizes the coefficient matrix and that can be passed to the `scipy.linalg.cho_solve()` which is way faster than the option above.

- Another option (but don't tell anyone) is to invert the coefficient matrix and just solve the equation with a matrix multiplication. This is way faster but your coefficient matrix has to be invertible. If the determinant is close to zero, may cause numerical instability.

4.2.2 Contents

`data_tools.diffusion.`**`build_mat`**`(`*cent*, *neigh*, *dims*, *bcs='dirichlet'*`)`
　　Builds a (block) tri-diagonal coefficient matrix to solve a n-dimensional diffusion problem as a linear algebraic system.

- **Arguments:**
    - *cent* [float]: The coefficient corresponding to the central element of the stencil.
    - *neigh* [float]: The coefficient corresponding to the direct neighbors of the central element in the stencil.
    - *dims* [list]: Or [tuple], contains the size of finite elements [int] for each dimension. Note that the order is first dimension first (e.g.: `[x, y, z]`) as opposed to numpy's indexing order (last dimension first, e.g.: `[z, y, x]`).

– *bcs* [str]: Optional, `'dirichlet'` 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]: The (block) tri-diagonal coefficient matrix. Matrix will be square with size equal to the product of all dimension sizes.

data_tools.diffusion.**coef_mat_hetero**(*K*, *dt*, *dx*, *bcs='dirichlet'*)

Builds a block tri-diagonal coefficient matrix for a n-dimensional diffusion problem with heterogeneous diffusion coefficients.

- **Arguments:**

    – *K* [numpy.ndarray]: The diffusion coefficients matrix.

    – *dt* [float]: The discrete time step.

    – *dx* [float]: The discrete spatial step. It is assumed that the different dimension are equally discretized (e.g.: $\Delta x = \Delta y$).

    – *bcs* [str]: Optional, `'dirichlet'` by default. Determines the boundary conditions. Available options are `'periodic'`, `'dirichlet'` or `'neumann'`. Note that Dirichlet BCs do not hold mass conservation. Periodic BCs are not perfect.

- **Returns:**

    – [numpy.ndarray]: The (block) tri-diagonal coefficient matrix. Matrix will be square with size equal to the product of all dimension sizes.

4.3 data_tools.iterables

Iterable-type operations module.

4.3.1 Contents

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 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.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.**similarity**(*a*, *b*, *mode='j'*)

  Computes the similarity index between two sets. There are three options available:

  Jaccard (mode='j'):

  $$s_J(A, B) = \frac{|A \cap B|}{|A \cup B|}$$

  Sorensen-Dice (mode='sd'):

  $$s_{SD}(A, B) = \frac{2|A \cap B|}{|A| + |B|}$$

  Szymkiewicz–Simpson (mode='ss'):

  $$s_{SS}(A, B) = \frac{|A \cap B|}{\min(|A|, |B|)}$$

  - **Arguments:**

    - *a* [set]: One of the two sets to compute the similarity index.

    - *b* [set]: The other set to compute the similarity index.

    - *mode* [str]: Optional, 'j' (Jaccard) by default. Indicates which type of similarity index/coefficient is to be computed. Available options are: 'j' for Jaccard, 'sd' for Sorensen-Dice and 'ss' for Szymkiewicz–Simpson.

  - **Returns:**

    - [float]: The corresponding similarity index/coefficient according to the specified *mode*.

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}]
    >>> subsets(N)
    {'010': set([2]), '011': set([3]), '001': set([4]), '111': set([
    ]), '110': set([]), '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 contianing all keys and all values respectively from the dictionaries in
  *dicts.

- **Example:**

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

4.4 data_tools.models

Model classes module.

4.4.1 Contents

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 pa-
      rameter. 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 alpha-
      betical 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 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.

class data_tools.models.**Linear** (*x*, *y*)
    Linear regression model using least squares. We define the model as $y = mx + b$. The slope m is computed by dividing the covariance of x and y over the variance of x:

$$m = \frac{S_{xy}}{S_{xx}}$$

Which are defined as follows:

$$S_{xx} = \sum x^2 - \frac{(\sum x)^2}{n}$$
$$S_{xy} = \sum xy - \frac{(\sum x)(\sum y)}{n}$$

Where n is the number of (x, y) data points. The intercept is then obtained from:

$$b = \frac{\sum y + m \sum x}{n}$$

- **Arguments:**

    – *x* [numpy.ndarray]: The independent variable to fit the linear model.

