`covdepGE` versus `HeteroGGM` in heterogeneous structure recovery

Contents

Problem statement

Here, we compare the performance of `HeteroGGM` to `covdepGE` though a simulation study. In this example, `X` $\in \mathbb{R}^{180\times 5}$ and `Z` $\in \mathbb{R}^{180}$. `Z` is generated by drawing 60 times each from the uniform distribution on the intervals $(-3,-1), (-1,1)$, and $(1,3)$ (without loss of generality, we sort `Z` into ascending order). Then, we generate the l-th observation of `X` by drawing once from a 5 dimensional 0 mean Gaussian distribution with precision matrix $\Omega(z_l)$ defined as:

$$\Omega(z) = \begin{cases} \Omega^{(1)}(z) & z \in (-3,-1) \\ \Omega^{(2)}(z) & z \in (-1,1) \\ \Omega^{(3)}(z) & z \in (1,3) \end{cases} \tag{1}$$

Where $\Omega_1, \Omega_2, \Omega_3 \in \mathbb{R}^{5\times 5}$ are defined as:

$$\left[\Omega^{(1)}(z)\right]_{j,k} = \begin{cases} 2 & j = k \\ 1 & (j,k) \in \{(1,2),(2,1),(2,3),(3,2)\} \\ 0 & \text{otherwise} \end{cases} \quad \left[\Omega^{(2)}(z)\right]_{j,k} = \begin{cases} 2 & j = k \\ \frac{1-z}{2} & (j,k) \in \{(1,2),(2,1)\} \\ \frac{1+z}{2} & (j,k) \in \{(1,3),(3,1)\} \\ 1 & (j,k) \in \{(2,3),(3,2)\} \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

$$\left[\Omega^{(3)}(z)\right]_{j,k} = \begin{cases} 2 & j = k \\ 1 & (j,k) \in \{(1,3),(3,1),(2,3),(3,2)\} \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

Thus, as z approaches -1 from the right, $\Omega(z)$ approaches $\Omega^{(1)}(z)$ (more formally, $\|\Omega(z) - \Omega^{(1)}(z)\|$ goes to 0). Similarly, as z approaches 1 from the left, $\Omega(z)$ goes to $\Omega^{(3)}(z)$. We visualize these precision matrices and the corresponding structures below.

Note that `HeteroGGM` will attempt to recover the precision matrices without any help from the extraneous covariate, while `covdepGE` uses the extraneous covariate to calculate similarity weights between the observations to facilitate sharing of information.

Data generation

Here, we show how the data are generated.

```
# devtools::install_github("JacobHelwig/covdepGE")
library(HeteroGGM)
```

```
## Warning: package 'HeteroGGM' was built under R version 4.1.3
```

