data_tools Documentation

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Nicolàs Palacio

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

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Contact: nicolaspalacio91@gmail.com

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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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TWO

DEPENDENCIES

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

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.

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MODULES

4.1 data_tools.databases

Databases functions module.

```
data_tools.databases.up_query, in_mode='ACC', out_mode='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].
- *in_mode* [str]: Optional, 'ACC' by default. This is, UniProt accession number. You can check other options available in the URL above.
- out_mode [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.

• Example:

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 []: .
- dt []: .

- dx2 []: .
- **-** d []: .
- -bcs []: .

П: .

4.3 data_tools.models

Model classes module.

 $\verb|class| data_tools.models.Lasso| (\textit{Cs}=500, \textit{cv}=10, \textit{sampler}='\textit{skf'}, \textit{solver}='\textit{liblinear'}, **kwargs)|$

 $Wrapper\ class\ inheriting\ from\ {\tt sklearn.linear_model.LogisticRegressionCV}\ with\ L1\ regularization.$

• 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)

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- 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:

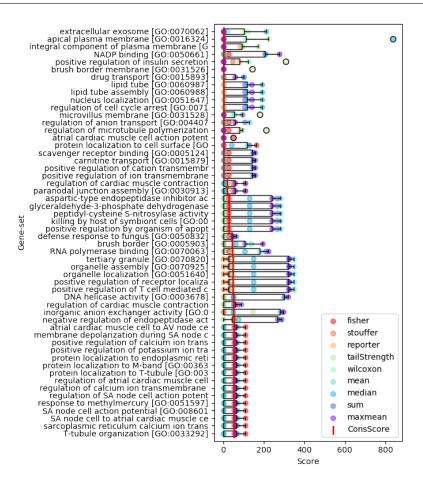
- df [pandas.DataFrame]: Values contained correspond to the scores of the gene-sets (consensus and each individual methods). Index must contain the gene-set labels. Columns are assumed to be ConsRank (ignored), ConsScore followed by the individual methods (e.g.: mean, median, sum, etc).

- 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 genesets 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].

- [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'], c=['C0', 'C1', 'C2', 'C3'], title=None, file-name=None, figsize=None)

Plots a Venn diagram from a list of sets N. Number of sets must be between 2 and 4 (inclusive).

• Arguments:

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- N [list]: Or any iterable type containing [set] objects.
- labels [list]: Optional, ['A', 'B', 'C', 'D'] by default. Labels for the sets following the same order as provided in N.
- c [list]: Optional, ['C0', 'C1' 'C2', 'C3'] 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].

- [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=('CO', 'CI'), legend=True, *title=None*, *filename=None*, *figsize=None*)

Generates a volcano plot from the differential expression data provided.

• Arguments:

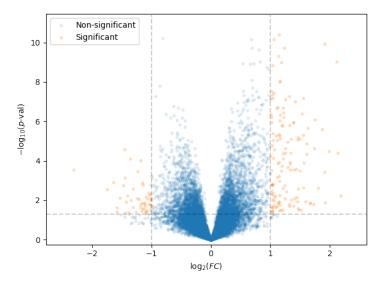
- logfc [list]: Or any iterable type. Contains the log (usually base 2) fold-change values. Must have the same length as logpval.

- *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].

- [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.

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- 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.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:

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

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