    – *y* [numpy.ndarray]: The dependent variable to fit the linear model.

- **Attributes:**

    – *n* [int]: Number of data points provided.

    – *varx* [float]: Variance of the independent variable.

- *vary* [float]: Variance of the dependent variable.

- *covar* [float]: Covariance between dependent and independent variables.

- *slope* [float]: The slope of the linear model fitted to the provided data.

- *intercept* [float]: The intercept of the fitted model.

- *pred* [numpy.array]: The dependent variable (y) predicted by the model.

- *sse* [float]: Sum of Squares of Errors of the model.

- *rmse* [float]: Root mean squared error, also known as the standard deviation of the model.

- *corr_coef* [float]: Pearson's correlation coefficient of the model.

- *coef_det* [float]: Coefficient of determination of the model. This is, the squared correlation coefficient value.

plot (*filename=None*, *figsize=None*)
Plots the data and the fitted model.

- **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.

class data_tools.models.**PowerLaw** (*x*, *y*)
Fits a power law model to the provided data. Given $y = ax^k$, the data is log-transformed and fitted to a linear model using least squares, since applaying log to both sides of the model:

$$\log(y) = k \log(x) + \log(a)$$

This can be interpreted as a linear model of slope k and intercept $\log(a)$.

- **Arguments:**

  - *x* [np.ndarray]: The independent variable to fit the model.

  - *y* [np.ndarray]: The dependent variable to fit the model.

- **Attributes:**

  - *lm* [data_tools.models.Linear]: The linear model of the data in log space.

  - *a* [float]: The constant of the power law distribution.

  - *k* [float]: The exponent of the power law distribution.

plot (*filename=None*, *figsize=None*, *grid=False*)
Plots the data and the fitted model in a log-log scale.

- **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].

  - *grid* [bool]: Optional, `False` by default. Whether to show the plot grid lines.

- **Returns:**

    – [matplotlib.figure.Figure]: Figure object containing the score plot.

4.5 data_tools.plots

Plotting functions module.

4.5.1 Contents

data_tools.plots.**chordplot**(*nodes*, *edges*, *alpha=0.2*, *plot_lines=False*, *labels=False*, *label_sizes=False*, *colors=None*, *title=None*, *filename=None*, *figsize=None*)

Generates a chord plot from a collection of nodes and edges (and their sizes). **NOTE**: Make sure that all nodes are involved in at least one edge (with size > 0).

- **Arguments:**

    – *nodes* [dict]: Can also be [pandas.DataFrame] or [pandas.Series]. Values contain the nodes sizes and the keys/ indices the node names (must correspond to the ones in *edges*).

    – *edges* [pd.DataFrame]: Can also be [numpy.ndarray] or [list] of [list] as long as contains *n* by 3 elements where *n* is the number of edges and their elements describe the source and target nodes and the size of that edge.

    – *alpha* [float]: Optional, `0.2` by default. Sets the transparency of the edges.

    – *plot_lines* [bool]: Optional, `False` by default. Whether to plot the edge borders or not.

    – *labels* [bool]: Optional, `False` by default. If `True` will label de nodes according to their index/key inputed in the first argument. Otherwise can be [list] or other iterable containing other labels (same order as provided in *nodes*).

    – *label_sizes* [bool]: Optional, `False` by default. Sets whether to append the node sizes when labelling the plot.

    – *colors* [list]: Optional, `None` by default (matplotlib default color sequence). 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 *nodes* (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 the chord plot, unless *filename* is provided.

