Package 'LipidTrend'

July 13, 2025

Title LipidTrend: Analysis and Visualization of Lipid Feature Tendencies

Version 0.99.1

Description ``LipidTrend'' is an R package that implements a permutation-based statistical test to identify significant differences in lipidomic features between groups. The test incorporates Gaussian kernel smoothing of region statistics to improve stability and accuracy, particularly when dealing with small sample sizes. This package also includes two plotting functions for visualizing significant tendencies in 1D and 2D feature data, respectively.

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URL https://github.com/BioinfOMICS/LipidTrend

BugReports https://github.com/BioinfOMICS/LipidTrend/issues

LazyData FALSE

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Contents

.analyzeSplitChain *Process Split Chain Analysis*

Description

Helper function to analyze even and odd chain lipids separately

Usage

```
.analyzeSplitChain(
  X,
  X.info,
  group,
  chain_col,
  radius,
  own_contri,
  test,
  permute_time,
  abund_weight
)
```

Arguments

X	Matrix. Lipid abundance data matrix.
X.info	Data frame. Lipid feature information.
group	Vector. Group assignments.
chain_col	Column name for chain length
radius	Numeric. Distance of neighbor to include.
own_contri	Numeric. Proportion of own contribution.
test	Character. Statistical test to use.
permute_time	Integer. Number of permutations.
abund_weight	Logical. Whether to use abundance weighting.

Value

A data frame with split chain results

.buildWall *Build Walls Between Different Regions*

Description

Identifies walls needed between different regions based on spatial relationships and region assignments

Usage

```
.buildWall(feature.idx, X.info, selected.region, x.distance, y.distance)
```

Arguments

`feature.idx`	Numeric. Index of the feature to analyze
`X.info`	Matrix or data.frame. Contains spatial coordinates
`selected.region`	Character vector. Region assignments for features
`x.distance`	Numeric. Scaling factor for x-coordinates
`y.distance`	Numeric. Scaling factor for y-coordinates

Value

Data frame with coordinates and wall positions

`.calcSegment` *Calculate Segment Coordinates*

Description

Calculates start and end coordinates for wall segments

Usage

```
.calcSegment(wall_data, direction, x_dist, y_dist)
```

Arguments

`wall_data`	Data frame. Wall position data
`direction`	Character. Wall direction
`x_dist`	Numeric. X-axis distance scale
`y_dist`	Numeric. Y-axis distance scale

Value

List of segment coordinates

`.countDistance` *Normalize Coordinate Matrix by Feature Distance*

Description

Normalizes coordinates by dividing each dimension by its minimum distance

Usage

```
.countDistance(dist_input)
```

Arguments

`dist_input`	Matrix or data.frame. Contains spatial coordinates.

Value

A list containing the normalized matrix and distance values for each dimension

---

.createSegmentLayer *Create Segment Layer for Wall Visualization*

Description

Creates a ggplot2 layer for wall segments

Usage

```
.createSegmentLayer(wall_data, direction, color, x_dist, y_dist)
```

Arguments

wall_data	Data frame. Wall coordinates
direction	Character. Wall direction
color	Character. Wall color
x_dist	Numeric. X-axis distance scale
y_dist	Numeric. Y-axis distance scale

Value

A ggplot2 layer object or NULL

.findNeighbor *Find Neighboring Features*

Description

Identifies neighboring features in specified directions

Usage

```
.findNeighbor(self, others, type = c("right", "left", "top", "bottom"))
```

Arguments

self	Numeric vector. Reference point coordinates
others	Matrix. Coordinates of other features
type	Character. Direction to check ("right", "left", "top", "bottom")

Value

Logical vector indicating neighbor presence

.formingFinalPlot *Add Data Points and Styling to Base Plot*

Description

Adds data points with fold change coloring, significance annotations, and styling to a base heatmap plot.

Usage

```
.formingFinalPlot(base_plot, heatmap.df)
```

Arguments

base_plot	A ggplot object containing the initial base plot structure
heatmap.df	A data frame with columns for visualization: **avg.abund** Numeric. Average abundance values for point sizing **log2.FC** Numeric. Log2 fold change values for point coloring **pval.annotate** Character. Significance symbols for annotations **label_vjust** Numeric. Vertical adjustment for text labels

Value

A ggplot object with enhanced visualization layers

.plotHeatmap *Plot Heatmap with Abundance Data and Region Walls*

Description

Creates a ggplot2 heatmap visualization showing abundance data with walls between regions, using vectorized operations.