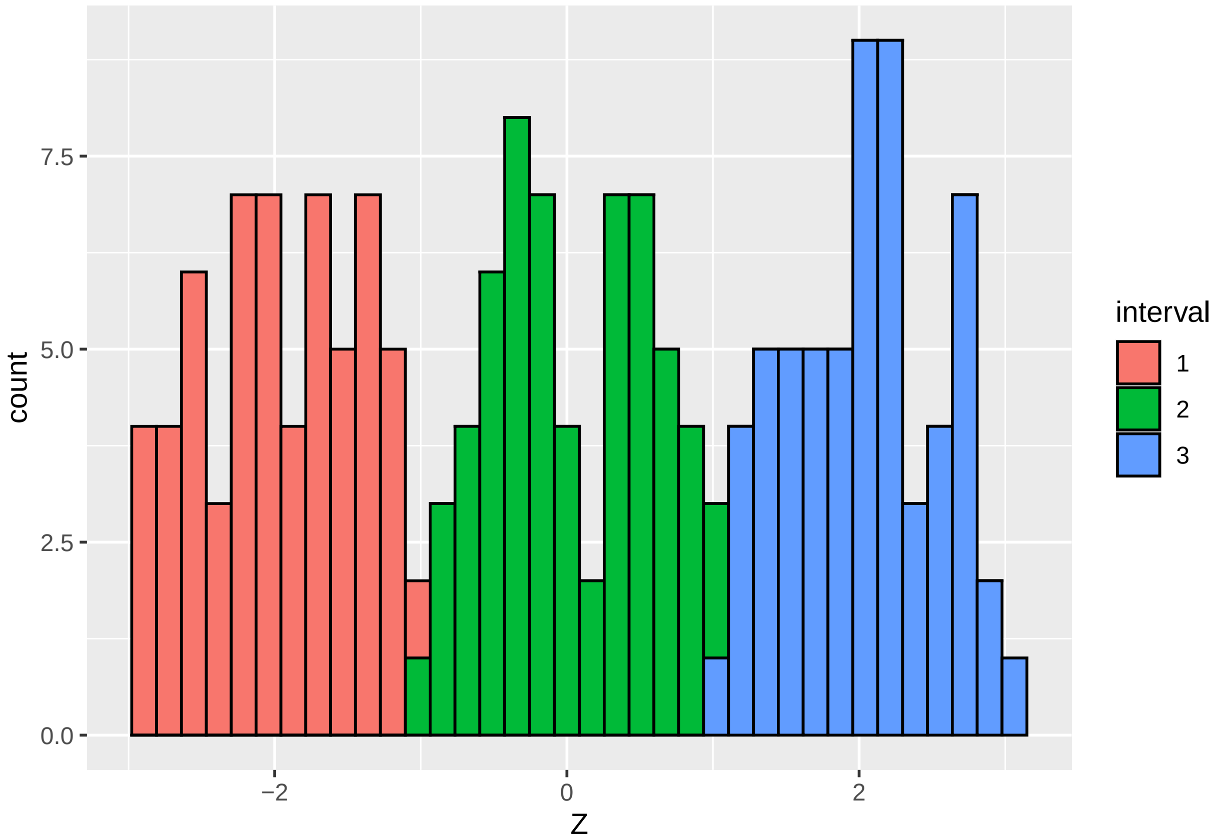
```
library(mclust)
```

```
## Package 'mclust' version 5.4.7
## Type 'citation("mclust")' for citing this R package in publications.
```

```
library(covdepGE)
library(ggplot2)
```

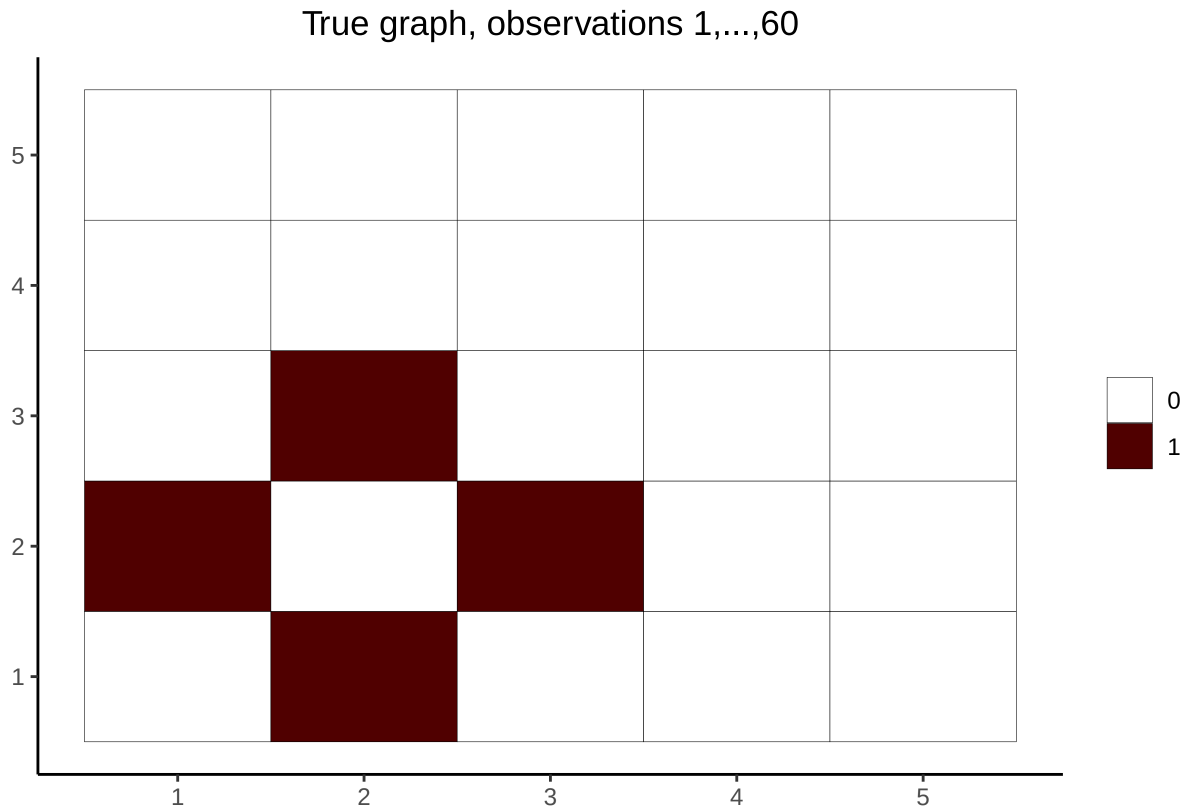
```
## Warning: package 'ggplot2' was built under R version 4.1.3
```

```
# get the data
set.seed(1)
data <- generateData()
X <- data$X
Z <- data$Z
interval <- data$interval
prec <- data$true_precision

# get overall and within interval sample sizes
n <- nrow(X)
n1 <- sum(interval == 1)
n2 <- sum(interval == 2)
n3 <- sum(interval == 3)

# visualize the distribution of the extraneous covariate
ggplot(data.frame(Z = Z, interval = as.factor(interval))) +
  geom_histogram(aes(Z, fill = interval), color = "black", bins = n %/% 5)
```