- **Example:**

```
>>> nodes = {'A':5, 'B':10, 'C':20, 'D':15, 'E':15}
>>> edges = [['A', 'B', 10],
...          ['A', 'C', 25],
...          ['B', 'C', 50],
```
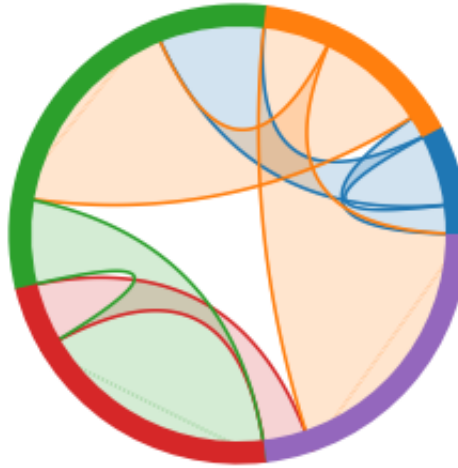
```
...                ['D', 'E', 5],
...                ['B', 'E', 30],
...                ['C', 'D', 20]]
>>> chordplot(nodes, edges, plot_lines=True)
```


data_tools.plots.**cluster_hmap**(*matrix*, *xlabels=None*, *ylabels=None*, *title=None*, *filename=None*, *figsize=None*, *cmap='viridis'*, *link_kwargs={}*, *hmap_kwargs={}*, *dendo_kwargs={}*)

Generates a heatmap with hierarchical clustering dendrograms attached. The linkage matrix and dendrogram are computed using the module `scipy.cluster.hierarchy`, you may check the corresponding documentation for available and default methods.

- **Arguments:**

    - *matrix* [numpy.ndarray]: Contains the values to generate the plot. It is assumed to be a 2-dimensional matrix.

    - *xlabels* [list]: Optional, `None` by default. Labels for the x-axis of the matrix following the same order as provided (e.g. sample names).

    - *ylabels* [list]: Optional, `None` by default. Labels for the y-axis of the matrix following the same order as provided (e.g. measurements).

    - *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].

    - *cmap* [str]: Optional, `'viridis'` by default. The colormap used for the plot (can also be a [matplotlib.colors.Colormap] object). See other [str] options available in Matplotlib's reference manual.

    - *link_kwargs* [dict]: Optional, `{}` by default. Dictionary containing the key-value pairs for keyword arguments passed to scipy.cluster.hierarchy.linkage.

- – *hmap_kwargs* [dict]: Optional, {} by default. Dictionary containing the key-value pairs for keyword arguments passed to **`matplotlib.axes.Axes.imshow`_**.

- – *dendo_kwargs* [dict]: Optional, {} by default. Dictionary containing the key-value pairs for keyword arguments passed to scipy.cluster.hierarchy.dendrogram.

- **Returns:**

  - – [matplotlib.figure.Figure]: The figure object containing the density plot, unless *filename* is provided.

data_tools.plots.**cmap_bkgr = <matplotlib.colors.LinearSegmentedColormap object>**
  Custom colormap, gradient from black (lowest) to lime green (highest).

data_tools.plots.**cmap_bkrd = <matplotlib.colors.LinearSegmentedColormap object>**
  Custom colormap, gradient from black (lowest) to red (highest).

data_tools.plots.**cmap_rdbkgr = <matplotlib.colors.LinearSegmentedColormap object>**
  Custom colormap, gradient from red (lowest) to black (middle) to lime green (highest).

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, unless *filename* is provided.

data_tools.plots.**pca**(*data*, *n_comp=2*, *groups=None*, *cmap='rainbow'*, *title=None*, *filename=None*, *figsize=None*)
  Computes the principal component analysis (PCA) and plots the results.

- **Arguments:**

  - – *data* [pandas.DataFrame]: Contains the high-dimensional data to compute the PCA. The samples (data points) are assumed to be rows and the measurements (features) in the columns.

  - – *n_comp* [int]: Optional, 2 by default. The number of first components to plot. Maximum is three (otherwise defaults to two).

  - – *groups* [dict]: Optional, None by default. Can also be a [pandas.Series]. Defines which samples (keys/index corresponding to row names in *data*) belong to a group (e.g. condition, treatment, . . .) to color the data points. If none is provided, all points are colored in black.

> - *cmap* [str]: Optional, `'rainbow'` by default. The colormap used to draw the groups' colors (can also be a user-defined [matplotlib.colors.Colormap] object). See other [str] options available in Matplotlib's reference manual. If no *groups* are provided, the argument is 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 the scatter plot of the PC's unless *filename* is provided.

