

Package ‘phase.portrait’

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Title Phase Portrait Analysis

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Description Tools for generating tables and plots needed for phase portrait analysis.

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calculate_derivatives	<i>Calculate Rate of Change (Delta) in Values Over Time This function calculates the rate of change (delta) in the value column over pseudotime. The calculation method can be specified as lead, lag, or lead-lag.</i>
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Description

Calculate Rate of Change (Delta) in Values Over Time This function calculates the rate of change (delta) in the value column over pseudotime. The calculation method can be specified as lead, lag, or lead-lag.

Usage

```
calculate_derivatives(
  df,
  derivative = "lead",
  delta_name = "delta",
  save = FALSE
)
```

Arguments

df	A data frame with value, pseudotime, sample, condition, and variable columns.
derivative	A character string specifying the derivative method to calculate the rate of change. Options are: <ul style="list-style-type: none"> • "lead" (default): Uses the next timepoint to calculate the change. • "lag": Uses the previous timepoint to calculate the change. • "lead-lag": Calculates the change over two surrounding timepoints, useful for datasets with more than two timepoints.
delta_name	A character string specifying the name of the new column for the rate of change. Default is "delta".
save	Logical, if TRUE, saves the resulting data frame to a file.

Value

A data frame with an added delta column (or specified name) representing the rate of change in value over pseudotime.

Examples

```
df <- data.frame(
  value = c(1, 2, 3, 4, 5),
  pseudotime = c(1, 2, 3, 4, 5),
  sample = "sample1",
  condition = "condition1",
  variable = "variable1"
)
calculate_derivatives(df, derivative = "lead-lag", delta_name = "rate_change")
```

iterate_plotting	<i>Generate Multiple Plots with Fixed or Dynamic Axes This function iterates over a dataset and generates multiple plots using a specified plotting function. It supports fixed or dynamic axis limits based on the overall dataset or additional arguments provided. Each subset of data is passed to the plotting function along with optional parameters.</i>
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Description

Generate Multiple Plots with Fixed or Dynamic Axes This function iterates over a dataset and generates multiple plots using a specified plotting function. It supports fixed or dynamic axis limits based on the overall dataset or additional arguments provided. Each subset of data is passed to the plotting function along with optional parameters.

Usage

```
iterate_plotting(
  df,
  fx,
  input = "standard",
  fixed_axes = TRUE,
  save = FALSE,
  ...
)
```

Arguments

df	A data frame containing the dataset with x, y, x_label, and y_label columns.
fx	A function to generate individual plots. It should accept arguments df_split, input, save, and optionally min_x, max_x, min_y, max_y.
input	A character string specifying the input type, either "standard" or "fraction". Default is "standard".
fixed_axes	Logical. If TRUE, uses global axis limits for all plots. If FALSE, each plot can have dynamic axis limits. Default is TRUE.
save	Logical. If TRUE, saves each plot generated by the fx function. Default is FALSE.
...	Additional arguments passed to fx, allowing custom axis limits (min_x, max_x, min_y, max_y).

Value

A list of plots generated by the fx function, each created based on a subset of df.

Examples

```
# Example usage:
# plots <- iterate_plotting(df, fx = plot_phase_portrait, input = "standard", fixed_axes = TRUE)
# ' @export
```

normalize_values	<i>Normalize Values This function normalizes a value column in a data frame using either max or min-max normalization.</i>
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Description

Normalize Values This function normalizes a value column in a data frame using either max or min-max normalization.

Arguments

df	A data frame with a value column to be normalized.
normalization	A character string specifying the normalization method. Options are: <ul style="list-style-type: none"> "max" (default): Scales value by dividing by the maximum absolute value. "min-max": Scales value to a 0-1 range by subtracting the minimum and dividing by the maximum.

Value

A data frame with the normalized value column.

