Package 'BioGSP'

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Description Implementation of Graph Signal Processing (GSP) methods including Spectral Graph Wavelet Transform (SGWT) for analyzing spatial patterns in biological data. Based on Hammond, Vandergheynst, and Gribonval (2011) ``Wavelets on Graphs via Spectral Graph Theory". Provides tools for multi-scale analysis of spatial signals, including forward and inverse transforms, energy analysis, and visualization functions tailored for biological applications.
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Description

The BioGSP package provides a comprehensive implementation of Graph Signal Processing (GSP) methods including Spectral Graph Wavelet Transform (SGWT) for analyzing spatial patterns in biological data. This implementation is based on Hammond, Vandergheynst, and Gribonval (2011) "Wavelets on Graphs via Spectral Graph Theory".

Details

The package enables multi-scale analysis of spatial signals by:

- Building graphs from spatial coordinates using k-nearest neighbors
- Computing graph Laplacian eigendecomposition for spectral analysis
- Designing wavelets in the spectral domain using various kernel functions
- Decomposing signals into scaling and wavelet components at multiple scales
- Providing reconstruction capabilities with error analysis
- · Offering comprehensive visualization and analysis tools

Main Functions

```
sgwt_forward Forward SGWT transform
sgwt_inverse Inverse SGWT transform
sgwt_energy_analysis Energy distribution analysis
plot_sgwt_decomposition Visualization of SGWT components
Cal_GCC Graph Cross-Correlation analysis
demo_sgwt Demonstration with synthetic data
```

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Applications

The BioGSP package is particularly useful for:

- Spatial biology: Analyzing cell distribution patterns in tissue imaging (CODEX, Visium, etc.)
- Single-cell genomics: Spatial transcriptomics and proteomics analysis
- Neuroscience: Brain connectivity and signal analysis
- Pathology: Tumor microenvironment and tissue architecture analysis
- Developmental biology: Spatial pattern formation and cell fate mapping
- Immunology: Immune cell spatial organization and interactions

Author(s)

BioGSP Development Team

References

Hammond, D. K., Vandergheynst, P., & Gribonval, R. (2011). Wavelets on graphs via spectral graph theory. Applied and Computational Harmonic Analysis, 30(2), 129-150.

```
## Not run:
# Load the package
library(BioGSP)
# Run a quick demo
demo_result <- demo_sgwt()</pre>
# Generate synthetic data
set.seed(123)
n < -100
data <- data.frame(</pre>
 x = runif(n, 0, 10),
  y = runif(n, 0, 10),
  signal = sin(runif(n, 0, 2*pi))
# Apply SGWT
result <- SGWT(data, signal = "signal", k = 8, J = 4)
# Analyze results
energy_analysis <- sgwt_energy_analysis(result)</pre>
print(energy_analysis)
## End(Not run)
```

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Cal_Eigen

Calculate eigenvalues and eigenvectors with knee detection

Description

Calculate eigenvalues and eigenvectors of a spatial graph with automatic detection of the low-frequency cutoff using knee detection

Usage

```
Cal_Eigen(data.in = NULL, k = 25, k_fold = 15, sensitivity = 2)
```

Arguments

```
data.in Data frame with x and y coordinates

k Number of nearest neighbors (default: 25)

k_fold Eigendecomposition parameter (default: 15)

sensitivity Sensitivity parameter for knee detection (default: 2)
```

Value

List containing knee point, eigenvectors, and eigenvalues

Examples

```
## Not run:
# Create spatial data
data <- data.frame(x = runif(100), y = runif(100))
result <- Cal_Eigen(data, k = 10)
## End(Not run)</pre>
```

Cal_GCC

Calculate Graph Cross-Correlation (GCC)

Description

Calculate Graph Cross-Correlation between two signals using Graph Fourier Transform

Usage

```
Cal_GCC(
  data.in = NULL,
  knee = NULL,
  signal1 = NULL,
  signal2 = NULL,
  eigenvector = NULL)
```

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Arguments

data.in	Data frame containing the signals
knee	Knee point for frequency cutoff
signal1	Name of first signal column
signal2	Name of second signal column
eigenvector	Matrix of eigenvectors

Value

Cosine similarity value

Examples

```
## Not run:
# Assuming you have data with two signals and eigenvectors
# gcc_value <- Cal_GCC(data, knee = 10, signal1 = "sig1", signal2 = "sig2", eigenvector =
## End(Not run)</pre>
```

cal_laplacian

Calculate Graph Laplacian Matrix

Description

Compute unnormalized, normalized, or random-walk Laplacian from an adjacency matrix.

