

PyIOmica is a general omics package with multiple tools for analyzing omics data.

Usage:

```
from pyiomica import pyiomica
```

Notes:

For additional information visit: <https://github.com/gmiaslab/pyiomica> and <https://mathiomica.org> by G. Mias Lab

Modules

appdirs	json	matplotlib.path	shutil
matplotlib.cm	matplotlib	pandas	sklearn
copy	multiprocessing	pickle	urllib
datetime	numpy	matplotlib.pyplot	zipfile
gzip	numba	pymysql	
h5py	networkx	importlib.resources	
scipy.cluster.hierarchy	os	scipy	

Functions

BenjaminiHochbergFDR(pValues, SignificanceLevel=0.05)

HypothesisTesting BenjaminiHochbergFDR correction

Args:

pValues: p-values (1D array of floats)
SignificanceLevel: default = 0.05.

Returns:

Corrected p-Values, p- and q-Value cutoffs

Usage:

```
result = BenjaminiHochbergFDR(pValues)
```

ExportEnrichmentReport(data, AppendString="", OutputDirectory=None)

Export results from enrichment analysis to Excel spreadsheets.

Args:

data: enrichment results
AppendString: custom report name, if empty then time stamp will be used
OutputDirectory: path of directories where the report will be saved

Returns:

None

Usage:

```
ExportEnrichmentReport(goExample1, AppendString='goExample1', OutputDirectory=None)
```

GOAnalysis(data, GetGeneDictionaryOptions={}, AugmentDictionary=True, InputID=['UniProt ID', 'Gene Symbol'], OutputID='UniProt ID', GOAnalysisAssignerOptions={'Species':'human', 'OntologyLengthFilter':2, 'ReportFilter':1, 'ReportFilterFunction':<ufunc 'greater_equal'>, 'pValueCutoff':0.05, 'TestFunction':<function <lambda> at 0x7fad40c80c80>, 'FilterSignificant':True, 'OBODictionaryVariable':None, 'OBOGODictionaryOptions':{}, 'MultipleListCorrection':False, 'GeneDictionary':None})

Calculate input data over-representation analysis for Gene Ontology (GO) categories.

Args:

data: data to analyze
GetGeneDictionaryOptions: a list of options that will be passed to this internal GetGeneDictionary function
AugmentDictionary: a choice whether or not to augment the current ConstantGeneDictionary global variable or create a new one
InputID: kind of identifiers/accessions used as input
OutputID: kind of IDs/accessions to convert the input IDs/accession numbers in the function's analysis
GOAnalysisAssignerOptions: a list of options that will be passed to the internal GOAnalysisAssigner function
BackgroundSet: background list to create annotation projection to limited background space, involves considering pathways/groups/sets and that provides a list of IDs (e.g. gene accessions) that should be considered as the background for the calculation
Species: the species considered in the calculation, by default corresponding to human
OntologyLengthFilter: function that can be used to set the value for which terms to consider in the computation, by excluding GO terms that have fewer items compared to the OntologyLengthFilter value. It is used by the internal GOAnalysisAssigner function
ReportFilter: functions that use pathways/ontologies/groups, and provides a cutoff for membership in ontologies/pathways/groups in selecting which terms/categories to return. It is typically used in conjunction with ReportFilterFunction
ReportFilterFunction: specifies what operator form will be used to compare against ReportFilter option value in selecting which terms/categories to return
HypothesisFunction: allows the choice of function for implementing multiple hypothesis testing considerations
FilterSignificant: can be set to True to filter data based on whether the analysis result is statistically significant, or if set to False to return all membership computations
OBODictionaryVariable: a GO annotation variable. If set to None, OBOGODictionary will be used internally to automatically generate the default GO annotation
OBOGODictionaryOptions: a list of options to be passed to the internal OBOGODictionary function that provides the GO annotations
MultipleListCorrection: specifies whether or not to correct for multi-omics analysis. The choices are None, Automatic, or a custom number, e.g protein+RNA
MultipleList: specifies whether the input accessions list constituted a multi-omics list input that is annotated so
GeneDictionary: points to an existing variable to use as a gene dictionary in annotations. If set to None the default ConstantGeneDictionary will be used

Returns:

Enrichment dictionary

Usage:

```
goExample1 = GOAnalysis(["TAB1", "TNFSF13B", "MALT1", "TIRAP", "CHUK",
"TNFRSF13C", "PARP1", "CSNK2A1", "CSNK2A2", "CSNK2B", "LTBR",
"LYN", "MYD88", "GADD45B", "ATM", "NFKB1", "NFKB2", "NFKBIA",
"IRAK4", "PIAS4", "PLAU"])
```

GOAnalysisAssigner(PyIOmicaDataDirectory=None, ImportDirectly=False, BackgroundSet=[], Species='human', LengthFilter=None, LengthFilterFunction=<ufunc 'g'
GOFileName=None, GOFileColumns=[2, 5], GOURL='http://current.geneontology.org/annotations/')
Download and create gene associations and restrict to required background set.

Args:
PyIOmicaDataDirectory: the directory where the default package data is stored
ImportDirectly: import from URL regardless is the file already exists
BackgroundSet: background list to create annotation projection to limited background space, involves considering pathways/groups/sets and that provides a list of IDs (e.g. gene accessions) that should be considered as the background for the calculation
Species: species considered in the calculation, by default corresponding to human
LengthFilterFunction: performs computations of membership in pathways/ontologies/groups/sets, that specifies which function to use to filter the number of members a reported category has compared to the number typically provided by LengthFilter
LengthFilter: argument for LengthFilterFunction
GOFileName: the name for the specific GO file to download from the GOURL if option ImportDirectly is set to True
GOFileColumns: columns to use for IDs and GO:accessions respectively from the downloaded GO annotation file, used when ImportDirectly is set to True to obtain a new GO association file
GOURL: the location (base URL) where the GO association annotation files are downloaded from

Returns:
IDToGO and GOTOID dictionary

Usage:
GOassignment = [GOAnalysisAssigner](#)()

GeneTranslation(InputList, TargetIDList, GeneDictionary, InputID=None, Species='human')

Use geneDictionary to convert inputList IDs to different annotations as indicated by targetIDList.

