MInfer: MInfer: Bridging MetaboAnalyst and Jacobian analysis for metabolomic networks

Overview

MInfer is an R package designed to streamline the analysis of metabolomics data. It offers tools for:

- Data preparation
- Covariance matrix generation
- Jacobian matrix computation
- Visualization of metabolite interaction networks

This package enables a seamless integration of MetaboAnalyst's capabilities with advanced Jacobian analysis, allowing researchers to explore dynamic interactions between metabolites comprehensively.

Installation

To begin using MInfer, follow these steps:

Prerequisites

Ensure that the `devtools` package is installed on your system:

```
install.packages("devtools")
```

Install MInfer from GitHub

Install the package directly from its repository:

```
devtools::install_github("cellbiomaths/MInfer")
```

Load the Package

Once installed, load the package into your R session:

```
library(MInfer)
```

Key Features

Targeted and Non-Targeted Data Support

- MInfer is designed for identified metabolites (targeted analysis).
- It also supports non-targeted metabolomics data, but only annotated compounds are mapped to pathways to ensure unbiased analysis.

Dynamic Interaction Analysis

- Generate Jacobian matrices to model interactions between metabolites under varying conditions.
- Visualize networks using heatmaps and 3D plots.

Flexible Data Preparation

- Select experimental conditions to focus your analysis.
- Generate covariance matrices for dynamic and network modeling.

Usage Examples

Workflow 1: Analyze a Metabolite Interaction Network (MIN)

Step 1: Define Metabolite IDs

Define a list of KEGG IDs to analyze. These IDs must be present in the dataset:

```
# Define metabolite IDs
input_ids <- c('C00042', 'C00149', 'C00036')

# Run the minfer function
results <- minfer(input_ids)

# Display the results
print(results)
```

Workflow 2: Compute and Visualize Jacobian Matrices

Step 1: Load Example Data

MInfer includes example datasets for quick testing:

```
# Load example data
data(example_data)
```

Step 2: Prepare Data

Select specific experimental conditions (e.g., 6°C and 16°C):

```
# Prepare data for two conditions
data_6C <- prepare_data(met_input, 6)
data_16C <- prepare_data(met_input, 16)
```

Step 3: Generate Covariance Matrices

Specify the number of time points using the `num_tp` parameter:

```
# Generate covariance matrices
cov_6C <- generate_covariance(data_6C, num_tp = 1)
cov_16C <- generate_covariance(data_16C, num_tp = 1)
```

Step 4: Calculate Jacobian Matrices

Use the covariance matrices to compute Jacobian matrices:

```
# Calculate Jacobian matrices
jacobian_6C <- calculate_jacobian(cov_6C[[1]], interactions_fin, icount = 15)
jacobian_16C <- calculate_jacobian(cov_16C[[1]], interactions_fin, icount =
15)
```

Step 5: Visualize Results

MInfer includes visualization tools for heatmaps and 3D plots:

```
# Heatmap visualization
visualize_heatmap(jacobian_6C$J, title = "Jacobian Matrix - 6°C")

# 3D visualization
visualize_3d(jacobian_16C$J)
```

Advanced Features

Targeted vs. Non-Targeted Data

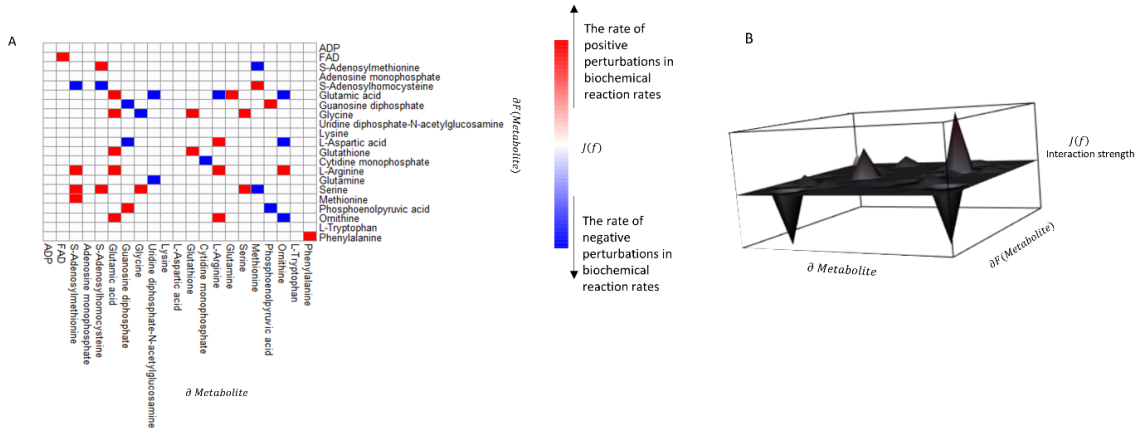
- **Targeted Analysis:** Works directly with identified metabolites for precise pathway mapping.
- **Non-Targeted Analysis:** Accepts datasets with unidentified metabolites but maps only annotated compounds to pathways, ensuring comprehensive yet unbiased results.

Time Point Flexibility

- The `num_tp` parameter allows modeling dynamic interactions across various time points.

Visualization

- Built-in tools offer both 2D (heatmap) (A) and 3D visualizations (B), facilitating clear interpretation of metabolite interactions.



Practical Tips

- **Ensure Data Compatibility:** Use datasets with KEGG IDs for accurate mapping.
- **Preprocess Data:** Focus on high-quality, annotated metabolites to enhance analysis reliability.
- **Combine Approaches:** Integrate MInfer results with external tools like MetaboAnalyst for broader insights.

Getting Help / Contact

For questions or support, contact the developers via the GitHub repository / https://github.com/cellbiomaths or https://github.com/JanaSchwarzerova / or email Jana.Schwarzerova@vut.cz / jana.schwarzerova2@fno.cz