Using sabinaHSBM for link prediction and network reconstruction using Hierarchical Stochastic Block Models

Example on how to use it to identify missing and spurious links with the full\_reconstruction method (with parallelized computation)

The *sabinaHSBM* package provides tools for link prediction and network reconstruction using hierarchical stochastic block models (HSBM). This document demonstrates a simple use for the full\_reconstruction method, showcasing how it handles missing and spurious links in an incomplete and error-prone network. To enhance computational efficiency during the prediction links step we leverage parallelized computation.

We use the example dataset dat included in the package to show key functionalities, including data preparation, link prediction, and network reconstruction.

# Loading Required Libraries

We begin by loading the required R packages. Missing packages are automatically installed.

# If the package is not installed, install it from GitHub  
# if (!requireNamespace("sabinaHSBM", quietly = TRUE)) {  
# library(remotes)  
# remotes::install\_github("h-lima/sabinaHSBM")  
# }  
  
# Load the sabinaHSBM package  
#library(sabinaHSBM)  
devtools::load\_all("/home/project\_hsbm/graph\_tool/sabinaHSBM/")

If the required packages are not already installed, install them from CRAN

list.of.packages <- c(  
 "dplyr",  
 "parallel",  
 "reshape2",  
 "reticulate",  
 "stringr",  
 "tidyr",  
 "ROCR",  
 "data.table"  
)  
  
new.packages <- list.of.packages[!(list.of.packages %in% installed.packages()[, "Package"])]  
if (length(new.packages) > 0) {  
 install.packages(new.packages, dependencies = TRUE)  
}  
  
for (package in list.of.packages) {  
 library(package, character.only = TRUE)  
}

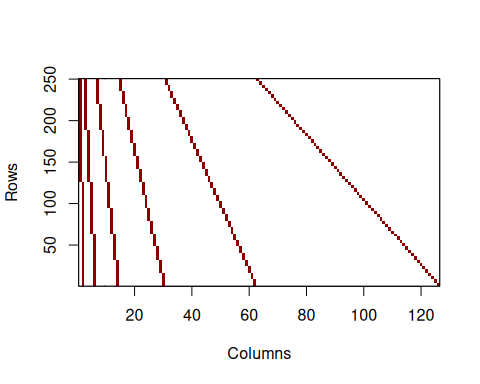
# Record starting time (optional)  
start\_time <- Sys.time()

# Load data

The dataset dat2 is a binary bipartite matrix representing a hypothetical species interactions network. Columns and rows correspond to two different types of nodes (e.g., hosts and parasites), and links (values of 1, in red) represent interaction between them while 0 (in black) represent lack of observed interaction. The distribution of these links follows a structured pattern.

# Load the dataset  
data(dat2, package = "sabinaHSBM")  
dat<- dat2

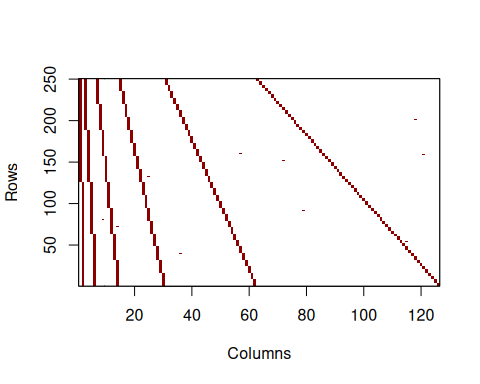
# Plot the original matrix  
plot\_interaction\_matrix(adj\_mat = dat, order\_mat = FALSE)



To simulate spurious links and address the full\_reconstruction method, we randomly add a small number of false positives (1) to the matrix. This controlled modification allows us to demonstrate how the method identifies both spurious links (observed but potentially erroneous interactions, false positives) and missing links (unobserved but likely interactions, false negatives).

# Add spurious links artificially  
set.seed(123)  
num\_spurious <- ceiling(sum(dat) \* 0.01) # Proportion of spurious links to add  
spurious\_links <- matrix(nrow = num\_spurious, ncol = 2)  
  
for (i in 1:num\_spurious) {  
 repeat {  
 random\_row <- sample(1:nrow(dat), 1)  
 random\_col <- sample(1:ncol(dat), 1)  
   
 if (dat[random\_row, random\_col] == 0) {  
 dat[random\_row, random\_col] <- 1  
 spurious\_links[i,] <- c(random\_row, random\_col)  
 break  
 }  
 }  
 }

# Plot the matrix with spurious  
plot\_interaction\_matrix(dat, order\_mat = FALSE)



# Preparing Input data for HSBM

The hsbm.input function pre-processes the dataset, creating cross-validation folds and edge lists required for modeling. Here, we use 5-fold cross-validation and the full\_reconstruction method.