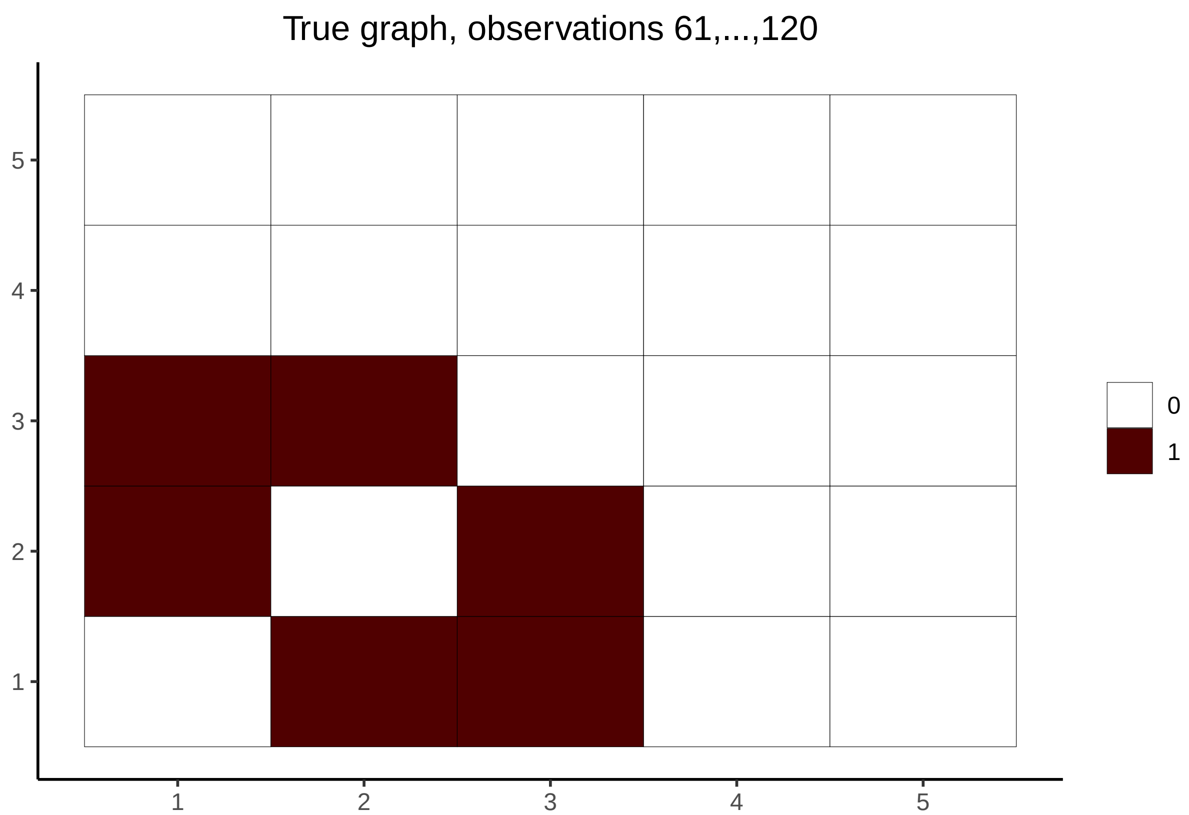



```r
# visualize the true conditional dependence structure in each of the intervals
titles <- paste0(rep("True graph, observations "), c(1, n1 + 1, n1 + n2 + 1),
                 rep(",...,", 3), c(n1, n1 + n2, n))
true_graphs <- lapply(lapply(lapply(prec, `!=`, 0), `*`, 1), `-`, diag(5))
lapply(1:3, function(j) matViz(unique(true_graphs)[[j]]) + ggtitle(titles[j]))
```

