

MeTime R Package

July 27, 2022

add_col_normality *Function to check normality and add data to col data*

Description

A method applied on the s4 object of class "metime_analyser" to check normality of the metabolites and add it to corresponding columns

Usage

```
add_col_normality(object, which_data, type, metab_names)
```

Arguments

object	An object of class metime_analyser
which_data	dataset on which the method is to be applied
type	type of test, currently only shapiro-wilk test is available under the choice "shapiro"
metab_names	column that has the metabolite names in col_data.

Value

S4 object with shapiro wilk test related data in the col_data

Examples

```
object <- add_col_normality(object=data, which_data=c("lipid_data", "nmr_data"), type="shapiro", metab_names=c("m
```

`add_screening_vars` *Function to add measurements taken at screening time for samples to be added to all timepoints*

Description

A method applied on the s4 object of class "metime_analyser" to add all those datapoints that were measured only during screening to all the respective samples at all timepoints

Usage

```
add_screening_vars(object, vars)
```

Arguments

<code>object</code>	An object of class metime_analyser
<code>vars</code>	A character naming the vars of interest

Value

phenotype data which can be replaced into the original object or use it separately with a different object

Examples

```
# adding APOEGrp, PTGENDER to all data points
new_with_apoegrp_sex <- add_screening_vars(object=metime_analyser_object, vars=c("APOEGrp", "PTGENDER"))
```

`calc_conservation_metabolite` *Function to calculate metabolite conservation index*

Description

Method applied on the object metime_analyser to calculate the metabotype conservation index

Usage

```
calc_conservation_metabolite(object, which_data, verbose)
```

Arguments

<code>object</code>	An object of class metime_analyser
<code>which_data</code>	Name of the dataset to be used
<code>verbose</code>	Information provided on steps being processed

Value

List of conservation index results

Examples

```
#calculating metabolite_conservation_index  
out <- calc_metabolite_conservation(object=metime_analyser_object, which_data="Name of the dataset")
```

calc_conservation_metabotype

Function to calculate metabotype conservation index

Description

Method applied on the object metime_analyser to calculate the metabotype conservation index

Usage

```
calc_conservation_metabotype(object, which_data, verbose)
```

Arguments

object	An object of class metime_analyser
which_data	Name of the dataset to be used
verbose	Information provided on steps being processed

Value

List of conservation index results

Examples

```
#calculating metabotype_conservation_index  
out <- calc_metabotype_conservation(object=metime_analyser_object, which_data="Name of the dataset")
```

calc_correlation_pairwise*Function to calculate correlation***Description**

calculate pairwise correlations This function creates a dataframe for plotting from a dataset.

Usage

```
calc_correlation_pairwise(object, which_data, method)
```

Arguments

- | | |
|------------|---|
| object | S4 Object of class metime_analyser |
| which_data | specify datasets to calculate on. One or more possible |
| method | default setting: method="pearson", Alternative "spearman" also possible |

Value

data.frame with pairwise results

Examples

```
# Example to calculate correlations
dist <- calc_correlation(object=metime_analyser_object, which_data="name of the dataset",
                           method="pearson")
```

calc_dimensionality_reduction*Function to calculate dimensionality reduction methods such as tsne, umap and pca.***Description**

A method to apply on s4 object of class metime_analyse in order to obtain information after dimensionality reduction on a dataset/s

Usage

```
calc_dimensionality_reduction(object, which_data, type)
```

Arguments

object	An object of class metime_analyser
which_data	a character vector - Names of the dataset from which the samples will be extracted
type	type of the dimensionality reduction method to be applied. Accepted inputs are "UMAP", "tSNE", "PCA"

Value

a list with two dataframes containing the dimensionality reduction information 1) samples - data of the individuals(".samples") 2) metabs - data of the metabolites(".metabs")

Examples

```
#calculate PCA
pca <- calc_dimensionality_reduction(object=metime_analyser_object, which_data="name/s of the dataset/s", type="PCA")
#calculate UMAP
pca <- calc_dimensionality_reduction(object=metime_analyser_object, which_data="name/s of the dataset/s", type="UMAP")
#calculate tSNE
pca <- calc_dimensionality_reduction(object=metime_analyser_object, which_data="name/s of the dataset/s", type="tSNE")
```

calc_distance_pairwise

Function to calculate dissimilarity using distance measures

Description

calculate pairwise distances This function creates a dataframe for plotting from a dataset.