# Prepare input data  
n\_folds <- 5 # Number of folds for cross-validation  
  
myInput <- hsbm.input(  
 dat, # Binary bipartite matrix of observed links  
 n\_folds = n\_folds,  
 add\_spurious = FALSE # Simulate spurious links  
)

## [1] "Actual cross-validation rate is 0.200"  
## [2] "Actual cross-validation rate is 0.200"  
## [3] "Actual cross-validation rate is 0.200"  
## [4] "Actual cross-validation rate is 0.200"  
## [5] "Actual cross-validation rate is 0.200"

For the purposes of this example, artificial spurious links are labeled with the “spurious\_edge” tag using the code below. This labeling allows for tracking these links throughout the analysis and network reconstruction process, although in typical use, such labeling would not be necessary.

myInput$edgelists <- lapply(myInput$edgelists,  
 function(x){  
 x$x <- 1  
 return(x)  
 })  
  
for(i in 1:length(myInput$edgelists)){  
 el <- myInput$edgelists[[i]]  
 rows <- as.numeric(el[, 1]) + 1  
 cols <- as.numeric(el[, 2]) - nrow(myInput$data) + 1  
 rows\_cols <- paste0(rows, "\_", cols)  
 spurious\_rows\_cols <- paste0(spurious\_links[, 1], "\_", spurious\_links[, 2])  
 spurious\_loc <- which(rows\_cols %in% spurious\_rows\_cols)  
 el[spurious\_loc, ]$x <- 1  
 el[spurious\_loc, ]$edge\_type <- "spurious\_edge"  
 myInput$edgelists[[i]] <- el  
}

# Summarizes network characteristics  
summary(myInput)

## n\_rows n\_cols n\_links rows\_single\_link cols\_single\_link possible\_links  
## 1 250 126 1515 0 0 31500

# Predict link probabilities

The hsbm.predict function applies the HSBM to predict probabilities of all links (observed and unobserved links). This step is crucial to identify spurious and missing links within the data, which are often present in incomplete or error-prone networks. The function works directly with the processed input created by hsbm.input. This step can be computationally intensive when working with large datasets or numerous folds. To improve performance, we use parallelized computation, distributing tasks across multiple cores.

# Define the number of cores to use  
#nCores <- detectCores() - 1  
nCores <- 2  
  
# Generate HSBM predictions  
myPred <- hsbm.predict(  
 myInput, # Input data processed by hsbm.input()  
 iter = 10000, # Number of iterations  
 wait= 10000, # Number of iterations for MCMC equilibration  
 method = "full\_reconstruction", # Method for link prediction  
 save\_blocks = TRUE, # Save group assignments   
 save\_pickle = FALSE, # Save results as pickle files  
 n\_cores = nCores  
)

Predicted link probabilities and group assignments are stored for each fold. Below, we extract the link probabilities (p) and groups assignments of links for fold 1.

# View probabilities for fold 1  
probabilities\_fold1 <- myPred$probs[[1]]  
head(probabilities\_fold1)

## v1 v2 p v1\_names v2\_names edge\_type  
## 1 0 250 1 sp1 SPa documented  
## 2 0 252 1 sp1 SPc documented  
## 3 0 256 1 sp1 SPg documented  
## 4 0 264 1 sp1 SPo documented  
## 5 0 280 1 sp1 SPeb documented  
## 6 0 312 1 sp1 SPkc documented

The group assignments provide the hierarchical clustering structure of nodes for each fold. Let’s extract and examine the group assignments for fold 1:

# View the group/block assignments for fold 1  
groups\_fold1 <- myPred$groups[[1]]  
  
# Filter one type of nodes (e.g., hosts, in columns)  
vnames <- colnames(myPred$data)  
groups\_fold1 <- groups\_fold1 %>% filter(names %in% vnames)  
g\_cols <- grep("^G", names(groups\_fold1))  
groups\_fold1[g\_cols] <- lapply(groups\_fold1[g\_cols], sort)  
  
print(head(groups\_fold1))

## nodes G1 G2 G3 G4 G5 names  
## 1 250 22 277 4 1 2 SPa  
## 2 251 55 277 4 1 2 SPb  
## 3 252 65 277 4 1 2 SPc  
## 4 253 65 277 4 1 2 SPd  
## 5 254 65 277 4 1 2 SPe  
## 6 255 65 277 4 1 2 SPf

Hierarchical group assignments provide insight into how nodes (e.g., hosts) are organized across multiple levels. At the first level (G1) nodes are divided into specific groups, reflecting fine-scale patterns. Moving to higher levels (G2, G3, G4) these groups (or communities) are progressively aggregated, revealing broader patterns and relationships or communities.