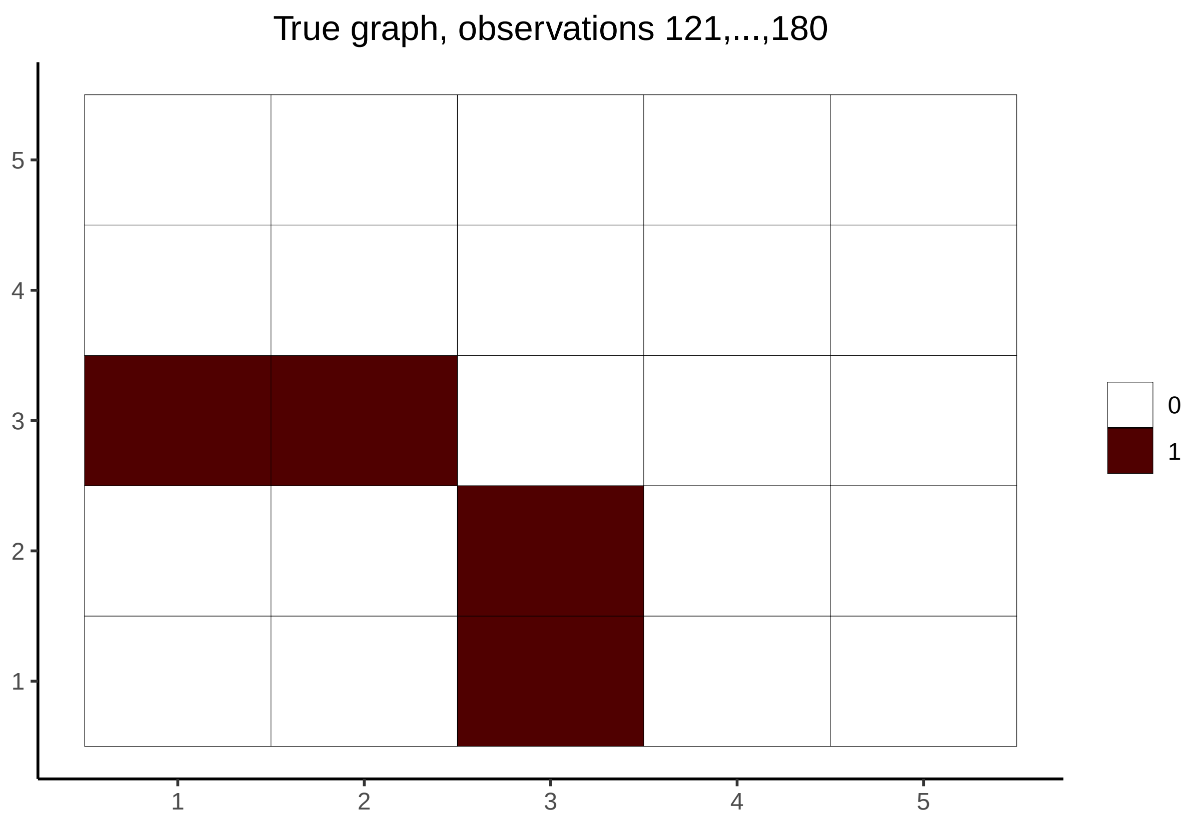
```
## [[1]]
```




```
##
## [[2]]
```




```
##
## [[3]]
```