`data_tools.plots.`**`phase_portrait`**(*f*, *x=0, 1*, *y=0, 1*, *ics=None*, *dt=0.1*, *title=None*, *file-name=None*, *figsize=None*)

Generates a phase portrait of a ODE system given the nullclines. This is, for a system of the form:

$$\begin{cases} \frac{\mathrm{d}u}{\mathrm{d}t} = f(u, v) \\ \frac{\mathrm{d}v}{\mathrm{d}t} = g(u, v) \end{cases}$$

The nullclines are obtained by equalizing the derivatives to zero and isolating v on each equation. The argument f is therefore expected to return the pair of values v in terms of u for each nullcline. See below for an example.

- **Arguments:**

> - *f* [function]: Defines the two nullclines of the system.
>
> - *x* [tuple]: Optional, `(0, 1)` by default. The range of values to span the x-axis.
>
> - *y* [tuple]: Optional, `(0, 1)` by default. The range of values to span the y-axis.
>
> - *ics* [tuple]: Optional, `None` by default. Set of initial conditions to plot a trajectory. Must have three elements: the initial values of each component and the amount of time the trajectory is simulated.
>
> - *dt* [float]: Optional `0.1` by default. The time-step to simulate the trajectory (given *ics* is provided).
>
> - *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].
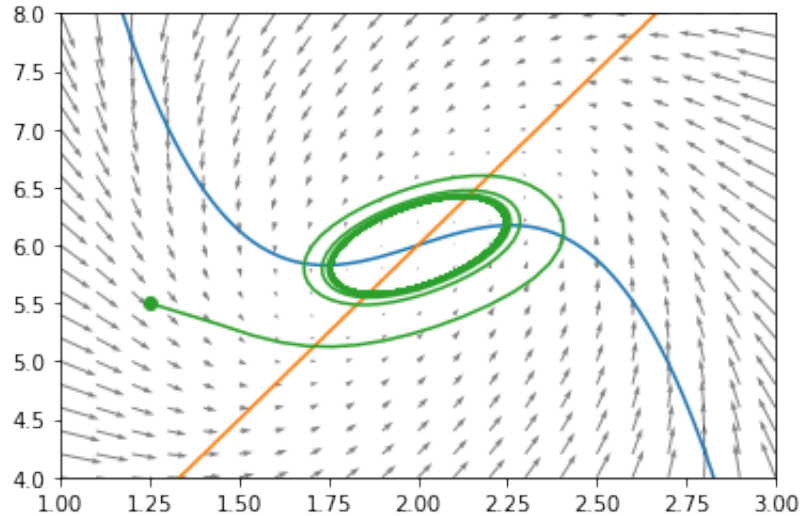
- **Returns:**

> - [matplotlib.figure.Figure]: The figure object containing the phase portrait of the system, unless *filename* is provided.

- **Example:** Let's assume we want the phase portait of the following system:

$$\begin{cases} \frac{\mathrm{d}u}{\mathrm{d}t} = u - 5(u - 2)^3 + 4 - v \\ \frac{\mathrm{d}v}{\mathrm{d}t} = 3u - v \end{cases}$$

> Then:

```
>>> def f(u):
...     return [u - 5 * (u - 2) ** 3 + 4,
...             3 * u]
>>> phase_portrait(f, x=(1, 3), y=(4, 8), ics=[1.25, 5.5, 100])
```


data_tools.plots.**piano_consensus**(*df*, *nchar=40*, *boxes=True*, *top=None*, *title=None*, *file-name=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.

    - *top* [int]: Optional, `None` by default. Sets the number of maximum enriched gene sets to plot (starting from the top ranked).

    - *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, unless *filename* is provided.