Examples

```
df <- data.frame(value = c(1, 2, 3, 4, 5), variable = "var1")
normalize_values(df, normalization = "min-max")
#' @export
```

phase_lines	<i>Generate Phase Lines for Visualization (Binned, Averaged, or all) This function generates a data frame for visualizing phase lines by creating either binned, averaged, or all types of phase line summaries, using x and y variables or their fractional representations. The result can be used to create phase line plots with separate facets for dx or dy, with flexibility to filter based on a minimum number of observations per bin.</i>
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Description

Generate Phase Lines for Visualization (Binned, Averaged, or all) This function generates a data frame for visualizing phase lines by creating either binned, averaged, or all types of phase line summaries, using x and y variables or their fractional representations. The result can be used to create phase line plots with separate facets for dx or dy, with flexibility to filter based on a minimum number of observations per bin.

Arguments

df	A data frame containing columns: x, y, dx, dy, x_variable, y_variable, x_label, y_label, dx_label, dy_label
n_bins	Integer specifying the number of bins to discretize x and y. Default is 4.
min_bin_n	Integer specifying the minimum number of observations required in each bin.
input	Character string specifying "standard" for direct values or "fraction" for fractional representation.
output	Character string specifying output type: "binned", "average", or "all".

Value

A data table with phase line summaries, including a column output_type indicating "binned" or "average".

Examples

```
# Example usage
phase_lines(df, n_bins = 5, min_bin_n = 2, input = "standard", output = "all")
```

phase_portrait	<i>Generate Phase Portrait Summary (Standard or Fraction-Based) This function generates a phase portrait by binning x and y variables into discrete intervals and calculating the median rate of change (dx and dy) within each bin. It can be used to visualize the dynamics of two variables over binned states, either as a standard portrait or as a fraction-based portrait where x values are represented as fractions of the sum (x + y).</i>
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Description

Generate Phase Portrait Summary (Standard or Fraction-Based) This function generates a phase portrait by binning x and y variables into discrete intervals and calculating the median rate of change (dx and dy) within each bin. It can be used to visualize the dynamics of two variables over binned states, either as a standard portrait or as a fraction-based portrait where x values are represented as fractions of the sum (x + y).

Arguments

df	A data frame containing the following columns: <ul style="list-style-type: none"> • condition: Factor or character column indicating the experimental or observational condition. • x: Numeric column representing values for the x-axis variable. • y: Numeric column representing values for the y-axis variable. • dx: Numeric column representing the rate of change of x. • dy: Numeric column representing the rate of change of y. • x_variable, y_variable: Character or factor columns identifying the variables.
n_bins	Integer specifying the number of bins to discretize x and y variables. Default is 4.
min_bin_n	Integer specifying the minimum number of observations required in each bin for it to be included in the output. Default is 1.
input	Character string specifying the input of data, either "standard" for standard binning or "fraction" for fraction-based binning.

Value

A data frame with summarized phase portrait data containing:

- condition, x_variable, y_variable: Grouping columns from the input.
- x, y: Discretized values of x and y or fractional representation of x and total size as y.
- dx, dy: Median values of dx and dy within each bin.
- n: Number of observations in each bin.
- x_label, y_label: Labels for x and y variables, adapted based on the input.
- dx_label, dy_label: Labels for rate of change for x and y variables.
- input: The input of the data ("standard" or "fraction").

Examples

```
# Example usage
phase_portrait(df, n_bins = 5, min_bin_n = 2, input = "standard")
phase_portrait(df, n_bins = 5, min_bin_n = 2, input = "fraction")
```

phase_space	<i>Generate Phase Space for Pairwise Variable Analysis with Parallel Processing This function calculates the phase space for all pairwise combinations of variables within a data frame. It computes phase portraits by pairing each variable's values and their derivatives, then merges them into a combined phase space data frame. Parallel processing is supported for improved performance.</i>
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Description

Generate Phase Space for Pairwise Variable Analysis with Parallel Processing This function calculates the phase space for all pairwise combinations of variables within a data frame. It computes phase portraits by pairing each variable's values and their derivatives, then merges them into a combined phase space data frame. Parallel processing is supported for improved performance.