Args:
InputList: list of names
TargetIDList: target ID list
GeneDictionary: an existing variable to use as a gene dictionary in annotations.
If set to None the default ConstantGeneDictionary will be used
InputID: the kind of identifiers/accessions used as input
Species: the species considered in the calculation, by default corresponding to human

Returns:
Dictionary

Usage:
GenDict = [GeneTranslation](#)(data, "UniProt ID", ConstantGeneDictionary, InputID = ["UniProt ID", "Gene Symbol"], Species = "human")

GetGeneDictionary(geneUCSCTable=None, UCSCSQLString=None, UCSCSQLSelectLabels=None, ImportDirectly=False, Species='human', KEGGUCSCSplit=[True])
Create an ID/accession dictionary from a UCSC search - typically of gene annotations.

Args:
geneUCSCTable: path to a geneUCSCTable file
UCSCSQLString: an association to be used to obtain data from the UCSC Browser tables. The key of the association must match the Species option value used (default: human). The value for the species corresponds to the actual MySQL command used
UCSCSQLSelectLabels: an association to be used to assign key labels for the data imported from the UCSC Browser tables. The key of the association must match the Species option value used (default: human). The value is a multi component string list corresponding to the matrices in the data file, or the tables used in the MySQL query provided by UCSCSQLString
ImportDirectly: import from URL regardless is the file already exists
Species: species considered in the calculation, by default corresponding to human
KEGGUCSCSplit: a two component list, {True/False, label}. If the first component is set to True the initially imported KEGG IDs, identified by the second component label, are split on + string to fix nomenclature issues, retaining the string following +

Returns:
Dictionary

Usage:
geneDict = [GetGeneDictionary](#)()

KEGGAnalysis(data, AnalysisType='Genomic', GetGeneDictionaryOptions={}, AugmentDictionary=True, InputID=['UniProt ID', 'Gene Symbol'], OutputID='KEGG C
[cpd]', MolecularOutputID='cpd', KEGGAnalysisAssignerOptions={}, BackgroundSet=[], KEGGOrganism='hsa', KEGGMolecular='cpd', KEGGDatabase='pathway', P
ReportFilter=1, ReportFilterFunction=<ufunc 'greater_equal', pValueCutoff=0.05, TestFunction=<function <lambda> at 0x7fad40c80f28>, HypothesisFunction=<funct
0x7fad40c81048>, FilterSignificant=True, KEGGDictionaryVariable=None, KEGGDictionaryOptions={}, MultipleListCorrection=None, MultipleList=False, GeneDicti
Species='human', MolecularSpecies='compound', NonUCSC=False, PyIOmicaDataDirectory=None)

Calculate input data over-representation analysis for KEGG: Kyoto Encyclopedia of Genes and Genomes pathways.
Input can be a list, a dictionary of lists or a clustering object.

Args:
data: data to analyze
AnalysisType: analysis methods that may be used, "Genomic", "Molecular" or "All"
GetGeneDictionaryOptions: a list of options that will be passed to this internal GetGeneDictionary function
AugmentDictionary: a choice whether or not to augment the current ConstantGeneDictionary global variable or create a new one
InputID: the kind of identifiers/accessions used as input
OutputID: a string value that specifies what kind of IDs/accessions to convert the input IDs/accession numbers in the function's analysis
MolecularInputID: a string list to indicate the kind of ID to use for the input molecule entries
KEGGAnalysisAssignerOptions: a list of options that will be passed to this internal KEGGAnalysisAssigner function
BackgroundSet: a list of IDs (e.g. gene accessions) that should be considered as the background for the calculation
KEGGOrganism: indicates which organism (org) to use for "Genomic" type of analysis (default is human analysis: org="hsa")
KEGGMolecular: which database to use for molecular analysis (default is the compound database: cpd)
KEGGDatabase: KEGG database to use as the target database
PathwayLengthFilter: pathways to consider in the computation, by excluding pathways that have fewer items compared to the PathwayLengthFilter value
ReportFilter: provides a cutoff for membership in ontologies/pathways/groups in selecting which terms/categories to return. It is typically used in conjunction with ReportFilterFunction

ReportFilterFunction: operator form will be used to compare against ReportFilter option value in selecting which terms/categories to return
pValueCutoff: a cutoff p-value for (adjusted) p-values to assess statistical significance
TestFunction: a function used to calculate p-values
HypothesisFunction: allows the choice of function for implementing multiple hypothesis testing considerations
FilterSignificant: can be set to True to filter data based on whether the analysis result is statistically significant, or if set to False to return all membership computations
KEGGDictionaryVariable: KEGG dictionary, and provides a KEGG annotation variable. If set to None, KEGGDictionary will be used internally to automatically generate the default KEGG annotation
KEGGDictionaryOptions: a list of options to be passed to the internal KEGGDictionary function that provides the KEGG annotations
MultipleListCorrection: specifies whether or not to correct for multi-omics analysis.
The choices are None, Automatic, or a custom number
MultipleList: whether the input accessions list constituted a multi-omics list input that is annotated so
GeneDictionary: existing variable to use as a gene dictionary in annotations. If set to None the default ConstantGeneDictionary will be used
Species: the species considered in the calculation, by default corresponding to human
MolecularSpecies: the kind of molecular input
NonUCSC: if UCSC browser was used in determining an internal GeneDictionary used in ID translations, where the KEGG identifiers for genes are number strings (e.g. 4790).The NonUCSC option can be set to True if standard KEGG accessions are used in a user provided GeneDictionary variable,
in the form OptionValue[KEGGOrganism] <>:<>numberString, e.g. hsa:4790
PyIomicaDataDirectory: directory where the default package data is stored