Usage

```
calc_distance_pairwise(object, which_data, method)
```

Arguments

object	S4 Object of class metime_analyser
which_data	specify datasets to calculate on. One or more possible
method	default setting: method="euclidean", Alternative "maximum", "minimum", "manhattan", "canberra", "minkowski" are also possible

Value

data.frame with pairwise results

Examples

```
# Example to calculate pairwise distances
dist <- calc_pairwise_distance(object=metime_analyser_object, which_data="name of the dataset",
                                 method="euclidean")
```

calc_featureselection_boruta*Function to calculate dependent variables***Description**

An S4 method to be applied on the metime_analyser object so as to calculate dependent variables

Usage

```
calc_featureselection_boruta(
  object,
  which_x,
  which_y,
  verbose,
  output_loc,
  file_name
)
```

Arguments

<code>object</code>	An object of class metime_analyser
<code>which_x</code>	Name of the dataset to be used for training
<code>which_y</code>	Name of the dataset to be used for testing
<code>verbose</code>	Information provided on steps being processed
<code>output_loc</code>	path to the parent directory where in the out file will be stored
<code>file_name</code>	name of the out file

Value

List of conservation index results

calc_ggm_genenet*An automated function to calculate GGM from genenet***Description**

automated funtion that can be applied on s3 object obtained after prep_data_for_ggms() to obtain geneNet network along with threshold used

Usage

```
calc_ggm_genenet(object, which_data, threshold, timepoints)
```

Arguments

object	S4 object of class metime_analyser
which_data	a character or a character vector naming the datasets of interest
threshold	type of threshold to be used for extracting significant edges
timepoints	timepoints of interest that are to be used to build networks(as per timepoints in rows)

Value

Network data with edgelist, partial correlation values and associated p-values and corrected p-values

calc_ttest

*Function to calculate students t-test***Description**

Method for S4 object of class metime_analyser for performing t-test

Usage

```
calc_ttest(object, which_data, split_var)
```

Arguments

object	S4 object of class metime_analyser
which_data	dataset or datasets to be used for the analysis
split_var	split variable for testing

Value

t-test result as a list or a list of t-test results

get_append_analyser_object

This function appends an object of class metime_analyser with a new dataset.

Description

function to apply on metime_analyse object to append a new dataset into the existing object

Usage

```
get_append_analyser_object(object, data, col_data, row_data, name)
```

Arguments

<code>object</code>	S4 object of class <code>metime_analyser</code>
<code>data</code>	<code>data.frame</code> containing data
<code>col_data</code>	<code>data.frame</code> containing <code>col_data</code> : id column of col data has to match colnames of data
<code>row_data</code>	<code>data.frame</code> containing <code>row_data</code> : id column of row data has to match rownames of data
<code>name</code>	Name of the new dataset

Value

An object of class `metime_analyser`

Examples

```
# append data frames into the metime_analyser object
appended_object <- get_append_metab_object(object=metime_analyser_object, data=data, row_data=data, col_data=col
```

`get_files_and_names` *Function to pack all the data into a single object of class "metime_analyser"*

Description

This function loads all the files from the parent directory. It assumes a certain naming pattern as follows: "datatype_Nonelcollrow_data.rds" Any other naming pattern is not allowed. The function first writes all files into a list and each type of data is packed into its respective class i.e. `col_data`, `row_data` or `data`

Usage

```
get_files_and_names(path, annotations_index)
```

Arguments

<code>path</code>	Path to the parent directory
<code>annotations_index</code>	a list to be filled as follows = <code>list(phenotype="Name or index of the files", medication="Name or index of the files")</code>