Arguments

df	<p>A data frame containing the following columns:</p> <ul style="list-style-type: none"> • value: Numeric values representing measurements or observations of interest. • delta: Numeric values representing the derivative (rate of change) of value. • variable: Factor or character column representing the variable or feature name. • condition: Factor or character column identifying different experimental or observational conditions. • sample: Factor or character column identifying different samples. • pseudotime: Numeric values representing temporal or sequential progression.
n_cores	Integer specifying the number of cores to use for parallel processing. If NULL, defaults to the total available cores minus two (if running on Unix). On Windows, n_cores is set to 1.

Value

A data frame containing phase space information with columns:

- x: Values of the first variable in each pairwise combination.
- dx: Derivative of the first variable.
- x_variable: Name of the first variable.
- y: Values of the second variable in each pairwise combination.
- dy: Derivative of the second variable.
- y_variable: Name of the second variable.
- Additional columns: condition, sample, and pseudotime.

Examples

```
# Example data frame
df <- data.frame(
  value = runif(100),
  delta = rnorm(100),
  variable = rep(c("var1", "var2", "var3", "var4"), each = 25),
  condition = rep("cond1", 100),
  sample = rep(1:5, each = 20),
  pseudotime = rep(1:20, 5)
)

# Generate phase space
phase_space(df)
```

plot_all_trajectories *Plot All Trajectories in Phase Space* This function creates a phase space plot of all trajectories by visualizing x and y values across pseudotime. The plot can handle both standard and fraction-based input types, and provides options to customize axis limits, fix aspect ratio, and save the plot to a file.

Description

Plot All Trajectories in Phase Space This function creates a phase space plot of all trajectories by visualizing x and y values across pseudotime. The plot can handle both standard and fraction-based input types, and provides options to customize axis limits, fix aspect ratio, and save the plot to a file.

Arguments

df	A data frame containing x, y, pseudotime, sample, condition, x_variable, and y_variable.
input	A character string specifying the input type: either "standard" or "fraction". Default is "standard".
min_x	Numeric. Minimum x-axis limit for the plot. Default is NULL.
max_x	Numeric. Maximum x-axis limit for the plot. Default is NULL.
min_y	Numeric. Minimum y-axis limit for the plot. Default is NULL.
max_y	Numeric. Maximum y-axis limit for the plot. Default is NULL.
save	Logical, if TRUE, saves the plot as a PDF file. Default is FALSE.

Value

A ggplot object of the phase space trajectories.

Examples

```
plot_all_trajectories(df, input = "standard", min_x = -10, max_x = 10, min_y = -5, max_y = 5, save = TRUE)
```

plot_n	<i>Plot Cell Count (N) in Phase Space This function creates a phase space plot displaying the count (n) of observations in each bin. The plot can be generated for either standard or fraction-based input types, and provides options to customize axis limits, enforce a fixed aspect ratio, and save the plot to a file.</i>
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Description

Plot Cell Count (N) in Phase Space This function creates a phase space plot displaying the count (n) of observations in each bin. The plot can be generated for either standard or fraction-based input types, and provides options to customize axis limits, enforce a fixed aspect ratio, and save the plot to a file.

Arguments

df	A data frame containing x, y, n, condition, x_variable, and y_variable.
n_bins	Integer specifying the number of bins to use for x and y axes. Default is 4.
input	A character string specifying the input type, either "standard" or "fraction". Default is "standard".
min_x,	max_x Optional numeric values to set limits for the x-axis.
min_y,	max_y Optional numeric values to set limits for the y-axis.
save	Logical, if TRUE, saves the plot as a PDF file. Default is FALSE.

Value

A ggplot object showing the cell count (n) in phase space.

Examples

```
plot_n(df, n_bins = 4, input = "standard", min_x = -10, max_x = 10, min_y = -5, max_y = 5, save = TRUE)
```

plot_phase_line	<i>Plot Phase Lines in Phase Space This function generates a plot of phase lines in phase space, showing changes in x and y values (change rate) along with the grouping variable. It supports both standard and fraction-based input types and provides options to adjust axis limits, customize the plot's color scale, and save the plot as a PDF.</i>
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Description

Plot Phase Lines in Phase Space This function generates a plot of phase lines in phase space, showing changes in x and y values (change rate) along with the grouping variable. It supports both standard and fraction-based input types and provides options to adjust axis limits, customize the plot's color scale, and save the plot as a PDF.