Usage

```
cal_laplacian(W, type = c("unnormalized", "normalized", "randomwalk"))
```

Arguments

W A square adjacency matrix (can be dense or sparse).

type Type of Laplacian to compute: "unnormalized", "normalized", or "randomwalk".

Value

Laplacian matrix of the same class as input.

```
## Not run:
W <- matrix(c(0, 1, 1, 1, 0, 1, 1, 1, 0), nrow = 3)
cal_laplacian(W, type = "normalized")
## End(Not run)</pre>
```

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codex_toy_data

Toy CODEX Spatial Cell Type Data

Description

A synthetic dataset mimicking CODEX multiplexed imaging data for demonstrating Spectral Graph Wavelet Transform (SGWT) analysis on spatial cell type distributions. The dataset contains spatial coordinates and cell type annotations for multiple immune cell populations arranged in realistic spatial clusters.

Usage

```
codex_toy_data
```

Format

A data frame with 18604 rows and 5 columns:

cellLabel Character. Unique identifier for each cell

Y_cent Numeric. Y coordinate of cell centroid (0-115 range)

X_cent Numeric. X coordinate of cell centroid (0-116 range)

Annotation5 Character. Full descriptive cell type name

ROI_num Character. Region of interest identifier ("ROI_0" through "ROI_15")

Details

The dataset contains 16 regions of interest (ROI_0 through ROI_15) with different spatial patterns and varying cell counts (945-1497 cells per ROI). Each ROI represents a distinct tissue region with unique spatial arrangements of the same cell types.

ROI Distribution:

- **ROI_0**: 952 cells
- ROI_1: 945 cells
- ROI_2: 1155 cells
- **ROI_3**: 1421 cells
- **ROI_4**: 1096 cells
- ROI_5: 1420 cells
- ROI_6-ROI_15: 958-1497 cells each

Cell types across all ROIs include:

- BCL6- B Cell (~3719 cells): Primary B cell population
- CD4 T (~4092 cells): Helper T cells largest population
- CD8 T (~3346 cells): Cytotoxic T cells
- DC (~2233 cells): Dendritic cells
- M1 (~1490 cells): M1 macrophages
- CD4 Treg (~1490 cells): Regulatory T cells

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- BCL6+ B Cell (~931 cells): Activated B cells
- Endothelial (~746 cells): Vascular cells
- M2 (~370 cells): M2 macrophages
- Myeloid (~186 cells): Other myeloid cells
- Other (~1 cells): Miscellaneous cell types

This synthetic data is designed to demonstrate:

- Spatial clustering patterns of different cell types
- Multi-scale spatial analysis using SGWT
- Cross-cell type correlation analysis
- Graph construction and eigenvalue analysis
- Wavelet decomposition of spatial signals

Source

Generated synthetically using clustered normal distributions with realistic parameters based on real CODEX data characteristics.

```
# Load the toy dataset
data(codex_toy_data)
# Examine the structure
str(codex_toy_data)
head(codex_toy_data)
# Summary of cell types
table(codex_toy_data$Annotation5)
# Summary by ROI
table(codex_toy_data$ROI_num)
table(codex_toy_data$ROI_num, codex_toy_data$Annotation5)
# Quick visualization of spatial distribution
if (requireNamespace("ggplot2", quietly = TRUE)) {
  library(ggplot2)
  ggplot(codex\_toy\_data, aes(x = X\_cent, y = Y\_cent, color = Annotation5)) +
    geom\_point(size = 0.8, alpha = 0.7) +
    facet_wrap(~ROI_num, scales = "free") +
    labs(title = "Toy CODEX Spatial Cell Distribution by ROI",
         x = "X Coordinate", y = "Y Coordinate") +
    theme_minimal() +
    scale_y_reverse()
}
# Basic SGWT analysis example
## Not run:
# Focus on BCL6- B Cell cells in ROI_1 for SGWT analysis
bcl6nb_data <- codex_toy_data[codex_toy_data$Annotation5 == "BCL6- B Cell" &
                              codex_toy_data$ROI_num == "ROI_1", ]
# Create binned representation
```

```
library(dplyr)
binned_data <- codex_toy_data %>%
  filter(Annotation5 == "BCL6- B Cell", ROI_num == "ROI_1") %>%
    x_bin = cut(X_cent, breaks = 20, labels = FALSE),
    y_bin = cut(Y_cent, breaks = 20, labels = FALSE)
  ) 응>응
  group_by(x_bin, y_bin) %>%
  summarise(cell_count = n(), .groups = 'drop')
# Prepare for SGWT
complete_grid <- expand.grid(x_bin = 1:20, y_bin = 1:20)</pre>
sgwt_data <- complete_grid %>%
  left_join(binned_data, by = c("x_bin", "y_bin")) %>%
   cell_count = ifelse(is.na(cell_count), 0, cell_count),
   x = x_bin,
    y = y_bin,
    signal = cell_count / max(cell_count, na.rm = TRUE)
  select(x, y, signal)
# Apply SGWT
sgwt_result <- SGWT(data.in = sgwt_data,
                    signal = "signal",
                    k = 8,
                    J = 3,
                    kernel_type = "mexican_hat")
## End(Not run)
```

```
compare_kernel_families
```