Usage

```
.plotHeatmap(X.info, heatmap.df, walls, x.distance, y.distance)
```

Arguments

X.info	Matrix or data.frame. Contains coordinate information
heatmap.df	Data frame. Contains abundance and fold change data
walls	List. Contains wall coordinates for different regions
x.distance	Numeric. Distance between x-axis points
y.distance	Numeric. Distance between y-axis points

Value

A ggplot2 object

.pvalAnnotation *Create P-value Annotation*

Description

Converts p-values to significance symbols

Usage

```
.pvalAnnotation(pval)
```

Arguments

pval	Numeric. P-value to convert

Value

Character string with significance symbols

.regionStat *Region Statistics Calculation*

Description

Calculate region statistics using either t-test or Wilcoxon test

Usage

```
.regionStat(X, Y, test = "t.test", ...)
```

Arguments

X	Matrix. Lipid abundance data matrix.
Y	Matrix. Group information matrix.
test	Character. Statistical test to use ("t.test" or "Wilcoxon"). Default is "t.test".

Value

Numeric vector of statistical test results.

`.resultSummary` *Summarize Results*

Description

Summarize and format lipid trend analysis results

Usage

```
.resultSummary(
  X,
  X.info,
  group,
  smooth.stat,
  smooth.stat.permute,
  region.stat.obs,
  dimension,
  permute_time,
  ...
)
```

Arguments

`X`	Matrix. Lipid abundance data matrix.
`X.info`	Data frame. Lipid feature information.
`group`	Vector. Group assignments.
`smooth.stat`	Numeric vector. Smoothed statistics.
`smooth.stat.permute`	Matrix. Permutation results.
`region.stat.obs`	Numeric vector. Observed region statistics.
`dimension`	Integer. Dimension of the analysis.
`permute_time`	Integer. Number of permutations performed.
`...`	Additional arguments.

Value

Data frame containing formatted results.

.smooth_permutation *Smooth Permutation Analysis*

Description

Perform smooth permutation analysis for lipid trend data

Usage

```
.smooth_permutation(
  X,
  group,
  dist.mat,
  own_contri,
  test,
  abund_weight,
  permute_time,
  region.stat.obs
)
```

Arguments

X	Matrix. Lipid abundance data matrix.
group	Vector. Group assignments.
dist.mat	Matrix. Distance matrix.
own_contri	Numeric. Proportion of own contribution.
test	Character. Statistical test to use.
abund_weight	Logical. Whether to use abundance weighting.
permute_time	Integer. Number of permutations.
region.stat.obs	Numeric vector. Observed region statistics.

Value

List containing smooth statistics and permutation results.

.split_chain *Get Split Chain Status from LipidTrendSE*

Description

Get Split Chain Status from LipidTrendSE

Usage

```
.split_chain(object)
```

Arguments

object	A LipidTrendSE object

Value

Logical indicating if analysis was split by chain

.stat_lipidTrend *Statistical Analysis for lipidTrend*

Description

Perform statistical analysis for lipid trend data

Usage

```
.stat_lipidTrend(
  X,
  X.info,
  group,
  radius,
  own_contri,
  test,
  permute_time,
  abund_weight
)
```

Arguments

X	Matrix. Lipid abundance data matrix.
X.info	Data frame. Lipid feature information.
group	Vector. Group assignments.
radius	Numeric. Distance of neighbor to include.
own_contri	Numeric. Proportion of own contribution.
test	Character. Statistical test to use.
permute_time	Integer. Number of permutations.
abund_weight	Logical. Whether to use abundance weighting.

Value

Data frame containing analysis results.

.trendPlot1D *Create 1D result plot*

Description

Creates a ggplot visualization showing trends between case and control groups with highlighted significant regions.

Usage

```
.trendPlot1D(res, p_cutoff, y_scale)
```

Arguments

res	A data.frame containing columns for coordinates, abundance values, direction, and adjusted p-values
p_cutoff	Numeric value for significance cutoff. Default is 0.05
y_scale	Character. Choose one of the y-axis scales: "identity", "log2", "log10", or "sqrt". Default is "identity"

Value

A ggplot2 object

.trendPlot2D *Create 2D Trend Plot*

Description

Creates a 2D visualization of lipid trends with statistical annotations

Usage

```
.trendPlot2D(res, p_cutoff, log2FC_cutoff)
```

Arguments

res	Data frame containing analysis results
p_cutoff	Numeric significance level cutoff
log2FC_cutoff	Numeric log2 fold change cutoff

Value

A ggplot2 object representing the trend visualization

abundance_2D *Example lipid abundance data for two-dimensional LipidTrend analysis*

Description

Example lipid abundance data for two-dimensional LipidTrend analysis

Usage

```
data(abundance_2D)
```

Format

A `matrix` object of lipid abundance with 137 lipids over 6 samples

Source

Tomoyuki Shiota et al. ,Hepatoviruses promote very-long-chain fatty acid and sphingolipid synthesis for viral RNA replication and quasi-enveloped virus release. Sci Adv. 9(42):eadj4198 https://www.science.org/doi/10.1126/sciadv.adj4198.