Comparison

In this section, we fit each of the methods, calculate sensitivity and specificity, and visualize the resulting structures.

covdepGE

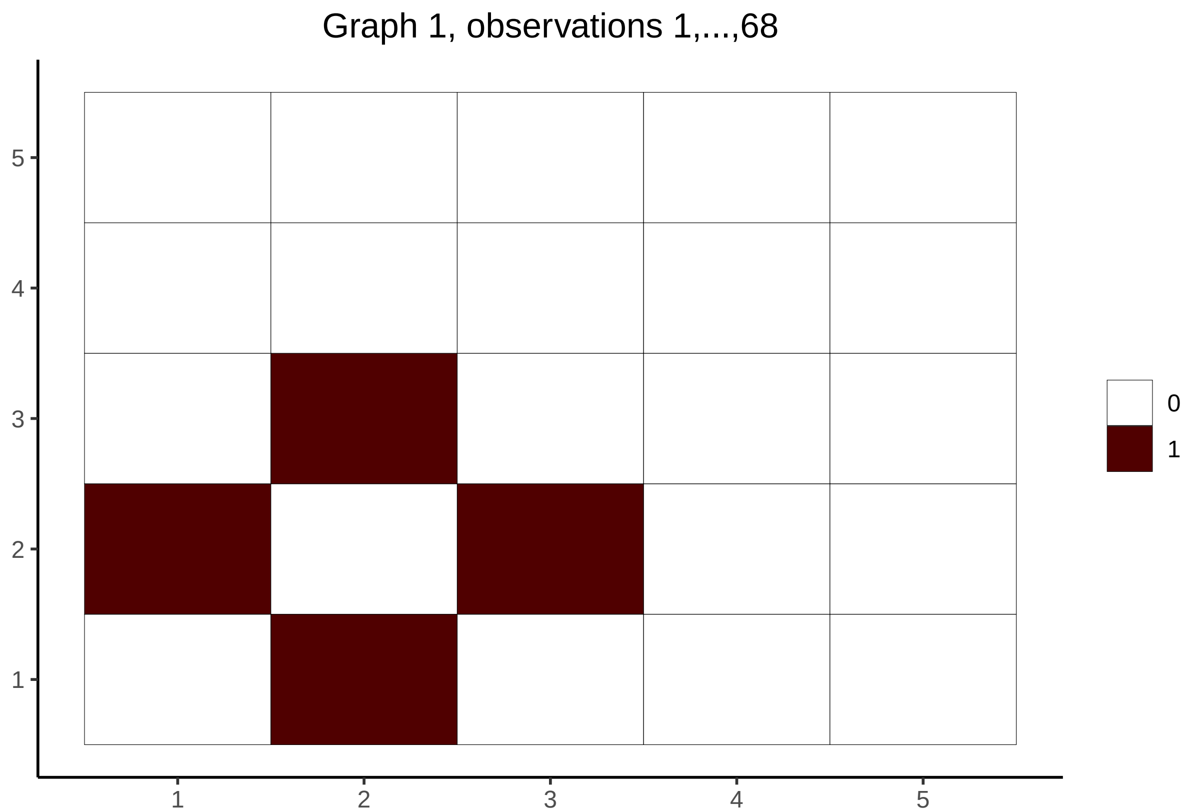
```
# covdepGE; factors paralellism along p
(out_covdepGE <- covdepGE(X, Z, parallel = T, num_workers = 5))
```

```
## Warning in covdepGE(X, Z, parallel = T, num_workers = 5): No registered workers
## detected; registering doParallel with 5 workers
```

```
##                       Covariate Dependent Graphical Model
##
## ELBO: -185642.35                                            # Unique Graphs: 3
## n: 180, variables: 5                       Hyperparameter grid size: 125 points
## Model fit completed in 3.84 secs
```

