Package: LipidTrend (via r-universe)

June 16, 2026

Title LipidTrend: Analysis and Visualization of Lipid Feature Tendencies

Version 1.2.0

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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Imports dplyr, ggnewscale, ggplot2, magrittr, methods, rlang, SummarizedExperiment, matrixTests

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Enhances data.table,

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Contents

`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

An object of class `matrix` (inherits from `array`) with 137 rows and 6 columns.

Value

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

An object of class `matrix` (inherits from `array`) with 29 rows and 6 columns.

Value

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

Performs region-based statistical analysis to identify lipidomic trends between groups. This function applies a two-stage procedure:

1. **Marginal Test**: Each lipid feature is first tested individually using either a t-test (with glog10 transformation) or a Wilcoxon test to obtain marginal statistics and p-values.
2. **Region-Based Permutation Test with Smoothing**: Marginal statistics are smoothed using a Gaussian kernel that incorporates neighborhood information (e.g., proximity in chain length or double bond count). Statistical significance is assessed by comparing the smoothed statistic against a null distribution generated through permutation.

This approach enhances statistical robustness, especially for small-sample datasets. It supports both one-dimensional and two-dimensional analyses depending on the number of features provided in the input.

The input must be a `SummarizedExperiment` object, and the output is a `LipidTrendSE` object, which can be used for result visualization or further downstream analysis.

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:

1. Assay: A matrix containing lipid abundance data, where rows represent lipids and columns represent samples.
2. 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.

3. 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 in `rowData` that specifies chain length. Must be provided if `split_chain=TRUE`, otherwise should be set to `NULL`. Default is `NULL`.

`radius` Numeric. Distance of neighboring features to be included in the smoothing kernel. Default is `3`.

`own_contri` Numeric. Proportion of self-contribution when smoothing. Default is `0.5`. Recommended range: 0.5–1 to avoid over-emphasizing neighbors.

`test` Character. Type of statistical test: either `"t.test"` or `"Wilcoxon"`. Default is `"t.test"`.

`abund_weight` Logical. Whether to use average abundance as a weight in calculating the region-based smoothed statistic. When set to TRUE, lipid species with higher mean abundance contribute more to the smoothed trend. Default is `TRUE`.

`permute_time` Integer. Number of permutations used to calculate empirical p-values in the region-based permutation test. Default is `100000`. For the Wilcoxon test (i.e., `test="Wilcoxon"`), we recommend setting `permute_time` to fewer than 10,000 to ensure reasonable runtime.

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, test="t.test",
    abund_weight=TRUE, 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

An object of class `data.frame` with 137 rows and 2 columns.

Value

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

An object of class `data.frame` with 29 rows and 1 columns.

Value

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. The result table includes the following columns:

1. Feature columns: Lipid feature values from the input `rowData`, such as chain length or double bond count. Column names vary depending on input.
2. avg.abund: Mean abundance of each lipid across all samples. For one-dimensional analysis, this may also include `avg.abund.ctrl` and `avg.abund.case` for group-wise means.
3. direction: Sign of the smoothed statistic:
   - + : Trend increases in the case group.
   - - : Trend decreases in the case group.
4. smoothing.pval.BH: Benjamini–Hochberg adjusted p-value from the region-based permutation test.
5. marginal.pval.BH: Benjamini–Hochberg adjusted p-value from the marginal test (per lipid).
6. log2.FC: Log2 fold-change in abundance between case and control groups.

7. significance: Overall significance label based on smoothed test and FC direction:
    - Increase: Significant positive trend in case group.
    - Decrease: Significant negative trend in case group.
    - NS: Not significant.

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

An object of class `data.frame` with 6 rows and 3 columns.

Value

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)
```

lipid_se_2D *Example Dataset for two-dimensional data*

Description

Example Dataset for two-dimensional data

Usage

```
data(lipid_se_2D)
```

Format

An object of class `SummarizedExperiment` with 137 rows and 6 columns.

Value

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

An object of class `SummarizedExperiment` with 29 rows and 6 columns.

Value

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)
```

LipidTrendSE-class *Class for storing analyzeLipidRegion analysis results*

Description

This class extends SummarizedExperiment to store analyzeLipidRegion analysis results

Slots

split_chain Logical. Indicates whether chains were split by parity (even vs. odd). When TRUE, results are stored in even_chain_result and odd_chain_result slots. 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_chain is TRUE)

odd_chain_result Data frame of results for odd chains (when split_chain is TRUE)

abund_weight Logical. Logical. Set to TRUE to incorporate average lipid abundance as a weight in the test statistic.