Returns:
Enrichment dictionary

Usage:
keggExample1 = [KEGGAnalysis](#)(["TAB1", "TNFSF13B", "MALT1", "TIRAP", "CHUK", "TNFRSF13C", "PARP1", "CSNK2A1", "CSNK2A2", "CSNK2B", "GADD45B", "ATM", "NFKB1", "NFKB2", "NFKBIA", "IRAK4", "PIAS4", "PLAU", "POLR3B", "NME1", "CTF

KEGGAnalysisAssigner(PyIomicaDataDirectory=None, ImportDirectly=False, BackgroundSet=[], KEGGQuery1='pathway', KEGGQuery2='hsa', LengthFilter=None
<ufunc 'greater_equal'>, Labels=['IDToPath', 'PathToID'])

Create KEGG: Kyoto Encyclopedia of Genes and Genomes pathway associations, restricted to required background set, downloading the data if necessary.

Args:
PyIomicaDataDirectory: directory where the default package data is stored
ImportDirectly: import from URL regardless is the file already exists
BackgroundSet: a list of IDs (e.g. gene accessions) that should be considered as the background for the calculation
KEGGQuery1: make KEGG API calls, and sets string query1 in <http://rest.kegg.jp/link/><> query1 <> / <> query2.
Typically this will be used as the target database to find related entries by using database cross-references
KEGGQuery2: KEGG API calls, and sets string query2 in <http://rest.kegg.jp/link/><> query1 <> / <> query2.
Typically this will be used as the source database to find related entries by using database cross-references
LengthFilterFunction: option for functions that perform computations of membership in pathways/ontologies/groups/sets, that specifies which function to use to filter the number of members a reported category has compared to the number typically provided by LengthFilter
LengthFilter: allows the selection of how many members each category can have, as typically restricted by the LengthFilterFunction
Labels: a string list for how keys in a created association will be named

Returns:
IDToPath and PathToID dictionary

Usage:
KEGGAssignment = [KEGGAnalysisAssigner](#)()

KEGGDictionary(PyIomicaDataDirectory=None, ImportDirectly=False, KEGGQuery1='pathway', KEGGQuery2='hsa')

Create a dictionary from KEGG: Kyoto Encyclopedia of Genes and Genomes terms - typically association of pathways and members therein.

Args:
PyIomicaDataDirectory: directory where the default package data is stored
ImportDirectly: import from URL regardless is the file already exists
KEGGQuery1: make KEGG API calls, and sets string query1 in <http://rest.kegg.jp/link/><> query1 <> / <> query2.
Typically this will be used as the target database to find related entries by using database cross-references
KEGGQuery2: KEGG API calls, and sets string query2 in <http://rest.kegg.jp/link/><> query1 <> / <> query2.
Typically this will be used as the source database to find related entries by using database cross-references

Returns:
Dictionary of definitions

Usage:
KEGGDict = [KEGGDictionary](#)()

LombScargle(inputTimes, inputData, inputSetTimes, FrequenciesOnly=False, NormalizeIntensities=False, OversamplingRate=1, UpperFrequencyFactor=1)
Calculate Lomb-Scargle periodogram.

Args:
inputTimes: times corresponding to provided data points (1D array of floats)
inputData: data points (1D array of floats)
inputSetTimes: a complete set of all possible N times during which data could have been collected
FrequenciesOnly: return frequencies only
NormalizeIntensities: normalize intensities to unity
OversamplingRate: oversampling rate
UpperFrequencyFactor: upper frequency factor

Returns:
Periodogram with a list of frequencies.

Usage:
pgram = [LombScargle](#)(inputTimes, inputData, inputSetTimes)

MassDictionary(PyIomicaDataDirectory=None)

Load PyIomica's current mass dictionary.

Args:
PyIomicaDataDirectory: directory where the default package data is stored

Returns:
Mass dictionary

Usage:
MassDict = [MassDictionary\(\)](#)

MassMatcher(data, accuracy, MassDictionaryVariable=None, MolecularSpecies='cpd')
Assign putative mass identification to input data based on monoisotopic mass (using PyIOmica's mass dictionary). The accuracy in parts per million.

Args:
data: input data
accuracy: accuracy
MassDictionaryVariable: mass dictionary variable. If set to None, inbuilt mass dictionary (MassDictionary) will be loaded and used
MolecularSpecies: the kind of molecular input

Returns:
List of IDs

Usage:
result = [MassMatcher](#)(18.010565, 2)

OBOGODictionary(FileURL='http://purl.obolibrary.org/obo/go/go-basic.obo', ImportDirectly=False, PyIOmicaDataDirectory=None, OBOFile='goBasicObo.txt')
Generate Open Biomedical Ontologies (OBO) Gene Ontology (GO) vocabulary dictionary.

Args:
FileURL: provides the location of the Open Biomedical Ontologies (OBO) Gene Ontology (GO) file in case this will be downloaded from the web
ImportDirectly: import from URL regardless is the file already exists
PyIOmicaDataDirectory: path of directories to data storage
OBOFile: name of file to store data in (file will be zipped)

Returns:
Dictionary of definitions

Usage:
OBODict = [OBOGODictionary\(\)](#)

PlotHorizontalVisibilityGraph(A, data, times, fileName, id)
Bar-plot style horizontal visibility graph.