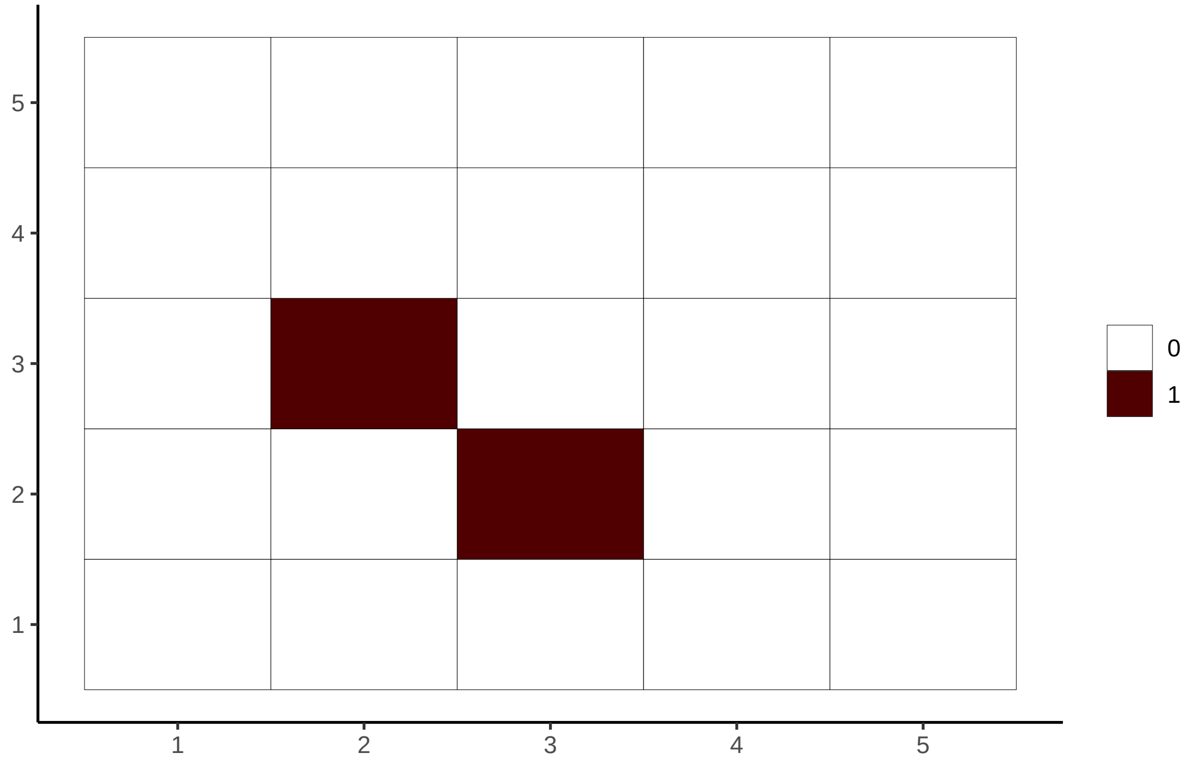
```
plot(out_covdepGE)
```

```
## [[1]]
```