Arguments

df	A data frame containing columns x, y, n, group_var, condition, facet, x_variable, and y_variable.
input	Character string specifying the input type, either "standard" or "fraction". Default is "standard".
min_x,	max_x Optional numeric values to set limits for the x-axis.
min_y,	max_y Optional numeric values to set limits for the y-axis.
save	Logical, if TRUE, saves the plot as a PDF file. Default is FALSE.

Value

A ggplot object representing phase lines in phase space.

Examples

```
plot_phase_line(df, input = "standard", min_x = -10, max_x = 10, min_y = -5, max_y = 5, save = TRUE)
```

plot_phase_portrait	<i>Plot Phase Portrait This function generates a phase portrait plot, visualizing the dynamics of two variables (x and y) with arrows representing the rate of change (dx and dy). The plot uses color to indicate the magnitude of change and can optionally enforce axis limits, aspect ratios, and save the plot to a file.</i>
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Description

Plot Phase Portrait This function generates a phase portrait plot, visualizing the dynamics of two variables (x and y) with arrows representing the rate of change (dx and dy). The plot uses color to indicate the magnitude of change and can optionally enforce axis limits, aspect ratios, and save the plot to a file.

Usage

```
plot_phase_portrait(
  df,
  input = "standard",
  min_x = NULL,
  max_x = NULL,
  min_y = NULL,
  max_y = NULL,
  save = FALSE
)
```

Arguments

df	A data frame containing x, y, dx, dy, condition, x_variable, and y_variable.
input	A character string indicating the type of input. Defaults to "standard".
min_x	Numeric. Minimum x-axis limit for the plot. Default is NULL.
max_x	Numeric. Maximum x-axis limit for the plot. Default is NULL.

min_y	Numeric. Minimum y-axis limit for the plot. Default is NULL.
max_y	Numeric. Maximum y-axis limit for the plot. Default is NULL.
save	Logical, if TRUE saves the plot to a PDF file. Default is FALSE.

Value

A ggplot object showing the phase portrait.

Examples

```
plot_phase_portrait(df, input = "standard", min_x = -10, max_x = 10, min_y = -5, max_y = 5, save = TRUE)
```

plot_stream	<i>Plot Phase Streamline This function creates a phase streamline plot, visualizing the dynamics of two variables (x and y) across conditions. It supports both standard and fraction-based input types, with options for binning, custom axis limits, fixed aspect ratio, and saving the plot.</i>
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Description

Plot Phase Streamline This function creates a phase streamline plot, visualizing the dynamics of two variables (x and y) across conditions. It supports both standard and fraction-based input types, with options for binning, custom axis limits, fixed aspect ratio, and saving the plot.

Usage

```
plot_stream(
  df,
  input = "standard",
  n_bins = 4,
  min_x = NULL,
  max_x = NULL,
  min_y = NULL,
  max_y = NULL,
  save = FALSE
)
```

Arguments

df	A data frame containing columns x, y, dx, dy, condition, x_variable, and y_variable.
input	A character string indicating the type of input, either "standard" or "fraction". Default is "standard".
n_bins	Integer specifying the number of bins for discretizing x and y. Default is 4.
min_x	Numeric. Minimum x-axis limit for the plot. Default is NULL.
max_x	Numeric. Maximum x-axis limit for the plot. Default is NULL.
min_y	Numeric. Minimum y-axis limit for the plot. Default is NULL.
max_y	Numeric. Maximum y-axis limit for the plot. Default is NULL.
save	Logical, if TRUE, saves the plot as a PDF file. Default is FALSE.

Value

A ggplot object showing the phase streamline.