Args:
A: Adjacency matrix
data: Numpy 2-D array of floats
times: Numpy 1-D array of floats
fileName: name of the figure file to save
id: label to add to the figure title

Returns:
None

Usage:
[PlotHorizontalVisibilityGraph](#)(A, data, times, 'Figure.png', 'Test Data')

PlotVisibilityGraph(A, data, times, fileName, id)
Bar-plot style visibility graph.

Args:
A: Adjacency matrix
data: Numpy 2-D array of floats
times: Numpy 1-D array of floats
fileName: name of the figure file to save
id: label to add to the figure title

Returns:
None

Usage:
[PlotVisibilityGraph](#)(A, data, times, 'Figure.png', 'Test Data')

addVisibilityGraph(data, times, dataName='G1S1', coords=[0.05, 0.95, 0.05, 0.95], numberOfVGs=1, groups_ac_colors=['b'], fig=None, numberOfCommunities=6, pri
fontsize=None, nodesize=None, level=0.55, commLineWidth=0.5, lineWidth=1.0, withLabel=True, withTitle=False, layout='circle', radius=0.07, noplot=False)
Draw a Visibility graph of data on a provided Matplotlib figure.

Args:
data: array of data to visualize
times: times corresponding to each data point, used for labels
dataName: label to include in file name
coords: coordinates of location of the plot on the figure
numberOfVGs: number of plots to add to this figure
groups_ac_colors: colors corresponding to different groups of graphs
fig: figure object
printCommunities: print communities details to screen
fontsize: size of labels
nodesize: size of nodes
level: distance of the community lines to nodes
commLineWidth: width of the community lines
lineWidth: width of the edges between nodes
withLabel: include label on plot
withTitle: include title on plot

Returns:
None

Usage:
`addVisibilityGraph(exampleData, exampleTimes, fig=fig, fontsize=16, nodesize=700,
level=0.85, commLineWidth=3.0, lineWidth=2.0, withLabel=False)`

ampSquaredNormed(func, freq, times, data)

Lomb-Scargle core function

Calculate the different frequency components of our spectrum: project the cosine/sine component and normalize it:

Args:
func: Sin or Cos
freq: frequencies (1D array of floats)
times: input times (starting point adjusted w.r.t. dataset times), Zero-padded
data: input Data with the mean subtracted from it, before zero-padding.

Returns:
Squared amplitude normalized.

Usage:
coef = `ampSquaredNormed`(np.cos, frequency, inputTimesNormed, inputDataCentered)
Intended for internal use only.

autocorrelation(inputTimes, inputData, inputSetTimes, UpperFrequencyFactor=1)

Autocorrelation function

Args:
inputTimes: times corresponding to provided data points (1D array of floats)
inputData: data points (1D array of floats)
inputSetTimes: a complete set of all possible N times during which data could have been collected.

Returns:
Array of time lags with corresponding autocorrelations

Usage:
result = `autocorrelation`(inputTimes, inputData, inputSetTimes)

boxCoxTransform(subset, lmbda=None, giveLmbda=False)

Power transform from scipy.stats

Args:
subset: pandas Series.
lmbda: Lambda parameter, if not specified optimal value will be determined
giveLmbda: also return Lambda value

Returns:
Transformed subset and Lambda parameter

Usage:
myData = `boxCoxTransform`(myData)

boxCoxTransformDataframe(df)

Box-cox transform data.

Args:
df: pandas DataFrame

Returns:
Processed pandas Dataframe

Usage:
df_data = `boxCoxTransformDataframe`(df_data)

chop(expr, tolerance=1e-10)

Equivalent of Mathematica.Chop Function.

Args:
expr: a number or a python sequence of numbers
tolerance: default is the same as in Mathematica

Returns:
Chopped data

Usage:
data = `chop`(data)

compareTimeSeriesToPointDataframe(df, point='first')

Subtract a particular point of each time series (row) of a Dataframe.

Args:
df: pandas DataFrame
point: 'first', 'last', 0, 1, ... , 10, or a value.

Returns:
Processed pandas Dataframe

Usage:
df_data = `compareTimeSeriesToPointDataframe`(df_data)

compareTwoTimeSeriesDataframe(df1, df2, function=<ufunc 'subtract'>, compareAllLevelsInIndex=True, mergeFunction=<function mean at 0x7fad301bd840>)

Create a new Dataframe based on comparison of two existing Dataframes.

Args:
df1: pandas DataFrame
df2: pandas DataFrame
function: np.subtract (default), np.add, np.divide, or another <ufunc>.
compareAllLevelsInIndex: True (default), if False only "source" and "id" will be compared,
mergeFunction: input Dataframes are merged with this function, i.e. np.mean (default), np.median, np.max, or another <ufunc>.

Returns:
New merged pandas Dataframe

Usage:
df_data = [compareTwoTimeSeriesDataframe](#)(df_dataH2, df_dataH1, function=np.subtract, compareAllLevelsInIndex=False, mergeFunction=n

createDirectories(path)
Create a path of directories, unless the path already exists.

Args:
path: path directory

Returns:
None

Usage:
[createDirectories](#)("/pathToFolder1/pathToSubFolder2")

createReverseDictionary(inputDictionary)
Efficient way to create a reverse dictionary from a dictionary.
Utilizes Pandas.DataFrame.groupby and Numpy arrays indexing.

Args:
inputDictionary: a dictionary to reverse

Returns:
Reversed dictionary

Usage:
revDict = [createReverseDictionary](#)(Dict)

exportClusteringObject(ClusteringObject, saveDir, dataName, includeData=True, includeAutocorr=True)
Export a clustering Groups-Subgroups dictionary object to a SpreadSheet.
Linkage data is not exported.