- **Example:**

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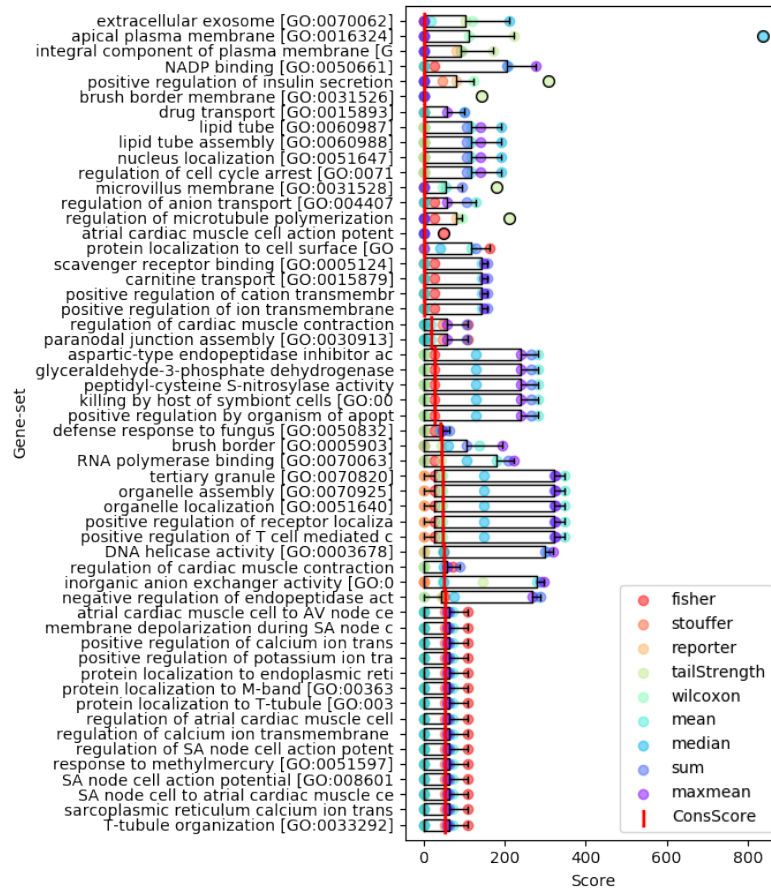

data_tools.plots.**similarity_heatmap**(*groups*, *labels=None*, *mode='j'*, *cmap='nipy_spectral'*, *title=None*, *filename=None*, *figsize=None*)

Given a group of sets, generates a heatmap with the similarity indices across each possible pair.

- **Arguments:**

    - *groups* [list]: Or any iterable of [set] objects.

    - *labels* [list]: Optional, `None` by default. Labels for the sets following the same order as provided in *groups*.

    - *mode* [str]: Optional, `'j'` (Jaccard) by default. Indicates which type of similarity index/coefficient is to be computed. Available options are: `'j'` for Jaccard, `'sd'` for Sorensen-Dice and `'ss'` for Szymkiewicz–Simpson. See `data_tools.iterables.similarity()` for more information.

    - *cmap* [str]: Optional, `'nipy_spectral'` by default. The colormap used for the plot (can also be a [matplotlib.colors.Colormap] object). See other [str] options available in Matplotlib's reference manual.

    - *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, unless *filename* is provided.

data_tools.plots.**similarity_histogram**(*groups*, *mode='j'*, *bins=10*, *title=None*, *filename=None*, *figsize=None*)

Given a group of sets, generates a histogram of the similarity indices across each possible pair (same-element pairs excluded).

- • **Arguments:**

  - – *groups* [list]: Or any iterable of [set] objects.

  - – *mode* [str]: Optional, `'j'` (Jaccard) by default. Indicates which type of similarity index/coefficient is to be computed. Available options are: `'j'` for Jaccard, `'sd'` for Sorensen-Dice and `'ss'` for Szymkiewicz–Simpson. See *data_tools.iterables.similarity()* for more information.

  - – *bins* [int]: Optional, `10` by default. Number of bins to show in the histogram.

  - – *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, unless *filename* is provided.

data_tools.plots.**upset_wrap**(*N*, *labels=None*, *drop_empty=False*, ***kwargs*)

Wrapper for UpSetPlot package. Mostly just generates the Boolean multi-indexed `pandas.Series` the `upsetplot.plot` function needs as input.

- • **Arguments:**

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

  - – *labels* [list]: Optional, `None` by default. Labels for the sets following the same order as provided in *N*. If none is passed they will be labelled `'set0'`, `'set1'` and so on.