Compare different kernel families

Description

Visualize and compare different kernel families (both scaling and wavelet filters)

Usage

```
compare_kernel_families(
  x_range = c(0, 3),
  scale_param = 1,
  plot_results = TRUE
)
```

Arguments

```
x_range Range of x values to evaluate (default: c(0,3))
scale_param Scale parameter for all functions (default: 1)
plot_results Whether to plot the comparison (default: TRUE)
```

compute_sgwt_filters 9

Value

Data frame with x values and kernel values for each family

Examples

Description

Compute wavelet and scaling function coefficients in the spectral domain

Usage

```
compute_sgwt_filters(
  eigenvalues,
  scales,
  lmax = NULL,
  kernel_type = "mexican_hat"
)
```

Arguments

Value

List of filters (scaling function + wavelets)

```
eigenvals <- c(0, 0.1, 0.5, 1.0, 1.5)
scales <- c(2, 1, 0.5)
filters <- compute_sgwt_filters(eigenvals, scales)
filters_meyer <- compute_sgwt_filters(eigenvals, scales, kernel_type = "meyer")
filters_heat <- compute_sgwt_filters(eigenvals, scales, kernel_type = "heat")</pre>
```

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```
cosine_similarity Calculate cosine similarity between two vectors
```

Description

Calculate cosine similarity between two numeric vectors

Usage

```
cosine_similarity(x, y)
```

Arguments

```
x First vectory Second vector
```

Value

Cosine similarity value (between -1 and 1)

Examples

```
x \leftarrow c(1, 2, 3)

y \leftarrow c(2, 3, 4)

similarity \leftarrow cosine\_similarity(x, y)
```

demo_sgwt

 $Demo\ function\ for\ SGWT$

Description

Demonstration function showing basic SGWT usage with synthetic data

Usage

```
demo_sgwt()
```

Value

List containing demo data, SGWT results, and energy analysis

```
## Not run:
demo_result <- demo_sgwt()
print(demo_result$energy)
## End(Not run)</pre>
```

FastDecompositionLap

Fast eigendecomposition of Laplacian matrix

Description

Perform fast eigendecomposition using RSpectra for large matrices

Usage

```
FastDecompositionLap(
  laplacianMat = NULL,
  k_fold = 1.5,
  which = "LM",
  sigma = NULL,
  opts = list(),
  lower = TRUE,
  ...
)
```

Arguments

```
laplacianMat Laplacian matrix

k_fold Multiplier for number of eigenvalues to compute (default: 1.5)

which Which eigenvalues to compute ("LM", "SM", etc.)

sigma Shift parameter for eigenvalue computation

opts Additional options for eigenvalue computation

lower Whether to compute from lower end of spectrum

... Additional arguments
```

Value

List with eigenvalues (evalues) and eigenvectors (evectors)

```
## Not run:
# Create a Laplacian matrix and decompose
L <- matrix(c(2, -1, -1, -1, 2, -1, -1, -1, 2), nrow = 3)
decomp <- FastDecompositionLap(L, k_fold = 2)
## End(Not run)</pre>
```

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find_knee_point

Find knee point in a curve

Description

Simple knee point detection using the maximum curvature method

Usage

```
find_knee_point(y, sensitivity = 1)
```

Arguments

```
y Numeric vector of y values sensitivity Sensitivity parameter (not used in this simple implementation)
```

Value

Index of the knee point

Examples

```
y \leftarrow c(1, 2, 3, 10, 11, 12) # curve with a knee knee_idx <- find_knee_point(y)
```

gft

Graph Fourier Transform

Description

Compute the Graph Fourier Transform (GFT) of a signal using Laplacian eigenvectors.

Usage

```
gft(signal, U)
```

Arguments

signal Input signal (vector or matrix)

U Matrix of eigenvectors (dense matrix preferred)

Value

Transformed signal in the spectral domain (vector or matrix)

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hello_sgwt

Hello function for SGWT package demonstration

Description

Simple hello function to demonstrate package loading

Usage