Value

An object of class `metime_analyser`

Examples

```
# Input in the parent directory from which the data files are to be extracted along with annotations_index to specify
get_files_and_names(path=/path/to/parent/directory, annotations_index=list(phenotype="Name of phenotype file", m
```

get_ggm_genenet	<i>Function to calculate a dynamic GeneNet GGM from a longitudinal data matrix</i>
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Description

calculates GGM on longitudinal data matrix and returns a dataframe with edges, partial correlation and associated p-values

Usage

```
get_ggm_genenet(data, threshold = c("bonferroni", "FDR", "li"))
```

Arguments

data	data matrix in a longitudinal format
threshold	type of multiple hypothesis correction. Available are Bonferroni("bonferroni"), Benjamini-Hochberg("FDR") and independent tests method("li", also see Li et al)

Value

a dataframe with edges, partial correlation and associated p-values

get_make_analyser_object	<i>Function to pack all the data into a single object of class "metime_analyser"</i>
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Description

This function creates an object of class metime_analyser from a dataset.

Usage

```
get_make_analyser_object(  
  data,  
  col_data,  
  row_data,  
  annotations_index,  
  name = NULL  
)
```

Arguments

data	data.frame containing data
col_data	data.frame containing col_data: id column of col data has to match colnames of data
row_data	data.frame containing row_data: id column of row data has to match rownames of data
annotations_index	a list to be filled as follows = list(phenotype="Name or index of the file/list", medication="Name or index of the files/list")
name	character. Name you want to assign to the new dataset that is being added on

Value

An object of class metime_analyser

Examples

```
# new_metime_analyser_object <- get_make_metab_object(data=data_frame, col_data=col_data_frame, row_data=row_data,
                                                      annotations_index=list(phenotype="name of phenotype", medication="name of medication"))
```

get_make_plotter_object

Function to make a plottable object for viz functions

Description

function to generate metime_plotter object from plot data and metadata

Usage

```
get_make_plotter_object(data, metadata, calc_type, calc_info, plot_type, style)
```

Arguments

data	dataframe of plotable data obtained from any calc object
metadata	dataframe with the metadata for the plot table mentioned above. To obtain these see get_metadata_for_rows() and get_metadata_for_columns()
calc_type	A character to specify type of calculation - will be used for comp_functions
calc_info	A string to define the information about calculation
plot_type	type of the plot you want to build. eg: "box", "dot" etc. Its a character vector
style	Style of plot, accepted inputs are "ggplot", "circos" and "visNetwork". Is a singular option.

```
get_metadata_for_columns
```

Get metadata for columns(in most cases for metabolites)

Description

function to generate a metadata list for building the MeTime plotter object

Usage

```
get_metadata_for_columns(object, which_data, columns, names, index_of_names)
```

Arguments

object	S4 object of class MeTime Analyser
which_data	Names of dataset/s to be used
columns	A list of character vectors for the columns of interest. Length of the list should be same as length of which_data
names	A Character vector with the new names for the columns mentioned above
index_of_names	character vector to define the name of the column in which names of the variables are stored

Value

data.frame with metadata information

```
get_metadata_for_rows  Get metadata for rows(in most cases for samples)
```

Description

function to generate a metadata list for building the MeTime plotter object

Usage

```
get_metadata_for_rows(object, which_data, columns, names)
```

Arguments

object	S4 object of class MeTime Analyser
which_data	Names of dataset/s to be used
columns	A list of character vectors for the columns of interest. Length of the list should be same as length of which_data
names	A Character vector with the new names for the columns mentioned above

Value

`data.frame` with metadata information for rows

`get_palette`

Get a palette of "n" distinct colorblind friendly colors

Description

Function to get a palette of distinct colorblind friendly colors, the distinctiveness is determined by the difference in their hue values.

Usage

```
get_palette(n)
```

Arguments

n	number of colors wanted in the palette
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Value

a color palette vector with colors in the form of hex codes

Examples

```
# colors=get_palette(n=10)
```

`get_samples_and_timepoints`

Function to know the number of timepoints and the total number of samples available at that point

Description

A method applied onto s4 object of class "metime_analyser" so as to obtain the number of unique samples available at each timepoint.