  - – *drop_empty* [bool]: Optional, `False` by default. Whether to remove the empty set intersections from the plot or not.

  - – ***kwargs*: Optional. Additional keyword arguments passed to `upsetplot.UpSet` class.

- • **Returns:** [dict]: Contains the `matplotlib.axes.Axes` instances for the UpSetPlot figure.

data_tools.plots.**venn**(*N*, *labels=['A', 'B', 'C', 'D', 'E']*, *c=['C0', 'C1', 'C2', 'C3', 'C4']*, *pct=False*, *sizes=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.

  - – *sizes* [bool]: Optional, `False` by default. Whether to include the size of the sets in the 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]: The figure object containing a combination of box and scatter plots of the gene-set scores, unless *filename* is provided.

- • **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'*, *labels=None*, *maxlabels=25*, *legend=True*, *title=None*, *filename=None*, *figsize=None*, *txt_size=7*, *adj_txt_kwargs={}*)

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.

- *labels* [list]: Optional, `None` by default. List of labels of the points, only the significant ones will be labeled. Must be in the same order as *logfc* and *logpval*.

- *maxlabels* [int]: Optional, `25` by default. Maximum number of labels to show to avoid overcrowding. If the number of labels to show is above, there will be only shown the top data points up to the threshold. This ranking is computed as the product of the *logpval* and absolute *logfc*.

- *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].

- *txt_size* [int]; Optional, `7` by default. The size of the labels (if applicable).

- *adj_txt_kwargs* [dict]: Optional, `{}` by default. The key, value pairs of keyword arguments to pass to adjust_text function (see adjustText reference manual for more information).

- **Returns:**

  - [matplotlib.figure.Figure]: Figure object containing the volcano plot, unless *filename* is provided.

- **Example:**

```
>>> volcano(my_log_fc, my_log_pval)
```
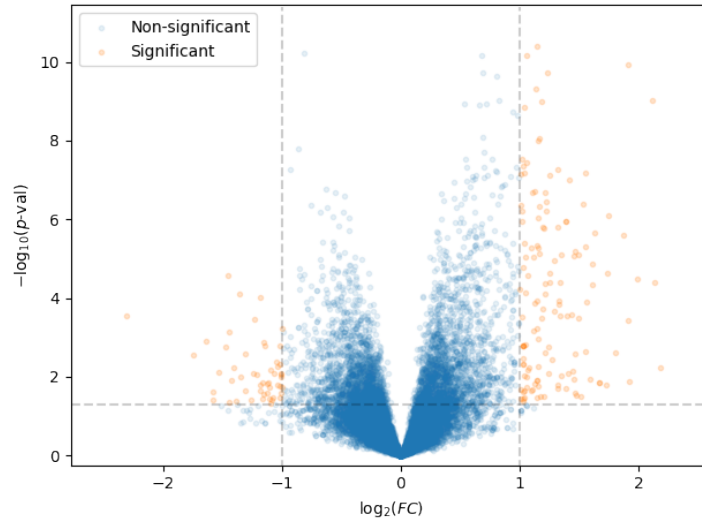
4.6 data_tools.signal

Signal processing module.

4.6.1 Contents

data_tools.signal.**fconvolve**(*u*, *v*)
　　Convolves two vectors or arrays using Fast Fourier Transform (FFT). According to Fourier theory, the convolution theorem states that:

$$g(x) = u(x) * v(x) = \mathcal{F}^{-1}\left\{\mathcal{F}\{u(x)\}\mathcal{F}\{v(x)\}\right\}$$

- **Arguments:**

　　- *u* [numpy.ndarray]: First array to convolve.

　　- *v* [numpy.ndarray]: The other array to be convolved.

- **Returns:**

　　- [numpy.ndarray]: The convolved array of *u* and *v*.

data_tools.signal.**gauss_kernel**(*size*, *sd=1*, *ndim=2*)
　　Returns a N-dimensional Gaussian kernel. The kernel is defined as follows:

$$k(\vec{x}) = \frac{1}{(\sqrt{2\pi}\sigma)^N}e^{-\frac{||\vec{x}||_2^2}{2\sigma^2}}$$

Where :math`N` is the number of dimensions and σ is the standard deviation of the kernel.