```
hello_sgwt()
```

Value

Character string with greeting

Examples

```
hello_sgwt()
```

install_and_load Install and load packages

Description

Utility function to install and load packages from CRAN or GitHub

Usage

```
install_and_load(packages)
```

Arguments

packages

Named vector where names are package names and values are source URLs

Value

NULL (side effect: installs and loads packages)

```
## Not run:
packages <- c("ggplot2" = "ggplot2", "devtools" = "r-lib/devtools")
install_and_load(packages)
## End(Not run)</pre>
```

Description

Plot frequency modes from graph Fourier analysis

Usage

```
plot_FM(input = NULL, FM_idx = c(1:20), ncol = 5)
```

Arguments

input Input data (currently not used, for future compatibility)

FM_idx Indices of frequency modes to plot (default: 1:20)

ncol Number of columns in plot layout (default: 5)

Value

Combined plot of frequency modes

Examples

```
## Not run:
# This function requires specific data structure (df_hex_combine)
# plot_FM(FM_idx = 1:10, ncol = 5)
## End(Not run)
```

```
plot_sgwt_decomposition
```

Plot SGWT decomposition results

Description

Visualize SGWT decomposition components including original signal, scaling function, wavelet coefficients, and reconstructed signal

Usage

```
plot_sgwt_decomposition(sgwt_result, data.in, plot_scales = NULL, ncol = 3)
```

Arguments

```
sgwt_result SGWT result object from SGWT() function
data.in Original data frame with spatial coordinates
plot_scales Which wavelet scales to plot (default: first 4)
ncol Number of columns in the plot layout (default: 3)
```

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Value

ggplot object with combined plots

Examples

```
## Not run:
# Assuming you have SGWT results
plots <- plot_sgwt_decomposition(sgwt_result, data.in)
print(plots)
## End(Not run)</pre>
```

SGWT

Spectral Graph Wavelet Transform (SGWT)

Description

Main function for performing Spectral Graph Wavelet Transform analysis on spatial data. Provides a comprehensive interface for multi-scale analysis of spatial signals using graph wavelets.

Usage

```
SGWT(
  data.in = NULL,
  signal = NULL,
  k = 25,
  scales = NULL,
  J = 5,
  scaling_factor = 2,
  kernel_type = "mexican_hat",
  laplacian_type = "normalized",
  k_fold = 15,
  return_all = TRUE
)
```

Arguments

data.in	Data frame containing spatial coordinates and signal data. Must contain columns 'x' and 'y' for spatial coordinates.				
signal	Character string specifying the column name of the signal to analyze, or a numeric vector of signal values.				
k	Number of nearest neighbors for graph construction (default: 25)				
scales	Vector of scales for the wavelets. If NULL, scales are auto-generated.				
J	Number of scales to generate if scales is NULL (default: 5)				
scaling_factor					
	Scaling factor between consecutive scales (default: 2)				
kernel_type	Kernel family ("mexican_hat", "meyer", or "heat") that defines both scaling and wavelet filters				

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Value

```
If return_all = TRUE, returns a list containing:

decomposition SGWT decomposition results

reconstructed_signal Reconstructed signal for validation

reconstruction_error RMSE between original and reconstructed signal

original_signal Original input signal

graph_info Graph construction information (adjacency matrix, Laplacian, eigenvalues, eigenvectors)

data Original input data

parameters Analysis parameters used

If return_all = FALSE, returns only the SGWT decomposition.
```

References

Hammond, D. K., Vandergheynst, P., & Gribonval, R. (2011). Wavelets on graphs via spectral graph theory. Applied and Computational Harmonic Analysis, 30(2), 129-150.

Examples

```
## Not run:
# Generate synthetic spatial data
set.seed(123)
n_points <- 100
x_coords <- rep(1:10, each = 10) + rnorm(n_points, 0, 0.1)
y_coords <- rep(1:10, times = 10) + rnorm(n_points, 0, 0.1)
signal_data <- sin(0.5 * x_coords) * cos(0.3 * y_coords) + rnorm(n_points, 0, 0.1)
demo_data <- data.frame(x = x_coords, y = y_coords, signal = signal_data)
# Apply SGWT
result <- SGWT(data.in = demo_data, signal = "signal", k = 8, J = 4)
# View reconstruction error
print(result$reconstruction_error)
## End(Not run)</pre>
```

sgwt-globals

Global variables used in ggplot2 aesthetics

Description

This file declares global variables used in ggplot2 aesthetics to avoid R CMD check NOTEs about undefined global functions or variables.

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```
sgwt_auto_scales Generate
```

