

Package: LipidTrend (via r-universe)

October 8, 2026

Title LipidTrend: Analysis and Visualization of Lipid Feature Tendencies

Version 1.3.1

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>

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Contents

abundance_2D	2
abundance_CL	3
analyzeLipidRegion	4
char_table_2D	5
char_table_CL	6
even_chain_result	7
group_info	8
lipid_se_2D	8
lipid_se_CL	9
LipidTrendSE-class	9
LipidTrendSE-validity	10
odd_chain_result	10
plotRegion1D	11
plotRegion2D	12
regionalTestFC	14
result	15
show,LipidTrendSE-method	16
Index	18

abundance_2D	<i>Example lipid abundance data for two-dimensional LipidTrend analysis</i>
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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	<i>Conduct statistical to analyze lipid features tendencies</i>
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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). The kernel weights a feature's own marginal statistic equally against its neighbors' (fixed 0.5 self-contribution, not user-adjustable, to prevent tuning this parameter toward a desired result). 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, test="t.test", abund_weight=TRUE,
  permute_time=100000)
```

Arguments

lipid_se	A <code>SummarizedExperiment</code> 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 <code>RowData</code> contains one column, a one-dimensional analysis will be performed. If <code>rowData</code> 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 <code>colData\$group</code> 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.
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, test="t.test",
  abund_weight=TRUE, permute_time=100)
```

char_table_2D	<i>Example lipid characteristics table for two-dimensional LipidTrend analysis</i>
---------------	--

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	<i>Example lipid characteristics table for one-dimensional LipidTrend analysis</i>
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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	<i>Get Even Chain Result from LipidTrendSE</i>
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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, 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)
```

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)
```

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, 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. Blue and red ribbons highlight regions where the trend significantly decreases or increases, respectively, in the case group compared to the control group; a direction is shaded only after its region-level paired t-test (see [regionalTestFC](#)) passes at regional_p_cutoff. 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.

The paired t-test is only reliable with more than 5 significant features in a direction. When either direction in a figure has 5 or fewer, there are too few features to run the test, and the whole figure falls back to shading by the smoothed permutation test alone (smoothing.pval.BH < p_cutoff) instead, so a single figure never mixes two different statistical criteria.

Usage

```
plotRegion1D(object, p_cutoff=0.05, regional_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 that defines region membership: a feature belongs to a region when its smoothed permutation p-value falls below this threshold (<code>smoothing.pval.BH < p_cutoff</code>). This membership determines both which regions are shaded by default and, when more than 5 features qualify in a direction, which features are fed into the region-level paired t-test used by regionalTestFC . Default is 0.05.
regional_p_cutoff	Numeric. Significance threshold applied afterward to the region-level paired t-test p-value itself (see regionalTestFC), deciding whether an already-defined region stays shaded. Only takes effect when both directions have more than 5 significant features (per p_cutoff); otherwise ignored, and shading falls back to p_cutoff alone. 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 [regionalTestFC](#) for the region-level validation statistics

Examples