Examples

```
plot_stream(df, input = "standard", n_bins = 4, min_x = 0, max_x = 1, min_y = 0, max_y = 1, save = TRUE)
```

plot_trajectory	<i>Plot Trajectory in Phase Space This function creates a phase space trajectory plot, visualizing x and y values along pseudotime. It connects x1 to x and x to x3 as well as y1 to y and y to y3, representing directional flows with arrows. This enables a clear depiction of how each point in phase space progresses over time.</i>
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Description

Plot Trajectory in Phase Space This function creates a phase space trajectory plot, visualizing x and y values along pseudotime. It connects x1 to x and x to x3 as well as y1 to y and y to y3, representing directional flows with arrows. This enables a clear depiction of how each point in phase space progresses over time.

Arguments

df	A dataframe containing columns for coordinates (x, y), pseudotime, and directional endpoints (x1, x3, y1, y3). Optionally includes input (plot label), condition (facet label), x_variable, and y_variable.
input	Character. Input type for the plot label. Default is "standard". If df\$input exists, it will override this parameter.
min_x	Numeric. Minimum x-axis limit for the plot. Default is NULL.
max_x	Numeric. Maximum x-axis limit for the plot. Default is NULL.
min_y	Numeric. Minimum y-axis limit for the plot. Default is NULL.
max_y	Numeric. Maximum y-axis limit for the plot. Default is NULL.
save	Logical. If TRUE, saves the plot as a PDF file. Default is FALSE.

Details

This function creates a phase space trajectory plot where points and paths are visualized with arrows to indicate directionality. It uses pseudotime as a color gradient to show progression through phase space. Faceting by the condition column allows for separate plots by specified condition.

Value

A ggplot object of the trajectory plot, with customizable color and axis limits.

Examples

```
# Example usage:
df <- data.frame(
  x = c(1, 2, 3), y = c(3, 2, 1),
  x1 = c(1.1, 2.1, 3.1), x3 = c(0.9, 1.9, 2.9),
  y1 = c(3.1, 2.1, 1.1), y3 = c(2.9, 1.9, 0.9),
  pseudotime = c(0.1, 0.5, 0.9),
  condition = c("A", "B", "A"),
  x_variable = "X Axis", y_variable = "Y Axis",
  input = "custom_label"
)
plot_trajectory(df, min_x = 0, max_x = 5, min_y = 0, max_y = 5)
```

pseudotime_trajectory *Calculate Pseudotime Trajectory Summary Statistics* This function calculates summary statistics (median and quantiles) for x and y variables along a pseudotime trajectory within each condition. It groups data by condition and pseudotime, then computes the 25th and 75th percentiles, as well as the median, for each group. This can be used to analyze trends or patterns in x and y over pseudotime.

Description

Calculate Pseudotime Trajectory Summary Statistics This function calculates summary statistics (median and quantiles) for x and y variables along a pseudotime trajectory within each condition. It groups data by condition and pseudotime, then computes the 25th and 75th percentiles, as well as the median, for each group. This can be used to analyze trends or patterns in x and y over pseudotime.

Arguments

df	<p>A data frame containing the following columns:</p> <ul style="list-style-type: none"> condition: Factor or character column indicating the experimental or observational condition. pseudotime: Numeric column indicating pseudotime or a sequential progression. x: Numeric column representing values for the x-axis variable. y: Numeric column representing values for the y-axis variable. x_variable: Character or factor column identifying the name of the x variable. y_variable: Character or factor column identifying the name of the y variable.
input	Either "standard" or "fraction" to specify the type of analysis.
save	Logical, if TRUE saves the resulting data frame as a CSV file. Default is FALSE.

Value

A data frame containing the calculated summary statistics for each combination of condition and pseudotime. Columns in the returned data frame include:

- x1: 25th percentile of x values.
- y1: 25th percentile of y values.
- x3: 75th percentile of x values.
- y3: 75th percentile of y values.
- x: Median of x values.
- y: Median of y values.
- n: Number of observations in each group.