Args:
ClusteringObject: clustering object
saveDir: path of directories to save the object to
dataName: label to include in the file name
includeData: export data
includeAutocorr: export autocorrelations of data

Returns:
File name of the exported clustering object

Usage:
[exportClusteringObject](#)(myObj, '/dir1', 'myObj')

filterOutAllZeroSignalsDataframe(df)
Filter out all-zero signals from a DataFrame.

Args:
df: pandas DataFrame

Returns:
Processed pandas Dataframe

Usage:
df_data = [filterOutAllZeroSignalsDataframe](#)(df_data)

filterOutFirstPointZeroSignalsDataframe(df)
Filter out out first time point zeros signals from a DataFrame.

Args:
df: pandas DataFrame

Returns:
Processed pandas Dataframe

Usage:
df_data = [filterOutFirstPointZeroSignalsDataframe](#)(df_data)

filterOutFractionZeroSignalsDataframe(df, max_fraction_of_allowed_zeros)
Filter out fraction-zero signals from a DataFrame.

Args:
df: pandas DataFrame
max_fraction_of_allowed_zeros: maximum fraction of allowed zeros

Returns:
Processed pandas Dataframe

Usage:
df_data = [filterOutFractionZeroSignalsDataframe](#)(df_data, 0.75)

getAdjacencyMatrixOfHorizontalVisibilityGraph(data)
Calculate adjacency matrix of horizontal visibility graph.
JIT-accelerated version (a bit faster than NumPy-accelerated version).
Single-threaded beats NumPy up to 2k data sizes.
Allows use of Multiple CPUs.

Args:
data: Numpy 2-D array of floats

Returns:

Adjacency matrix

Usage:

```
A = getAdjacencyMatrixOfHorizontalVisibilityGraph(data)
```

getAdjacencyMatrixOfHorizontalVisibilityGraph_NUMPY(data)

Calculate adjacency matrix of horizontal visibility graph.
NumPy-accelerated version.
Use with datasets larger than 2k.
Use in serial applications.

Args:

data: Numpy 2-D array of floats

Returns:

Adjacency matrix

Usage:

```
A = getAdjacencyMatrixOfHorizontalVisibilityGraph\_NUMPY(data)
```

getAdjacencyMatrixOfVisibilityGraph(data, times)

Calculate adjacency matrix of visibility graph.
JIT-accelerated version (a bit faster than NumPy-accelerated version).
Allows use of Multiple CPUs.

Args:

data: Numpy 2-D array of floats

times: Numpy 1-D array of floats

Returns:

Adjacency matrix

Usage:

```
A = getAdjacencyMatrixOfVisibilityGraph\_serial(data, times)
```

getAdjacencyMatrixOfVisibilityGraph_NUMPY(data, times)

Calculate adjacency matrix of visibility graph.
NumPy-accelerated version. Somewhat slower than JIT-accelerated version.
Use in serial applications.

Args:

data: Numpy 2-D array of floats

times: Numpy 1-D array of floats

Returns:

Adjacency matrix

Usage:

```
A = getAdjacencyMatrixOfVisibilityGraph\_serial(data, times)
```

getAutocorrelationsOfData(params)

Calculate autocorrelation using Lomb-Scargle Autocorrelation.
NOTE: there should be already no missing or non-numeric points in the input Series or Dataframe

Args:

params: a tuple of parameters in the form (df_data, setAllInputTimes), where
df_data is a pandas Series or Dataframe,
setAllInputTimes is a complete set of all possible N times during which data could have been collected.

Returns:

Array of autocorrelations of data.

Usage:

```
result = autocorrelation(df_data, setAllInputTimes)
```

getEstimatedNumberOfClusters(data, cluster_num_min, cluster_num_max, trials_to_do, numberOfAvailableCPUs=4, plotID=None, printScores=False)

Get estimated number of clusters using ARI with KMeans

Args:

data: data to analyze
cluster_num_min: minimum possible number of clusters
cluster_num_max: maximum possible number of clusters
trials_to_do: number of trials to do in ARI function
numberOfAvailableCPUs: number of processes to run in parallel
plotID: label for the plot of peaks
printScores: print all scores

Returns:

Largest peak, other possible peaks.

Usage:

```
n_clusters = getEstimatedNumberOfClusters(data, 1, 20, 25)
```

getGroupingIndex(data, n_groups=None, method='weighted', metric='correlation', significance='Elbow')

Cluster data into N groups, if N is provided, else determine N
return: linkage matrix, cluster labels, possible cluster labels.

Args:

data: data to analyze
n_groups: number of groups to split data into
method: linkage calculation method
metric: distance measure
significance: method for determining optimal number of groups and subgroups

Returns:

Linkage matrix, cluster index, possible groups


```
Usage:
    x, y, z = getGroupingIndex(data, method='weighted', metric='correlation', significance='Elbow')
```

getLobmScarglePeriodogramOfDataframe(df_data, NumberOfCPUs=4, parallel=True)

Calculate Lobm-Scargle periodogram of DataFrame.

```
Args:
    df: pandas DataFrame
    parallel: calculate in parallel mode (>1 process)
    NumberOfCPUs: number of processes to create if parallel
```

```
Returns:
    New pandas Dataframe
```

```
Usage:
    df_periodograms = getLobmScarglePeriodogramOfDataframe(df_data)
```

getRandomAutocorrelations(df_data, NumberOfRandomSamples=100000, NumberOfCPUs=4)