```
data("lipid_se_CL")
res_se <- analyzeLipidRegion(
  lipid_se=lipid_se_CL, ref_group="sgCtrl", split_chain=FALSE,
  chain_col=NULL, radius=2, test="t.test",
  abund_weight=TRUE, permute_time=100)
plot <- plotRegion1D(res_se, p_cutoff=0.05, y_scale='identity')
```

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; a direction is shaded only after its region-level paired t-test (see [regionalTestFC](#)) passes at `regional_p_cutoff`.

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.

The paired t-test is only reliable with more than 5 significant features in a direction. When either direction in a figure has 5 or fewer, there are too few features to run the test, and the whole figure falls back to shading by the smoothed permutation test alone (`smoothing.pval.BH < p_cutoff`) instead, so a single figure never mixes two different statistical criteria.

Usage

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

Arguments

<code>object</code>	A <code>LipidTrendSE</code> object generated by <code>analyzeLipidRegion()</code> for two-dimensional analysis.
<code>p_cutoff</code>	Numeric. Significance threshold that defines region membership: a feature belongs to a region when its smoothed permutation p-value falls below this threshold (<code>smoothing.pval.BH < p_cutoff</code>). This membership determines both which regions are shaded by default and, when more than 5 features qualify in a direction, which features are fed into the region-level paired t-test used by regionalTestFC . Default is 0.05.
<code>regional_p_cutoff</code>	Numeric. Significance threshold applied afterward to the region-level paired t-test p-value itself (see regionalTestFC), deciding whether an already-defined region stays shaded. Only takes effect when both directions have more than 5 significant features (per <code>p_cutoff</code>); otherwise ignored, and shading falls back to <code>p_cutoff</code> alone. Default is 0.05.
<code>log2FC_cutoff</code>	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 [regionalTestFC](#) for the region-level validation statistics

Examples

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

regionalTestFC

*Regional Paired T-Test and Fold-Change for Significant Trend Regions***Description**

For each significant trend region identified by [analyzeLipidRegion](#) (Increase / Decrease), performs an independent region-level paired t-test on feature-wise group-mean abundances (feature = pairing unit), and summarizes the region's fold-change. This provides an explainable, permutation-free statistic to accompany the smoothed permutation test result, and is also used internally by [plotRegion1D](#)/[plotRegion2D](#) to validate large regions before coloring them (see their `regional_p_cutoff` argument for the significance level applied to `regional.test.pval` in that decision).

Usage

```
regionalTestFC(object, p_cutoff = 0.05)

## S4 method for signature 'LipidTrendSE'
regionalTestFC(object, p_cutoff = 0.05)
```

Arguments

object	A LipidTrendSE object generated by analyzeLipidRegion() .
p_cutoff	Numeric. Significance threshold used to define which features belong to a region, based on the smoothed permutation test (<code>smoothing.pval.BH < p_cutoff</code>). Should match the <code>p_cutoff</code> used when visualizing the same result with plotRegion1D / plotRegion2D . Default is 0.05.

Value

A data frame with one row per direction (Increase/Decrease):

direction "Increase" or "Decrease".

n.features Number of significant features in that direction.

regional.test.pval Paired t-test p-value on feature-wise group-mean abundance across the significant features. NA when `n.features <= 5` (a paired t-test on 5 or fewer pairs is too underpowered to be trustworthy).

regional.FC Regional fold-change on the linear scale. This is the **median** fold-change across the significant features in that direction – a median rather than a mean, so that a single extreme feature cannot dominate the summary of the region.

log2.regional.FC The same quantity on the log2 scale: the median log2 fold-change across those features. Equal to `log2(regional.FC)`.

If `split_chain=TRUE` in the analysis, a list with `even_result`/`odd_result` data frames as above.

See Also

[analyzeLipidRegion](#) for generating the input `LipidTrendSE` object [plotRegion1D](#) and [plotRegion2D](#) for 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, permute_time=100)
tab <- regionalTestFC(res_se)
```

result	<i>Get Result from LipidTrendSE</i>
--------	-------------------------------------

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, 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

abundance_2D, [2](#)
abundance_CL, [3](#)
analyzeLipidRegion, [4](#), [12](#), [14](#), [15](#)

char_table_2D, [5](#)
char_table_CL, [6](#)

even_chain_result, [7](#)
even_chain_result, LipidTrendSE-method
 (even_chain_result), [7](#)

group_info, [8](#)

lipid_se_2D, [8](#)
lipid_se_CL, [9](#)
LipidTrendSE-class, [9](#)
LipidTrendSE-validity, [10](#)

odd_chain_result, [10](#)
odd_chain_result, LipidTrendSE-method
 (odd_chain_result), [10](#)

plotRegion1D, [5](#), [11](#), [14](#), [15](#)
plotRegion1D, LipidTrendSE-method
 (plotRegion1D), [11](#)
plotRegion2D, [5](#), [12](#), [14](#), [15](#)
plotRegion2D, LipidTrendSE-method
 (plotRegion2D), [12](#)

regionalTestFC, [11–13](#), [14](#), [14](#)
regionalTestFC, LipidTrendSE-method
 (regionalTestFC), [14](#)
result, [15](#)
result, LipidTrendSE-method (result), [15](#)

show, LipidTrendSE-method, [16](#)