Examples

```
# Example usage:
pseudotime_trajectory(df)
```

run_analysis	<i>Run Analysis and Generate Phase Portrait Plots This function performs an in-depth analysis on a dataset to produce various visualizations, including phase portraits, trajectory plots, and other dynamic plots in phase space. Users can specify different analysis options (standard or fraction-based), save individual or combined plot outputs, and control the granularity of binning and parallel processing.</i>
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Description

Run Analysis and Generate Phase Portrait Plots This function performs an in-depth analysis on a dataset to produce various visualizations, including phase portraits, trajectory plots, and other dynamic plots in phase space. Users can specify different analysis options (standard or fraction-based), save individual or combined plot outputs, and control the granularity of binning and parallel processing.

Arguments

df	A data frame containing the dataset with columns x, y, dx, dy, x_variable, y_variable.
option	A character string specifying the analysis type. Options include "all" (default), "standard", or "fraction".
n_bins	Integer specifying the number of bins to discretize x and y in phase line calculations. Default is 4.
min_bin_n	Integer specifying the minimum number of observations required in each bin. Default is 1.
save_tables	Logical. If TRUE, saves intermediary data tables generated during analysis. Default is FALSE.
plot_individual	Logical. If TRUE, saves each individual plot generated during the analysis. Default is FALSE.

plot_combined	Logical. If TRUE, saves combined plots into one file for easy comparison. Default is TRUE.
n_cores	Integer specifying the number of cores to use for parallel processing. Default is NULL (auto-detect).
phase_line_tables	Character string specifying phase line table output format: "binned", "average", or "all". Default is "all".

Details

The `run_analysis` function is designed to process and visualize phase space data comprehensively, providing flexibility for standard and fraction-based representations of the data. The function offers several customizable options for binning, minimum observations per bin, and parallel processing. Users can select to save intermediary data tables, individual plots, or combined plots based on their analysis needs. The main components of this function include:

- **Phase Space Calculation:** Calls `phase_space()` to compute the core phase space dataset, using parallel processing if specified.
- **Data Preparation for Plotting:** Computes additional summary tables, including `pseudotime_trajectory()`, `phase_portrait()`, and `phase_lines()` based on the selected option. Both standard and fraction-based versions can be generated, providing an in-depth view of phase space dynamics.
- **Plot Generation:** Creates various types of plots to visualize dynamics, including:
 - `trajectory_plots`: Displays pseudotime trajectories in phase space.
 - `all_trajectory_plots`: Shows all sample trajectories over pseudotime.
 - `stream_plots`: Displays dynamic phase portrait streams, representing variable changes over time.
 - `phase_portrait_plots`: Shows a static view of the phase portrait, summarizing variable interactions.
 - `phase_line_plots`: Visualizes phase lines across binned data, providing insights into directional trends.
 - `n_plots`: Highlights the observation count within each phase space bin.
- **Fraction-Based Plots:** Mirrors the standard plots but operates on a fraction-based representation of the data, with plot types prefixed by `fract_`.
- **Plot Merging:** If `plot_combined` is TRUE, combines selected plots into a single layout for easier comparison and visualization of results, saving it as a single PDF file.
- **Error Handling:** Each data processing and plotting step is wrapped in error handling, ensuring any issues are reported without halting the entire workflow.
- **Parallel Processing:** Supports parallel processing with `n_cores` to optimize performance for large datasets.

This function is well-suited for exploratory data analysis and visual interpretation of phase space dynamics, especially valuable when examining complex systems over time. Enabling `save_tables` or `plot_individual` can result in multiple file outputs for detailed analysis, while combined plots are saved as a single PDF for convenience.

Value

This function saves the generated plots and does not return a value.

Examples

```
# Example usage:
df <- data.frame(x = rnorm(100), y = rnorm(100), dx = rnorm(100), dy = rnorm(100),
                 x_variable = "X Axis", y_variable = "Y Axis")
run_analysis(df, option = "all", n_bins = 4, min_bin_n = 1, save_tables = TRUE, plot_individual = TRUE)
```