Next, we will explore how the model assigns specific probabilities to different types of links (“documented,” “held out,” and “spurious\_edge”) for each fold to evaluate HSBM ability to correctly identify them. Documented links, which are real observations (true positives), should have probabilities close to 1. Held-out links, which are real observations but transformed to 0s during training for validation, should also show high probabilities. In contrast, spurious edges, artificially generated (initially unobserved links transformed to 1s), should have probabilities close to 0, as the model should recognize them as false links (false negatives).

for(i in 1:5){  
 cat("Fold ", i, "\n")  
 cat("\tDocumented\n\t")  
 print(dplyr::filter(myPred$probs[[i]], edge\_type == "documented", p < 0.95))  
 cat("\tHeld out\n\t")  
 print(dplyr::filter(myPred$probs[[i]], edge\_type == "held\_out", p < 0.95))  
 cat("\tSpurious edge\n\t")  
 print(dplyr::filter(myPred$probs[[i]], edge\_type == "spurious\_edge", p < 0.95))  
}

## Fold 1   
## Documented  
## [1] v1 v2 p v1\_names v2\_names edge\_type  
## <0 rows> (or 0-length row.names)  
## Held out  
## [1] v1 v2 p v1\_names v2\_names edge\_type  
## <0 rows> (or 0-length row.names)  
## Spurious edge  
## v1 v2 p v1\_names v2\_names edge\_type  
## 1 42 350 0.4431443 sp43 SPwd spurious\_edge  
## 2 90 306 0.2087209 sp91 SPec spurious\_edge  
## 3 91 370 0.1713171 sp92 SPqe spurious\_edge  
## 4 158 328 0.4190419 sp159 SPad spurious\_edge  
## 5 194 291 0.7128713 sp195 SPpb spurious\_edge  
## 6 210 285 0.5653565 sp211 SPjb spurious\_edge  
## 7 49 367 0.0000000 sp50 SPne spurious\_edge  
## 8 89 340 0.0000000 sp90 SPmd spurious\_edge  
## 9 98 321 0.0000000 sp99 SPtc spurious\_edge  
## Fold 2   
## Documented  
## [1] v1 v2 p v1\_names v2\_names edge\_type  
## <0 rows> (or 0-length row.names)  
## Held out  
## [1] v1 v2 p v1\_names v2\_names edge\_type  
## <0 rows> (or 0-length row.names)  
## Spurious edge  
## v1 v2 p v1\_names v2\_names edge\_type  
## 1 98 321 0.7568757 sp99 SPtc spurious\_edge  
## 2 136 342 0.2511251 sp137 SPod spurious\_edge  
## 3 194 291 0.5510551 sp195 SPpb spurious\_edge  
## 4 210 285 0.2969297 sp211 SPjb spurious\_edge  
## 5 42 350 0.0000000 sp43 SPwd spurious\_edge  
## 6 49 367 0.0000000 sp50 SPne spurious\_edge  
## 7 91 370 0.0000000 sp92 SPqe spurious\_edge  
## Fold 3   
## Documented  
## [1] v1 v2 p v1\_names v2\_names edge\_type  
## <0 rows> (or 0-length row.names)  
## Held out  
## [1] v1 v2 p v1\_names v2\_names edge\_type  
## <0 rows> (or 0-length row.names)  
## Spurious edge  
## v1 v2 p v1\_names v2\_names edge\_type  
## 1 42 350 0.22822282 sp43 SPwd spurious\_edge  
## 2 49 367 0.38733873 sp50 SPne spurious\_edge  
## 3 90 306 0.27042704 sp91 SPec spurious\_edge  
## 4 117 274 0.00040004 sp118 SPy spurious\_edge  
## 5 136 342 0.93399340 sp137 SPod spurious\_edge  
## 6 210 285 0.71267127 sp211 SPjb spurious\_edge  
## 7 91 370 0.00000000 sp92 SPqe spurious\_edge  
## 8 98 321 0.00000000 sp99 SPtc spurious\_edge  
## 9 194 291 0.00000000 sp195 SPpb spurious\_edge  
## Fold 4   
## Documented  
## [1] v1 v2 p v1\_names v2\_names edge\_type  
## <0 rows> (or 0-length row.names)  
## Held out  
## [1] v1 v2 p v1\_names v2\_names edge\_type  
## <0 rows> (or 0-length row.names)  
## Spurious edge  
## v1 v2 p v1\_names v2\_names edge\_type  
## 1 90 306 0.57505751 sp91 SPec spurious\_edge  
## 2 91 370 0.05750575 sp92 SPqe spurious\_edge  
## 3 98 321 0.12511251 sp99 SPtc spurious\_edge  
## 4 117 274 0.45384538 sp118 SPy spurious\_edge  
## 5 194 291 0.00470047 sp195 SPpb spurious\_edge  
## 6 210 285 0.25442544 sp211 SPjb spurious\_edge  
## 7 42 350 0.00000000 sp43 SPwd spurious\_edge  
## 8 49 367 0.00000000 sp50 SPne spurious\_edge  
## Fold 5   
## Documented  
## [1] v1 v2 p v1\_names v2\_names edge\_type  
## <0 rows> (or 0-length row.names)  
## Held out  
## [1] v1 v2 p v1\_names v2\_names edge\_type  
## <0 rows> (or 0-length row.names)  
## Spurious edge  
## v1 v2 p v1\_names v2\_names edge\_type  
## 1 49 367 0.36423642 sp50 SPne spurious\_edge  
## 2 89 340 0.47754775 sp90 SPmd spurious\_edge  
## 3 117 274 0.45744574 sp118 SPy spurious\_edge  
## 4 169 258 0.66976698 sp170 SPi spurious\_edge  
## 5 210 285 0.00110011 sp211 SPjb spurious\_edge  
## 6 42 350 0.00000000 sp43 SPwd spurious\_edge  
## 7 91 370 0.00000000 sp92 SPqe spurious\_edge  
## 8 136 342 0.00000000 sp137 SPod spurious\_edge  
## 9 194 291 0.00000000 sp195 SPpb spurious\_edge