Examples

```
data(abundance_2D)
```

abundance_CL *Example lipid abundance data for one-dimensional LipidTrend analysis*

Description

Example lipid abundance data for one-dimensional LipidTrend analysis

Usage

```
data(abundance_CL)
```

Format

A `matrix` object of lipid abundance with 29 lipids over 6 samples

Source

Tomoyuki Shiota et al. ,Hepatoviruses promote very-long-chain fatty acid and sphingolipid synthesis for viral RNA replication and quasi-enveloped virus release. Sci Adv. 9(42):eadj4198 https://www.science.org/doi/10.1126/sciadv.adj4198.

Examples

```
data(abundance_CL)
```

`analyzeLipidRegion` *Conduct statistical to analyze lipid features tendencies*

Description

Calculate p-value of lipidomic features by permutation test. The test of region statistics smoothing with Gaussian kernel integrates neighbor's information and provides a stable testing result under small sample size.

Usage

```
analyzeLipidRegion(
  lipid_se,
  ref_group,
  split_chain = FALSE,
  chain_col = NULL,
  radius = 3,
  own_contri = 0.5,
  test = "t.test",
  abund_weight = TRUE,
  permute_time = 1e+05
)
```

Arguments

`lipid_se`	A SummarizedExperiment object. Must contain following data: **Assay** A matrix containing lipid abundance data, where rows represent lipids and columns represent samples. **RowData** A data frame of lipid features (e.g., double bond count, chain length), with rows as lipids and columns as lipid features (limited to 1 or 2 columns). The order of lipids must match the abundance data. If RowData contains one column, a one-dimensional analysis will be performed. If RowData includes two columns, a two-dimensional analysis will be conducted. **ColData** A data frame containing group information, where rows represent sample names and columns must include sample name, label name, and group, arranged accordingly.
`ref_group`	Character. Group name of the reference group. It must be one of the group names in the colData group column.
`split_chain`	Logical. If TRUE the results will split to shown by odd and even chain. Default is `FALSE`.
`chain_col`	Character. The column name of chain length. Set to NULL if split_chain is FALSE. Default is `'NULL'`.
`radius`	Numeric. Distance of neighbor to be included. Default is `3`.
`own_contri`	Numeric. Proportion of own contribution. Default is `0.5`. To not over-emphasize the neighbor information, we suggest to choose a value from 0.5 to 1.
`test`	String. Choose statistic test from "t.test" and "Wilcoxon". Default is `'t.test'`.
`abund_weight`	Logical. Consider the average abundance as the weight in the test statistic. Default is `TRUE`.
`permute_time`	Integer. Permutation times. Default is `100000`.

Value

A LipidTrendSE object containing lipidomic feature testing result.

See Also

plotRegion1D for one-dimensional visualization plotRegion2D for two-dimensional visualization

Examples

```
data("lipid_se_CL")
res_se <- analyzeLipidRegion(
    lipid_se=lipid_se_CL, ref_group="sgCtrl", split_chain=FALSE,
    chain_col=NULL, radius=3, own_contri=0.5, permute_time=100)
```

---

char_table_2D *Example lipid characteristics table for two-dimensional LipidTrend analysis*

Description

Example lipid characteristics table for two-dimensional LipidTrend analysis

Usage

```
data(char_table_2D)
```

Format

A data.frame object of total chain length and total double bond characteristics over 137 lipids

Source

Tomoyuki Shiota et al. ,Hepatoviruses promote very-long-chain fatty acid and sphingolipid synthesis for viral RNA replication and quasi-enveloped virus release. Sci Adv. 9(42):eadj4198 https://www.science.org/doi/10.1126/sciadv.adj4198.