Generate autocorrelation null-distribution from permuted data using Lomb-Scargle Autocorrelation.
NOTE: there should be already no missing or non-numeric points in the input Series or DataFrame

```
Args:
    df_data: pandas Series or Dataframe
    NumberOfRandomSamples: size of the distribution to generate
    NumberOfCPUs: number of processes to run simultaneously
```

```
Returns:
    DataFrame containing autocorrelations of null-distribution of data.
```

```
Usage:
    result = getRandomAutocorrelations(df_data)
```

getRandomPeriodograms(df_data, NumberOfRandomSamples=100000, NumberOfCPUs=4)

Generate periodograms null-distribution from permuted data using Lomb-Scargle function.

```
Args:
    df_data: pandas Series or Dataframe
    NumberOfRandomSamples: size of the distribution to generate
    NumberOfCPUs: number of processes to run simultaneously
```

```
Returns:
    New Pandas DataFrame containing periodograms
```

```
Usage:
    result = getRandomPeriodograms(df_data)
```

getSpikes(inputData, func, cutoffs)

Get sorted index of signals with statistically significant spikes,
i.e. those that pass the provided cutoff.

```
Args:
    inputData: data points (2D array of floats) where rows are normalized signals
    func: np.max or np.min
    cutoffs: a dictionary of cutoff values
```

```
Returns:
    Index of data with statistically significant spikes
```

```
Usage:
    index = getSpikes(inputData, np.max, cutoffs)
```

getSpikesCutoffs(df_data, p_cutoff, NumberOfRandomSamples=1000)

Calculate spikes cutoffs from a bootstrap of provided data,
gived the significance cutoff p_cutoff.

```
Args:
    df_data: pandas DataFrame where rows are normalized signals
    p_cutoff: p-Value cutoff, e.g. 0.01
    NumberOfRandomSamples: size of the bootstrap distribution
```

```
Returns:
    Dictionary of spike cutoffs.
```

```
Usage:
    cutoffs = getSpikesCutoffs(df_data, 0.01)
```

get_optimal_number_clusters_from_linkage_Elbow(Y)

Get optimal number clusters from linkage.
A point of the highest acceleration of the fusion coefficient of the given linkage.

```
Args:
    Y: linkage matrix
```

```
Returns:
    Optimal number of clusters
```

```
Usage:
    n_clusters = get\_optimal\_number\_clusters\_from\_linkage\_Elbow(Y)
```

get_optimal_number_clusters_from_linkage_Silhouette(Y, data, metric)

Determine the optimal number of cluster in data maximizing the Silhouette score.

```
Args:
    Y: linkage matrix
    data: data to analyze
```



```

    metric: distance measure

Returns:
    Optimal number of clusters

Usage:
    n_clusters = get\_optimal\_number\_clusters\_from\_linkage\_Elbow(Y, data, 'euclidean')

```

hdf5_usage_information()

```

Store/export any lagge datasets in hdf5 format via 'pandas' or 'h5py'

# mode='w' creates/recreates file from scratch
# mode='a' creates (if no file exists) or appends to the existing file, and reads it
# mode='r' is read only

# Save data to file using 'pandas':
df_example = pd.DataFrame({'A': [1, 2, 3], 'B': [4, 5, 6]}, index=['a', 'b', 'c'])
df_example.to_hdf('data.h5', key='my_df1', mode='a')
or
series_example = pd.Series([1, 2, 3, 4])
series_example.to_hdf('data.h5', key='my_series', mode='a')

# Create groups and datasets using 'h5py' and 'numpy' arrays:
tempFile = h5py.File('data.h5', 'a')
tempArray = np.array([[1,2,3,4,5],[6,7,8,9,10]]).astype(float)
if not 'arrays/my_array' in tempFile:
    dataset_example = tempFile.create_dataset('arrays/my_array', data=tempArray, maxshape=(None,2), dtype=tempArray.dtype,
                                              chunks=True) #auto-chunked, else use e.g. chunks=(100, 2)
                                              #compression='gzip', compression_opts=6

else:
    dataset_example = tempFile['arrays/my_array']

group_example = tempFile.create_group('more_data/additional')

# Modify values by slicing the dataset or replacing etire one using [...]
dataset_example[:] = np.array([[10,2,3,4,1],[60,7,8,9,1]])

# New shapes cannot be broadcasted, the dataset needs to be resized explicitly
dataset_example.resize(dataset_example.shape[0]+10, axis=0) #add more rows (initiated with zeros)

# Read data from h5 file:
df_example = pd.read_hdf('data.h5', 'my_df1')

tempFile = h5py.File('data.h5', 'r')
array_example = tempFile['arrays/my_array'].value

```

internalAnalysisFunction(data, multiCorr, MultipleList, OutputID, InputID, Species, totalMembers, pValueCutoff, ReportFilterFunction, ReportFilter, TestFunction, HyFilterSignificant, AssignmentForwardDictionary, AssignmentReverseDictionary, prefix, infoDict)

Analysis for Multi-Omics or Single-Omics input list
The function is used internally and not intended to be used directly by user.

```

Usage:
    Intended for internal use

```

makeClusteringObject(df_data, df_data_autocorr, significance='Elbow')

Make a clustering Groups-Subgroups dictionary object.

```

Args:
    df_data: data to analyze in DataFrame format
    df_data_autocorr: autocorrelations or periodograms in DataFrame format
    significance: method for determining optimal number of groups and subgroups

Returns:
    Clustering object

Usage:
    myObj = makeClusteringObject(df_data, df_data_autocorr, significance='Elbow')

```

makeDataHistograms(df, saveDir, dataName)

Make a histogram for each pandas Series (time point) in a pandas Dataframe.

```

Args:
    df: DataFrame containing data to visualize
    saveDir: path of directories to save the object to
    dataName: label to include in the file name

Returns:
    None

Usage:
    makeDataHistograms(df, '/dir1', 'myData')