# Network Reconstruction

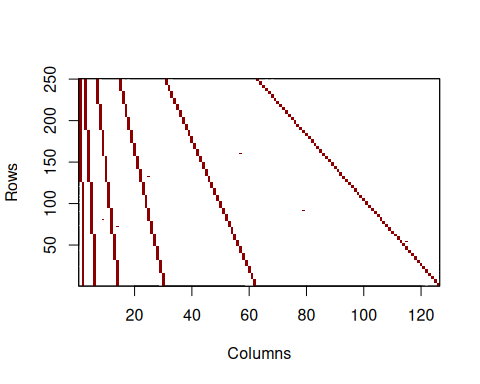
The hsbm.reconstructed function generates a reconstructed binary interaction matrix by combining predictions from all folds. The predicted matrix is binarized using a user-specified threshold.

# Network reconstruction  
myReconst <- hsbm.reconstructed(  
 myPred, # Predictions processed by hsbm.predict  
 rm\_documented=FALSE, # Remove documented links during validation  
 na\_treatment = "ignore\_na", # Handle NA values in predictions  
 threshold = 0.5, # Binarization threshold  
 new\_matrix\_method = "average\_thresholded", # Combine fold predictions  
 spurious\_edges = TRUE,  
)

## Warning in get\_hsbm\_results(hsbm\_out, input\_names = TRUE, na\_treatment =  
## na\_treatment): Predictions obtained for 13.46% of the links. Consider  
## increasing the number of iterations.

This output includes the final averaged probability matrix, the final reconstructed binary matrix, and evaluation metrics. These results highlight the predicted interactions, showcasing the method’s ability to detect spurious and missing links effectively. Let’s explore some of the key outputs.

# Visualize the reconstructed binary matrix  
plot\_interaction\_matrix(myReconst$new\_mat, order\_mat = FALSE)



# View the reconstruction summary and evaluation metrics  
summary(myReconst)

## $`Reconstructed Network Metrics`  
## obs\_links unobs\_links pred\_links kept\_links spurious\_links missing\_links  
## 1 1515 29985 1509 1509 6 0  
##   
## $`Evaluation Metrics`  
## mean\_RLRR mean\_auc mean\_aucpr mean\_yPRC mean\_prec mean\_sens mean\_spec  
## 1 0.9966997 0.9989746 1.033572 0.04809524 1 0.9960396 1  
## mean\_ACC mean\_ERR mean\_tss  
## 1 0.9998095 0.0001904762 0.9960396

The summary provides the number of spurious and missing links, as well as key evaluation metrics, such as the retained link recovery rate (RLRR).

Let’s now examine the top 10 predicted links that are most likely to be spurious (false positives) by visualizing the probabilities of “documented” links.

# Visualize the top most likely spurious links  
# top\_links\_spurious <- top\_links(hsbm\_out, n = 10, edge\_type = "documented")  
# print(top\_links\_spurious)

This document demonstrates the use of the *sabinaHSBM* package for network reconstruction. By applying the full reconstruction method, we showcased how spurious and missing links can be effectively identified and addressed in complex networks.

# Computing characteristics

Show processing time and computer characteristics

end\_time <- Sys.time()  
cat("The processing time of this script took: \n")

## The processing time of this script took:

end\_time - start\_time

## Time difference of 2.34626 hours

This analysis was performed on a Dynabook with the following characteristics:

* Processor (CPU): Intel Core i7-1165G7 @ 2.80GHz (11th Gen)
* Memory (RAM): 32 GB
* Operating System: Windows 11 Pro, Version 24H2
* R Version: 4.3.3