Generate automatic scales for SGWT

Description

Generate logarithmically spaced scales for SGWT

Usage

```
sgwt_auto_scales(lmax, J = 5, scaling_factor = 2)
```

Arguments

Scaling factor between consecutive scales

Value

Vector of scales

Examples

```
scales <- sgwt_auto_scales(lmax = 2.0, J = 5, scaling_factor = 2)</pre>
```

```
sgwt_energy_analysis
```

Analyze SGWT energy distribution across scales

Description

Calculate and analyze energy distribution across different scales in the SGWT decomposition

Usage

```
sgwt_energy_analysis(sgwt_result)
```

Arguments

Value

Data frame with energy analysis results

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Examples

```
## Not run:
# Assuming you have SGWT results
energy_analysis <- sgwt_energy_analysis(sgwt_result)
print(energy_analysis)
## End(Not run)</pre>
```

sgwt_forward

Forward SGWT transform

Description

Decompose signal into wavelet coefficients using SGWT

Usage

```
sgwt_forward(
  signal,
  eigenvectors,
  eigenvalues,
  scales,
  lmax = NULL,
  kernel_type = "mexican_hat"
)
```

Arguments

```
signal Input signal vector

eigenvectors Eigenvectors of the graph Laplacian

eigenvalues Eigenvalues of the graph Laplacian

scales Vector of scales for the wavelets

lmax Maximum eigenvalue (optional)

kernel_type Kernel family that defines both scaling and wavelet filters (default: "mexican_hat", options: "mexican_hat", "meyer", "heat")
```

Value

List containing coefficients, filters, scales, eigenvalues, and eigenvectors

```
## Not run:
# Assuming you have eigenvalues, eigenvectors, and a signal
result <- sgwt_forward(signal, eigenvectors, eigenvalues, scales)
result_meyer <- sgwt_forward(signal, eigenvectors, eigenvalues, scales, kernel_type = "meresult_heat <- sgwt_forward(signal, eigenvectors, eigenvalues, scales, kernel_type = "heat"
## End(Not run)</pre>
```

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sgwt_get_kernels

Get a unified kernel family (low-pass and band-pass) by kernel_type

Description

Returns a pair of functions implementing the scaling (low-pass) and wavelet (band-pass) kernels for a given kernel family. This enforces consistency: a single kernel_type defines both filters.

Usage

```
sgwt_get_kernels(kernel_type = "mexican_hat")
```

Arguments

```
kernel_type Kernel family name ("mexican_hat", "meyer", or "heat")
```

Value

A list with two functions: $list(scaling = function(x, scale_param), wavelet = function(x, scale_param))$

sgwt_inverse

Inverse SGWT transform

Description

Reconstruct signal from wavelet coefficients

Usage

```
sgwt_inverse(sgwt_decomp)
```

Arguments

```
\verb|sgwt_decomp| SGWT | decomposition | object | from | sgwt_forward |
```

Value

Reconstructed signal vector

```
## Not run:
# Assuming you have an SGWT decomposition
reconstructed <- sgwt_inverse(sgwt_decomp)
## End(Not run)</pre>
```

```
visualize_sgwt_kernels
```

Visualize SGWT kernels and scaling functions

Description

Visualize the scaling function and wavelet kernels used in SGWT based on the eigenvalue spectrum and selected parameters

Usage

```
visualize_sgwt_kernels(
  eigenvalues,
  scales = NULL,
  J = 4,
  scaling_factor = 2,
  kernel_type = "mexican_hat",
  lmax = NULL,
  eigenvalue_range = NULL,
  resolution = 1000
)
```

Arguments

```
eigenvalues Vector of eigenvalues from graph Laplacian
scales Vector of scales for the wavelets (if NULL, auto-generated)

J Number of scales to generate if scales is NULL (default: 4)
scaling_factor
Scaling factor between consecutive scales (default: 2)
kernel_type Type of wavelet kernel ("mexican_hat" or "meyer", default: "mexican_hat")
lmax Maximum eigenvalue (optional, computed if NULL)
eigenvalue_range
Range of eigenvalues to plot (default: full range)
resolution Number of points for smooth curve plotting (default: 1000)
```

Value

List containing the filter visualization plot and filter values

```
## Not run:
# Generate some example eigenvalues
eigenvals <- seq(0, 2, length.out = 100)
# Visualize kernels with specific parameters
viz_result <- visualize_sgwt_kernels(
   eigenvalues = eigenvals,
   J = 4,
   scaling_factor = 2,</pre>
```

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```
kernel_type = "mexican_hat"
)
print(viz_result$plot)
## End(Not run)
```

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