```

makeDendrogramHeatmap(ClusteringObject, saveDir, dataName, AutocorrNotPeriodogr=True, textScale=1.0, vectorImage=True)

Make Dendrogram-Heatmap plot along with Visibility graphs.

```

Args:
    ClusteringObject: clustering object
    saveDir: path of directories to save the object to
    dataName: label to include in the file name
    AutocorrNotPeriodogr: export data
    textScale: scaling of text size
    vectorImage: Boolean for exporting vector graphics or PNG format

Returns:
    None

```

Usage:
[makeDendrogramHeatmap](#)(myObj, '/dir1', 'myData', AutocorrNotPeriodogr=True)

makeLombScarglePeriodograms(df, saveDir, dataName)

Make a combined plot of the signal and its Lomb-Scargle periodogram for each pandas Series (time point) in a pandas Dataframe.

Args:
df: DataFrame containing data to visualize
saveDir: path of directories to save the object to
dataName: label to include in the file name

Returns:
None

Usage:
[makeLombScarglePeriodograms](#)(df, '/dir1', 'myData')

mergeDataframes(listOfDataframes)

Merge a list of Dataframes (outer join).

Args:
listOfDataframes: list of pandas DataFrames

Returns:
New pandas Dataframe

Usage:
df_data = [mergeDataframes](#)([df_data1, df_data2])

metricCommonEuclidean(u,v)

Metric to calculate 'euclidean' distance between vectors u and v using only common non-missing points (not NaNs).

Args:
u: Numpy 1-D array
v: Numpy 1-D array

Returns:
Measure of the distance between u and v

Usage:
dist = [metricCommonEuclidean](#)(u,v)

modifiedZScore(subset)

Calculate modified z-score of a 1D array based on "Median absolute deviation". Use on 1-D arrays only.

Args:
subset: data to transform

Returns:
Transformed subset

Usage:
data = [modifiedZScore](#)(data)

modifiedZScoreDataframe(df)

Z-score (Median-based) transform data.

Args:
df: pandas DataFrame

Returns:
Processed pandas Dataframe

Usage:
df_data = [modifiedZScoreDataframe](#)(df_data)

normalizeSignalsToUnityDataframe(df)

Normalize signals to unity.

Args:
df: pandas DataFrame

Returns:
Processed pandas Dataframe

Usage:
df_data = [normalizeSignalsToUnityDataframe](#)(df_data)

obtainConstantGeneDictionary(GeneDictionary, GetGeneDictionaryOptions, AugmentDictionary)

Obtain gene dictionary - if it exists can either augment with new information or Species or create new, if not exist then create variable.

Args:
GeneDictionary: an existing variable to use as a gene dictionary in annotations.
If set to None the default ConstantGeneDictionary will be used
GetGeneDictionaryOptions: a list of options that will be passed to this internal GetGeneDictionary function
AugmentDictionary: a choice whether or not to augment the current ConstantGeneDictionary global variable or create a new one

Returns:
None

Usage:

```
obtainConstantGeneDictionary(None, {}, False)
```

pAutocorrelation(args)

Wrapper of Autocorrelation function for use with Multiprocessing.

Args:

args: a tuple of arguments in the form (inputTimes, inputData, inputSetTimes)

Returns:

Array of time lags with corresponding autocorrelations

Usage:

```
result = pAutocorrelation((inputTimes, inputData, inputSetTimes))
```

pLombScargle(args)

Wrapper of LombScargle function for use with Multiprocessing.

Args:

args: a tuple of arguments in the form (inputTimes, inputData, inputSetTimes)

Returns:

Array of frequencies with corresponding intensities

Usage:

```
result = pLombScargle((inputTimes, inputData, inputSetTimes))
```

prepareDataframe(dataDir, dataFileName, AlltimesFileName)

Make a DataFrame from CSV files.

Args:

dataDir: path of directories pointing to data

dataFileName: file name in dataDir

AlltimesFileName: file name in dataDir

Returns:

Pandas Dataframe

Usage:

```
df_data = prepareDataframe(dataDir, dataFileName, AlltimesFileName)
df_data.index = pd.MultiIndex.from_tuples([(item.split(':')[1], item.split(':')[0].split('_')[0],
(' '.join(item.split(':')[0].split('_')[1:])) for item in df_data.index.values],
names=['source', 'id', 'metadata'])
```

quantileNormalizeDataframe(df)

Quantile Normalize signals to normal distribution.

Args:

df: pandas DataFrame

Returns:

Processed pandas Dataframe

Usage:

```
df_data = quantileNormalizeDataframe(df_data)
```

read(fileName, withPKLZextension=True, hdf5fileName=None, jsonFormat=False)

Read object from a file recorded by function "write". Pandas and Numpy objects are read from HDF5 file when provided, otherwise attempt to read from PKLZ file.

Args:

fileName: path of directories ending with the file name

withPKLZextension: add ".pklz" to a pickle file

hdf5fileName: path of directories ending with the file name. If None then data is pickled

jsonFormat: save data into compressed json file

Returns:

data: data object to write into a file

Usage:

```
exampleDataFrame = read('/dir1/exampleDataFrame', hdf5fileName='/dir2/data.h5')
```

readMathIOmicaData(fileName)

Read text files exported by MathIOmica and convert to Python data

Args:

fileName: path of directories and name of the file containing data

Returns:

Python data

Usage:

```
data = readMathIOmicaData("../../MathIOmica/MathIOmica/MathIOmicaData/ExampleData/rnaExample")
```

removeConstantSignalsDataframe(df, theta_cutoff)

Remove constant signals.