Usage

```
get_samples_and_timepoints(object, which_data)
```

Arguments

object	An object of class metime_analyser
which_data	Name of the dataset in context

Value

A data table with timepoints and number of samples at each timepoint

Examples

```
# newdata <- get_samples_and_timepoints(object=metime_analyser_object, which_data="Name of dataset of interest")
```

get_text_for_plot *Function to Obtain textual information for visualization in interactive plots*

Description

a standard function to be applied on data matrices or dataframes with the colnames of interest such that the information from columns is visualized in the interactive plot

Usage

```
get_text_for_plot(data, colnames)
```

Arguments

data	a dataframe with plotting data along with other variables for visualization
colnames	a character vector with the names of the variables that you want to see on the plot

Value

a vector with strings that can be parsed into plot_ly text.

Examples

```
# text = get_text(data=data.frame, colnames=c("names", "of", "columns", "of", "interest"))
```

metime_analyser-class *Constructor to generate an object of class metime_analyser. contains slots - list_of_data: For the list of all data matrices. - list_of_col_data: list of all the col data files in the same order. - list_of_row_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.*

Description

Constructor to generate an object of class metime_analyser. contains slots - list_of_data: For the list of all data matrices. - list_of_col_data: list of all the col data files in the same order. - list_of_row_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.

Constructor to generate an object of class metime_analyser. contains slots - list_of_data: For the list of all data matrices. - list_of_col_data: list of all the col data files in the same order. - list_of_row_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.

Constructor to generate an object of class metime_analyser. contains slots - list_of_data: For the list of all data matrices. - list_of_col_data: list of all the col data files in the same order. - list_of_row_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.

Constructor to generate an object of class metime_analyser. contains slots - list_of_data: For the list of all data matrices. - list_of_col_data: list of all the col data files in the same order. - list_of_row_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.

Constructor to generate an object of class metime_analyser. contains slots - list_of_data: For the list of all data matrices. - list_of_col_data: list of all the col data files in the same order. - list_of_row_data: list of all the row data files in the same order. - annotations: list with phenotype and medication. Each of which is character that represents the name of the aforementioned dataset types.

<code>metime_plotter-class</code>	<i>creating metime_plotter class that converts calculations and metadata as a plotable object to parse into viz_plotter Contains slots - plot_data: list of Dataframe(s) with plotting data and metadata for visualization. Dataframes is an option only for visNetwork() plots. Need a list of two dataframes: Nodes dataframe and edge dataframe named as \$.node and \$.edge - plot: ggplot(), circos() or visNetwork() object - calc_type: A vector to specify type of calculation - will be used for comp_functions - calc_info: string to define the information about calculation - plot_type: A character vector to define the type of plots that are needed. - style: Character that defines the style of plot i.e. a ggplot(), circos() or visNetwork() plot. Is always a singular input. Cannot have two styles in one object.</i>
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Description

creating metime_plotter class that converts calculations and metadata as a plotable object to parse into viz_plotter Contains slots - plot_data: list of Dataframe(s) with plotting data and metadata for visualization. Dataframes is an option only for visNetwork() plots. Need a list of two dataframes: Nodes dataframe and edge dataframe named as \$.node and \$.edge - plot: ggplot(), circos() or visNetwork() object - calc_type: A vector to specify type of calculation - will be used for comp_functions - calc_info: string to define the information about calculation - plot_type: A character vector to define the type of plots that are needed. - style: Character that defines the style of plot i.e. a ggplot(), circos() or visNetwork() plot. Is always a singular input. Cannot have two styles in one object.

creating metime_plotter class that converts calculations and metadata as a plotable object to parse into viz_plotter Contains slots - plot_data: Dataframe with plotting data and metadata for visualization - plot: ggplot(), circos() or visNetwork() object with predefined aesthetics - calc_type: A vector to specify type of calculation - will be used for comp_functions - calc_info: string to define the information about calculation - plot_type: A character vector to define the type of plots that are needed.

<code>mod_convert_s4_to_s3</code>	<i>Function to Convert S4 object of class metime_analyser to an S3 object with same architecture</i>
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Description

converter function to be applied onto metime_analyse object to convert into a standard list of S3 type.