Examples

```
data(char_table_2D)
```

char_table_CL *Example lipid characteristics table for one-dimensional LipidTrend analysis*

Description

Example lipid characteristics table for one-dimensional LipidTrend analysis

Usage

```
data(char_table_CL)
```

Format

A `data.frame` object of chain characteristics over 29 lipids

Source

Tomoyuki Shiota et al. ,Hepatoviruses promote very-long-chain fatty acid and sphingolipid synthesis for viral RNA replication and quasi-enveloped virus release. Sci Adv. 9(42):eadj4198 https://www.science.org/doi/10.1126/sciadv.adj4198.

Examples

```
data(char_table_CL)
```

even_chain_result *Get Even Chain Result from LipidTrendSE*

Description

Get Even Chain Result from LipidTrendSE

Usage

```
even_chain_result(object)

## S4 method for signature 'LipidTrendSE'
even_chain_result(object)
```

Arguments

`object`	A LipidTrendSE object

Value

A data frame containing even chain result or NULL

Examples

```
data("lipid_se_CL")
sub <- lipid_se_CL[seq_len(10), ]
res_se <- analyzeLipidRegion(
    lipid_se=sub, ref_group="sgCtrl", split_chain=TRUE,
    chain_col="chain", radius=3, own_contri=0.5, permute_time=100)
# Get complete result summary
results <- even_chain_result(res_se)
```

`group_info` *Example group information table for LipidTrend analysis*

Description

Example group information table for LipidTrend analysis

Usage

```
data(group_info)
```

Format

A `data.frame` object of sample name, lable name, and group name over 6 samples

Source

Tomoyuki Shiota et al. ,Hepatoviruses promote very-long-chain fatty acid and sphingolipid synthesis for viral RNA replication and quasi-enveloped virus release. Sci Adv. 9(42):eadj4198 https://www.science.org/doi/10.1126/sciadv.adj4198.

Examples

```
data(group_info)
```

`LipidTrend` *LipidTrend: Analysis and Visualization of Lipid Feature Tendencies*

Description

The LipidTrend package provides tools for analyzing and visualizing trends in lipidomics data. It implements statistical methods for identifying significant changes in lipid abundances across different features, with support for both one-dimensional and two-dimensional analyses.

Main functions

- `analyzeLipidRegion`: Analyzing lipid trends using permutation tests and Gaussian kernel smoothing
- `plotRegion1D`: Visualize one-dimensional lipid trends
- `plotRegion2D`: Create two-dimensional visualizations of lipid trends

Vignettes

See the package vignettes for detailed workflows: `vignette('LipidTrend')`

Installation

To install from Bioconductor, use:

```
if (!requireNamespace('BiocManager', quietly=TRUE))
    install.packages('BiocManager')
BiocManager::install('LipidTrend')
```

Author(s)

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- Hung-Ching Chang [contributor]
- Meng-Hsin Tsai [contributor]

See Also

Useful links:

- https://github.com/BioinfOMICS/LipidTrend
- Report bugs at https://github.com/BioinfOMICS/LipidTrend/issues

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`LipidTrendSE-class` *Class for storing analyzeLipidRegion analysis results*

Description

This class extends SummarizedExperiment to store analyzeLipidRegion analysis results

Slots

`split_chain` Logical indicating whether chains were split by parity. When TRUE, results are stored in even_chain_result and odd_chain_result. When FALSE, results are stored in the result slot.

`result` Data frame of analysis results (for non-split data)

`even_chain_result` Data frame of results for even chains (when split)

`odd_chain_result` Data frame of results for odd chains (when split)

LipidTrendSE-validity *Validate LipidTrendSE object*

Description

Validate LipidTrendSE object

Arguments

object	A LipidTrendSE object to validate

Value

TRUE if valid, otherwise an error message

lipid_se_2D *Example Dataset for two-dimensional data*

Description

Example Dataset for two-dimensional data

Usage

```
data(lipid_se_2D)
```

Format

A SummarizedExperiment object with the following slots:

- colData A data frame with 6 observations on the following 3 variables, containing sample name, label name, and group name
- assay A 137*6 matrix containing lipid abundance data
- rowData A data frame with 137 observations on the following 2 variables containing total chain length and total double bond characteristic information

Examples

```
data(lipid_se_2D)
```

lipid_se_CL *Example Dataset for one-dimensional data*

Description

Example Dataset for one-dimensional data

Usage

```
data(lipid_se_CL)
```

Format

A SummarizedExperiment object with the following slots:

colData A data frame with 6 observations on the following 3 variables, containing sample name, label name, and group name

assay A 29*6 matrix containing lipid abundance data

rowData A data frame with 29 observations on the following 1 variables containing chain characteristic information