LipidTrendSE-validity *Validate LipidTrendSE object*

Description

Validate LipidTrendSE object

Arguments

object A LipidTrendSE object to validate

Value

TRUE if valid, otherwise an error message

`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. The result table includes the following columns:

1. Feature columns: Lipid feature values from the input `rowData`, such as chain length or double bond count. Column names vary depending on input.
2. avg.abund: Mean abundance of each lipid across all samples. For one-dimensional analysis, this may also include `avg.abund.ctrl` and `avg.abund.case` for group-wise means.
3. direction: Sign of the smoothed statistic:
   - + : Trend increases in the case group.
   - - : Trend decreases in the case group.
4. smoothing.pval.BH: Benjamini–Hochberg adjusted p-value from the region-based permutation test.
5. marginal.pval.BH: Benjamini–Hochberg adjusted p-value from the marginal test (per lipid).
6. log2.FC: Log2 fold-change in abundance between case and control groups.
7. significance: Overall significance label based on smoothed test and FC direction:
   - Increase: Significant positive trend in case group.
   - Decrease: Significant negative trend in case group.
   - NS: Not significant.

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 lipid trends from one-dimensional analysis results. The plot highlights regions of significant group differences based on the smoothed permutation test. Blue and red ribbons mark where the trend significantly decreases or increases, respectively, in the case group compared to the control group. Each point represents the mean abundance within each group (case vs. control) for a specific lipid feature. This visualization helps identify not only abundance differences but also the specific lipid feature regions where trends diverge between groups.

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 generated by analyzeLipidRegion() for one-dimensional feature analysis.
p_cutoff	Numeric. Significance threshold for highlighting regions based on smoothed permutation p-values. Default is 0.05.
y_scale	Character. Scale of the y-axis. Choose from "identity", "log2", "log10", or "sqrt". Default is "identity".

Value

If split_chain=TRUE in the analysis, the function returns a list containing two plots:

1. even_result: A ggplot object visualizing trends for even-chain lipids, or NULL if no such lipids exist.
2. odd_result: A ggplot object visualizing trends for odd-chain lipids, or NULL if no such lipids exist.

If split_chain=FALSE, the function returns a single ggplot object visualizing the trend for all lipids combined.

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, test="t.test",
    abund_weight=TRUE, permute_time=100)
plot <- plotRegion1D(res_se, p_cutoff=0.05, y_scale='identity')
```

---

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

Description

Visualize lipid trend analysis results in two-dimensional feature space (e.g., chain length vs. double bond count). The resulting heatmap highlights regions with significant trends between groups based on the smoothed permutation test.

Each point in the heatmap represents a lipid defined by two continuous features (such as chain length and double bond). Color indicates the log2 fold-change between groups, and asterisks denote levels of marginal significance. If `abund_weight=TRUE` during analysis, the point size reflects the mean abundance of each lipid. If `abund_weight=FALSE`, all points are displayed with equal size.

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 generated by `analyzeLipidRegion()` for two-dimensional analysis.
`p_cutoff`	Numeric. Significance threshold for smoothed permutation p-values. Default is `0.05`.
`log2FC_cutoff`	Numeric. Threshold for absolute log2 fold-change used to truncate the color scale in the heatmap. Values exceeding this threshold will be capped at the cutoff value for visualization purposes. Default is `3`.

Value

If `split_chain=TRUE` in the analysis, the function returns a list with:

1. even_result: A ggplot object for even-chain lipids, or `NULL` if none exist.
2. odd_result: A ggplot object for odd-chain lipids, or `NULL` if none exist.

If `split_chain=FALSE`, the function returns a single ggplot object visualizing all lipids together.

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, test="t.test",
    abund_weight=TRUE, permute_time=100)
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. The result table includes the following columns:

1. Feature columns: Lipid feature values from the input rowData, such as chain length or double bond count. Column names vary depending on input.
2. avg.abund: Mean abundance of each lipid across all samples. For one-dimensional analysis, this may also include avg.abund.ctrl and avg.abund.case for group-wise means.
3. direction: Sign of the smoothed statistic:
   - + : Trend increases in the case group.
   - - : Trend decreases in the case group.
4. smoothing.pval.BH: Benjamini–Hochberg adjusted p-value from the region-based permutation test.
5. marginal.pval.BH: Benjamini–Hochberg adjusted p-value from the marginal test (per lipid).
6. log2.FC: Log2 fold-change in abundance between case and control groups.
7. significance: Overall significance label based on smoothed test and FC direction:

- Increase: Significant positive trend in case group.
- Decrease: Significant negative trend in case group.
- NS: Not significant.

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