Usage

```
mod_convert_s4_to_s3(object)
```

Arguments

object An object of class metime_analyser

Value

An S3 object of the same data as metime_analyser in other words all slots are now converted into nested lists

Examples

```
# convert S4 object to a list
s3_list <- mod_convert_s4_to_s3(object=metime_analyser_object)
```

mod_extract_common_samples

Function to get only common samples from the dataframes in list_of_data

Description

A method applied on object of class metime_analyse to extract common samples across datasets.
Also has an option to split the data according timepoints(mod_split_acc_time()).

Usage

```
mod_extract_common_samples(object, time_splitter = FALSE)
```

Arguments

object An object of class metime_anaylser

time_splitter A boolean input: True leads to splitting of the data wrt time, False returns all the dataframes as they are with common rows

Value

list_of_data with common samples across all time points

Examples

```
# extracting common samples across all datasets
new_list_of_data <- mod_common_sample_extractor(object=metime_analyser_object)
```

mod_filter_tp*Functions for selecting time points*

Description

a method applied onto class metime_analyser in order to extract timepoints of interest from a dataset

Usage

```
mod_filter_tp(object, timepoints, full, which_data)
```

Arguments

object	An object of class metime_analyser
timepoints	time points to be selected
full	if TRUE subjects are only selected if measured in all selected time points
which_data	Name of the dataset to be used

Value

An object of class metime_analyser with processed data

Examples

```
#example to use this function
object <- mod_filter_tp(object, timepoints=c(0,12,24), full=TRUE, which_data="Name of the dataset")
```

mod_merge_metime_analysers*Function to merge one or more metime_analyser objects*

Description

function to merge multiple metime_analyser objects

Usage

```
mod_merge_metime_analysers(list_of_objects, annotations_index)
```

Arguments

list_of_objects	list of metime analyser objects that are to be merged
annotations_index	new list with annotations_index. Can also set to be NULL.

Value

A merged metime_analyser object

mod_split_acc_to_time *Function to split data according to time*

Description

Function to split the list of dataframes into a nested list with each dataframe being split into into dataframes of different timepoints

Usage

```
mod_split_acc_to_time(object)
```

Arguments

object	An object of class metime_analyser
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Value

list_of_data with each dataframe being broken into a list of dataframes with respect to the timepoint they belong to

Examples

```
#splitting data according to time
new_data <- mod_split_acc_to_time(object=metime_analyser_object)
```

mod_trans_log *Function to apply log transformation*

Description

Function to log transform data

Usage

```
mod_trans_log(object, which_data, base)
```

Arguments

object	An object of class metime_analyser
which_data	Name of the dataset to be used
base	base of log to be used

Value

An object of class metime_analyser with processed data

Examples

```
# example to apply log transformation  
object <- mod_logtrans(object, which_data="name of the dataset", base=2)
```

mod_trans_zscore *Function to scale the data*

Description

Functions for scaling

Usage

```
mod_trans_zscore(object, which_data)
```

Arguments

object	An object of class metime_analyser
which_data	Name of the dataset to be used

Value

An object of class metime_analyser with processed data

Examples

```
# example to apply scaling  
object <- mod_zscore(object, which_data="name of the dataset")
```

save_analyser_object *Function to extract analyser object data into a csv*

Description

extracts information from analyser object and saves it as a csv

Usage

```
save_analyser_object(object, which_data)
```

Arguments

- object** An object of class metime_plotter
which_data Character to specify the dataset

Value

saves the data in the working directory as a csv and returns nothing

Examples

```
see examples here
save_analyser_object(object, which_data="dataset")
```

save_plot_from_plotter

Function to save interactive plots

Description

extracts plot from plotter object and saves it as a widget

Usage

```
save_plot_from_plotter(object, out)
```

Arguments

- object** An object of class metime_plotter
out Character to specify path of the output file to save the widget in

Value

saves the plot and returns nothing

Examples

```
save_plot_from_plotter(object)
```

save_plotter_object *Function to extract plot data into a csv*

Description

extracts information from plotter object and saves it as a csv

Usage

```
save_plotter_object(object, out)
```

Arguments

object	An object of class metime_plotter
out	Character to specify path of the output file or character vector in case of visNetwork