Examples

```
data(lipid_se_CL)
```

odd_chain_result *Get Odd Chain Result from LipidTrendSE*

Description

Get Odd Chain Result from LipidTrendSE

Usage

```
odd_chain_result(object)

## S4 method for signature 'LipidTrendSE'
odd_chain_result(object)
```

Arguments

object A LipidTrendSE object

Value

A data frame containing odd chain result or NULL

Examples

```
data("lipid_se_CL")
res_se <- analyzeLipidRegion(
    lipid_se=lipid_se_CL, ref_group="sgCtrl", split_chain=TRUE,
    chain_col="chain", radius=3, own_contri=0.5, permute_time=100)
# Get complete result summary
results <- odd_chain_result(res_se)
```

`plotRegion1D` *Plot region trends for one-dimensional lipid feature*

Description

Visualize analysis results for one-dimensional features to identify lipid feature tendencies. The plots highlight regions of significant differences between case and control samples: blue areas indicate significantly lower abundance in case samples, while red areas indicate significantly higher abundance.

Usage

```
plotRegion1D(object, p_cutoff = 0.05, y_scale = "identity")

## S4 method for signature 'LipidTrendSE'
plotRegion1D(object, p_cutoff = 0.05, y_scale = "identity")
```

Arguments

`object`	A LipidTrendSE object containing analysis results.
`p_cutoff`	Numeric. Significance level. The range is 0 to 1. Default is `0.05`.
`y_scale`	Character. Choose one of the y-axis scales: "identity", "log2", "log10", or "sqrt". Default is `"identity"`.

Value

For split chain analyses, a list with two elements:

`even_result`	Plot for even chain features, or NULL if none exist
`odd_result`	Plot for odd chain features, or NULL if none exist

For non-split analyses, a single plot.

See Also

`analyzeLipidRegion` for generating the input LipidTrendSE object

Examples

```
data("lipid_se_CL")
res_se <- analyzeLipidRegion(
    lipid_se=lipid_se_CL, ref_group="sgCtrl", split_chain=FALSE,
    chain_col=NULL, radius=2, own_contri=0.5, permute_time=100,
    abund_weight=TRUE)
plot <- plotRegion1D(res_se, p_cutoff=0.05, y_scale='identity')
```

plotRegion2D *Plot region trends for two-dimensional lipid features*

Description

plotRegion2D visualizes lipid trend analysis results in two dimensions. The returned heatmap will show the results.

Usage

```
plotRegion2D(object, p_cutoff = 0.05, log2FC_cutoff = 3)

## S4 method for signature 'LipidTrendSE'
plotRegion2D(object, p_cutoff = 0.05, log2FC_cutoff = 3)
```

Arguments

object	A LipidTrendSE object containing analysis results.
p_cutoff	Numeric. Significance level. The range is 0 to 1. Default is 0.05.
log2FC_cutoff	Numeric. Significant level of log2-transformed fold change. Default is 3.

Value

For split chain analyses, a list with two elements:

even_result	Heatmap for even chain features, or NULL if none exist
odd_result	Heatmap for odd chain features, or NULL if none exist

For non-split analyses, a single heatmap.

See Also

analyzeLipidRegion for generating the input LipidTrendSE object

Examples

```
data("lipid_se_2D")
res_se <- analyzeLipidRegion(
    lipid_se=lipid_se_2D, ref_group="sgCtrl", split_chain=FALSE,
    chain_col=NULL, radius=3, own_contri=0.5, permute_time=100,
    abund_weight=TRUE)
plot_2D <- plotRegion2D(res_se, p_cutoff=0.05)
```

result *Get Result from LipidTrendSE*

Description

Get Result from LipidTrendSE

Usage

```
result(object)

## S4 method for signature 'LipidTrendSE'
result(object)
```

Arguments

object	A LipidTrendSE object

Value

A data frame containing analysis results or NULL

Examples

```
data("lipid_se_CL")
res_se <- analyzeLipidRegion(
    lipid_se=lipid_se_CL, ref_group="sgCtrl", split_chain=FALSE,
    chain_col=NULL, radius=3, own_contri=0.5, permute_time=100)
# Get complete result
results <- result(res_se)
```

show,LipidTrendSE-method *Show method for LipidTrendSE objects*

Description

Show method for LipidTrendSE objects

Usage

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

Arguments

object	A LipidTrendSE object

Value

LipidTrendSE object information

Index