Args:

df: pandas DataFrame

theta_cutoff: parameter for filtering the signals

Returns:

Processed pandas Dataframe

Usage:

```
df_data = removeConstantSignalsDataframe(df_data, 0.3)
```

runCPUs(NumberOfAvailableCPUs,func,list_of_tuples_of_func_params)
Parallelize function call with multiprocessing.Pool.

Args:
NumberOfAvailableCPUs: number of processes to create
func: function to apply, must take at most one argument
list_of_tuples_of_func_params: function parameters

Returns:
Results of func in a numpy array

Usage:
results = [runCPUs](#)(4, pAutocorrelation, [(times[i], data[i], allTimes) for i in range(10)])

runForClusterNum(arguments)
Calculate Adjusted Rand Index of the data for a range of cluster numbers.

Args:
arguments: a tuple of three parameters in the form
(cluster_num, data_array, trials_to_do), where
cluster_num: maximum number of clusters
data_array: data to test
trials_to_do: number of trials for each cluster number

Returns:
Numpy array

Usage:
instPool = multiprocessing.Pool(processes = NumberOfAvailableCPUs)
scores = instPool.map(runForClusterNum, [(cluster_num, copy.deepcopy(data), trials_to_do) for cluster_num in range(cluster_num_min, cluster_num_max)])
instPool.close()
instPool.join()

tagLowValuesDataframe(df,cutoff,replacement)
Tag low values with replacement value.

Args:
df: pandas DataFrame
cutoff: values below the "cutoff" are replaced with "replacement" value
replacement: replacement value

Returns:
Processed pandas Dataframe

Usage:
df_data = [tagLowValuesDataframe](#)(df_data, 1., 1.)

tagMissingValuesDataframe(df)
Tag missing (i.e. zero) values with NaN.

Args:
df: pandas DataFrame

Returns:
Processed pandas Dataframe

Usage:
df_data = [tagMissingValuesDataframe](#)(df_data)

timeSeriesClassification(df_data, dataName, saveDir, hdf5fileName=None, p_cutoff=0.05, NumberOfRandomSamples=100000, NumberOfCPUs=4, frequencyBasedClassification=False, calculateAutocorrelations=False, calculatePeriodograms=False)
Time series classification.

Args:
df_data: pandas DataFrame
dataName: data name, e.g. "myData_1"
saveDir: path of directories pointing to data storage
hdf5fileName: preferred hdf5 file name and location
p_cutoff: significance cutoff signals selection
NumberOfRandomSamples: size of the bootstrap distribution to generate
NumberOfCPUs: number of processes allowed to use in calculations
frequencyBasedClassification: whether Autocorrelation of Frequency based
calculateAutocorrelations: whether to recalculate Autocorrelations
calculatePeriodograms: whether to recalculate Periodograms

Returns:
None

Usage:
[timeSeriesClassification](#)(df_data, dataName, saveDir, NumberOfRandomSamples = 10**5, NumberOfCPUs = 4, p_cutoff = 0.05, frequencyBasedClassification=False, calculateAutocorrelations=False, calculatePeriodograms=False)

visualizeTimeSeriesClassification(dataName, saveDir, numberOfLagsToDraw=3, hdf5fileName=None, exportClusteringObjects=False, writeClusteringObjectToBinaries=False, AutocorrNotPeriodogr=True, vectorImage=True)
Visualize time series classification.

Args:
dataName: data name
saveDir: path of directories pointing to data storage
numberOfLagsToDraw: first top-N lags (or frequencies) to draw
hdf5fileName: HDF5 storage path and name
exportClusteringObjects: export clustering objects to xlsx files
writeClusteringObjectToBinaries: export clustering objects to binary (pickle) files
AutocorrNotPeriodogr: label to print on the plots

Returns:

None

Usage:

```
visualizeTimeSeriesClassification('myData_1', '/dir1/dir2/', AutocorrNotPeriodogr=True, writeClusteringObjectToBinaries=True)
```

write(data, fileName, withPKLZextension=True, hdf5fileName=None, jsonFormat=False)

Write object into a file. Pandas and Numpy objects are recorded in HDF5 format when 'hdf5fileName' is provided otherwise pickled into a new file.

Args:

data: data object to write into a file
fileName: path of directories ending with the file name
withPKLZextension: add ".pklz" to a pickle file
hdf5fileName: path of directories ending with the file name. If None then data is pickled.
jsonFormat: save data into compressed json file

Returns:

None

Usage:

```
write(exampleDataFrame, '/dir1/exampleDataFrame', hdf5fileName='/dir2/data.h5')
```

Data

ConstantGeneDictionary = None

ConstantPyIOMicaDataDirectory = '/Users/user/anaconda3/envs/pyiomicaTest/lib/python3.7/site-packages/pyiomica/data'

ConstantPyIOMicaExampleVideosDirectory = '/Users/user/anaconda3/envs/pyiomicaTest/lib/python3.7/site-packages/pyiomica/data/ExampleVideos'

ConstantPyIOMicaExamplesDirectory = '/Users/user/anaconda3/envs/pyiomicaTest/lib/python3.7/site-packages/pyiomica/data/ExampleData'

PackageDirectory = '/Users/user/anaconda3/envs/pyiomicaTest/lib/python3.7/site-packages/pyiomica'

UserDataDirectory = '/Users/user/anaconda3/envs/pyiomicaTest/lib/python3.7/site-packages/pyiomica/data'

path = '/Users/user/anaconda3/envs/pyiomicaTest/lib/python3.7/site-packages/pyiomica/data/ExampleVideos'

readIn = PosixPath('/Users/user/anaconda3/envs/pyiomica...thon3.7/site-packages/pyiomica/data/__init__.py')