- **Arguments:**

　　- *size* [int]: The number of discrete points of the kernel (will be the same on each dimension).

　　- *sd* [float]: Optional, `1` by default. The standard deviation of the gaussian kernel.

　　- *ndim* [int]: Optional, `2` by default. Number of dimensions for the desired kernel.

- **Returns:**

    – [numpy.ndarray]: The Gaussian kernel.

`data_tools.signal.`**`gauss_noise`**(*x*, *sd=1*)

    Applies additive Gaussian (white) noise to a given signal.

- **Arguments;**

    – *x* [numpy.ndarray]: The signal, can have any number of dimensions.

    – *sd* [float]: Optional, `1` by default. The standard deviation of the noise to apply.

- **Returns:**

    – [numpy.ndarray]: The signal *x* with the additive Gaussian noise applied.

4.7 data_tools.spatial

Spatial tools module.

4.7.1 Contents

`data_tools.spatial.`**`equidist_polar`**(*n*, *r=1*)

    For a given number of points (and optionally radius), returns the Cartesian coordinates of such number of equidistant points (in polar coordinates). This is, the (x, y) coordinates of *n* points equally spaced in a circle of radius *r*.

- **Arguments:**

    – *n* [int]: Number of points to retrieve the coordinates.

    – *r* [float]: Optional, `1` by default. The radius of the polar coordinates.

- **Returns:**

    – [list]: Contains *n* [tuple] pairs containing the (x, y) Cartesian coordinates.

`data_tools.spatial.`**`get_boundaries`**(*x*, *counts=False*)

    Given an array, returns either the mask where the boundary edges are or their counts if specified.

- **Arguments:**

    – x [numpy.ndarray]: The array where boundaries are to be identified or counted. Data type of its elements is totally irrelevant.

    – count [bool]: Optional, `False` by default. Whether to return the number of boundary edges or just their mask.

- **Returns:**

    – [numpy.ndarray]: Same shape as *x*. If `counts=False`, contains `True` on any cell that is on the boundary, `False` otherwise. If `counts=True`, will return a similar array but instead of [bool], there will be [int] denoting the number of boundary edges of the cells.

- **Examples:**

```
>>> x = numpy.ones((3, 3, 3))
>>> get_boundaries(x)
array([[[ True,  True,  True],
        [ True,  True,  True],
```

(continues on next page)

```
            [ True,  True,  True]],
          [[ True,  True,  True],
           [ True, False,  True],
           [ True,  True,  True]],
          [[ True,  True,  True],
           [ True,  True,  True],
           [ True,  True,  True]]])
>>> get_boundaries(x, counts=True)
array([[[3, 2, 3],
        [2, 1, 2],
        [3, 2, 3]],
       [[2, 1, 2],
        [1, 0, 1],
        [2, 1, 2]],
       [[3, 2, 3],
        [2, 1, 2],
        [3, 2, 3]]])
```

data_tools.spatial.**neighbour_count**(*x*)

> Given an array (up to three dimensions), returns another array with the same shape containing the counts of cells' neighbours whose value is zero.

> - **Arguments:**
>
>   - *x* [numpy.ndarray]: The array where to count the neighbours (zero-valued cells). Note that the cells can have any value or data type. As long as they be converted to [bool], the function will count all `False` around all `True` cells.
>
> - **Returns:**
>
>   - [numpy.ndarray]: Array with same shape as *x* containing the neighbour count.
>
> - **Examples:**

```
>>> x = numpy.random.randint(2, size=(5, 5))
>>> x
array([[0, 0, 1, 1, 0],
       [0, 0, 0, 1, 1],
       [1, 0, 1, 1, 1],
       [0, 0, 0, 0, 0],
       [1, 0, 0, 1, 1]])
>>> neighbour_count(x)
array([[0, 0, 2, 1, 0],
       [0, 0, 0, 1, 1],
       [3, 0, 3, 1, 1],
       [0, 0, 0, 0, 0],
       [2, 0, 0, 2, 1]])
```

4.8 data_tools.strings

String operations module.

4.8.1 Contents

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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