Value

saves the data into a csv and returns nothing

Examples

```
see examples here  
Network : save_plotter_object(object, out=c("edge.csv", "node.csv", "meta.csv"))  
Others : save_plotter_object(object, out="outfile.csv")
```

set_parallel_cores *register parallel backend*

Description

function to run in order to perform the analysis parallely thereby saving time

Usage

```
set_parallel_cores(n_cores = NULL)
```

Arguments

n_cores	A number of specified cores.
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Value

set a parallel backend

show,metime_analyser-method

Setting new print definition for the metime_analyser object

Description

function to see the structure of metime_analyser object

Usage

```
## S4 method for signature 'metime_analyser'
show(object)
```

Arguments

object S4 object of class metime_analyser

Value

structure of the S4 object

Examples

```
structure(object)
```

show,metime_plotter-method

Setting new print definition for the metime_plotter object

Description

function to see the structure of metime_plotter object

Usage

```
## S4 method for signature 'metime_plotter'
show(object)
```

Arguments

object S4 object of class metime_plotter

Value

structure of the S4 object

Examples

```
structure(object)
```

```
structure,metime_plotter-method
```

Setting new structure definition for the metime_plotter object

Description

function to see the structure of metime_plotter object

Usage

```
## S4 method for signature 'metime_plotter'  
structure(object)
```

Arguments

object S4 object of class metime_plotter

Value

structure of the S4 object

Examples

```
structure(object)
```

```
structure
```

Setting new structure definition for the metime_analyser object

Description

function to see the structure of metime_analyser object

Usage

```
structure(object)
```

Arguments

object S4 object of class metime_analyser

Value

structure of the S4 object

Examples

```
structure(object)
```

viz_distribution_plotter

Function for Plotting distributions of phenotypic variables

Description

A method to be applied onto s4 object so as to obtain distributions of various phenotypic variables

Usage

```
viz_distribution_plotter(object, colname, which_data, strats)
```

Arguments

object	An object of class metime_analyser
colname	Name of the variable whose distribution is of interest
which_data	Name of the dataset from which the samples will be extracted

Value

a list with either 1) density plot, mean table acc to timepoint and variable type or 2) bar plot, line plot, and variable type

Examples

```
# extracting distribuiton of Age from dataset1
```

```
plot <- viz_distribution_plotter(object, colname="Age", which_data="dataset1", strats="additional columns for fac
```

viz_plotter_circos

Setting up standard wrapper for all circos plots for a metime_plotter object.

Description

plot function for metime_plotter object with different inputs to specialize plots. Used for all calc outputs.

Usage

```
viz_plotter_circos(object, aesthetics, outfile)
```

Arguments

object	S4 object of class metime_plotter
aesthetics	list for aesthetics. eg: list(list(x="colname",y="colname",color="colname", shape="colname"), list(...)) for "dot" plot and "heatmap" plot, for heatmap: list(x="colname", y="colname", fill="colname"). Additionally two other character vectors are allowed namely \$.vis and \$.strats for text and for facet wrapping.

viz_plotter_ggplot*Setting up standard wrapper for all ggplot plots for a metime_plotter object.***Description**

plot function for metime_plotter object with different inputs to specialize plots. Used for all calc outputs.

Usage

```
viz_plotter_ggplot(object, aesthetics)
```

Arguments

object	S4 object of class metime_plotter
aesthetics	list for aesthetics. eg: list(list(x="colname",y="colname",color="colname", shape="colname"), list(...)) for "dot" plot and "heatmap" plot, for heatmap: list(x="colname", y="colname", fill="colname"). Additionally two other character vectors are allowed namely \$.vis and \$.strats for text and for facet wrapping.

Value

metime_plotter object with updated plot

viz_plotter_visNetwork*Setting up standard wrapper for network plots from visNetwork for a metime_plotter object.***Description**

plot function for metime_plotter object with different inputs to specialize plots. Used for all calc outputs.

Usage

```
viz_plotter_visNetwork(object, title)
```

Arguments

- | | |
|--------|--|
| object | S4 object of class metime_plotter |
| title | character/string that is the title of the graph output |

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