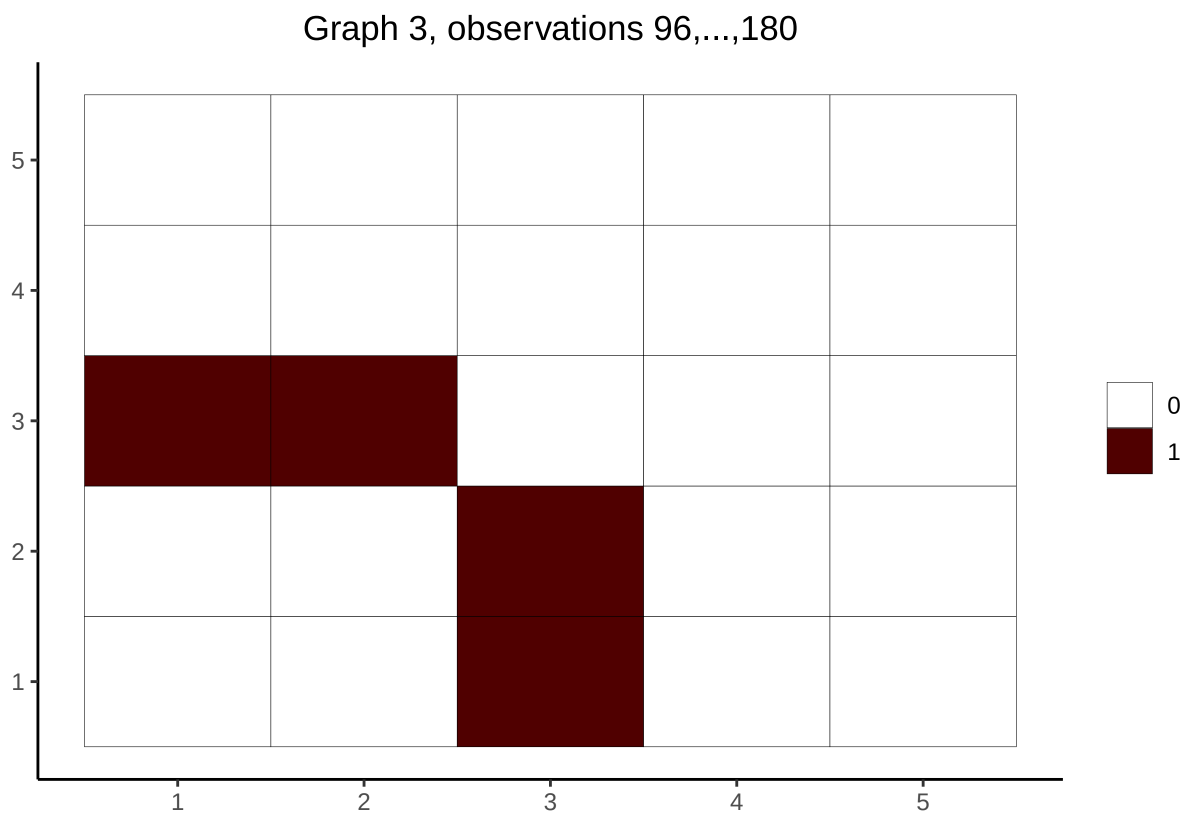



```
##
## [[2]]
```

Graph 2, observations 69,...,95




```
##
## [[3]]
```




```
# calculate number of true edges and non-edges (mask out diagonal)
n <- nrow(X)
p <- ncol(X)
trueGraphs0 <- lapply(true_graphs, `+`, diag(rep(NA, p)))
trueGraphs <- array(unlist(trueGraphs0), dim = c(p, p, n))
num_true1 <- sum(trueGraphs, na.rm = T)
num_true0 <- sum(trueGraphs == 0, na.rm = T)

# calculate number of correctly detected edges
pred_graphs <- out_covdepGE$graphs$graphs
predGraphs <- array(unlist(pred_graphs), dim = c(p, p, n))
correct1 <- sum(predGraphs == trueGraphs & trueGraphs == 1, na.rm = T)

# calculate number of correctly detected non-edges
correct0 <- sum(predGraphs == trueGraphs & trueGraphs == 0, na.rm = T)

# display sensitivity and specificity
sens <- correct1 / num_true1
spec <- correct0 / num_true0
cat("\nSensitivity:", round(sens, 3))
```

```
##
## Sensitivity: 0.793
```

```
cat("\nSpecificity:", round(spec, 3))
```

```
##
## Specificity: 1
```

```
rm(list = c("pred_graphs", "predGraphs", "correct1", "correct0", "sens", "spec"))
```

HeteroGGM

```
# HeteroGGM
clust <- Mclust(data$Z, verbose = F)
lambda <- genelambda.obo(lambda1_min = 0.01, lambda2_min = 0.2,
                         lambda3_min = 0.01)
start <- Sys.time()
out_hetGGM <- GGMPF(lambda, data$X + clust$classification * 10, clust$G)
elapsed <- round(Sys.time() - start, 3)
cat("\nTime to fit HeteroGGM:", elapsed, attr(elapsed, "units"), "\n")
```

```
##
## Time to fit HeteroGGM: 2.881 secs
```

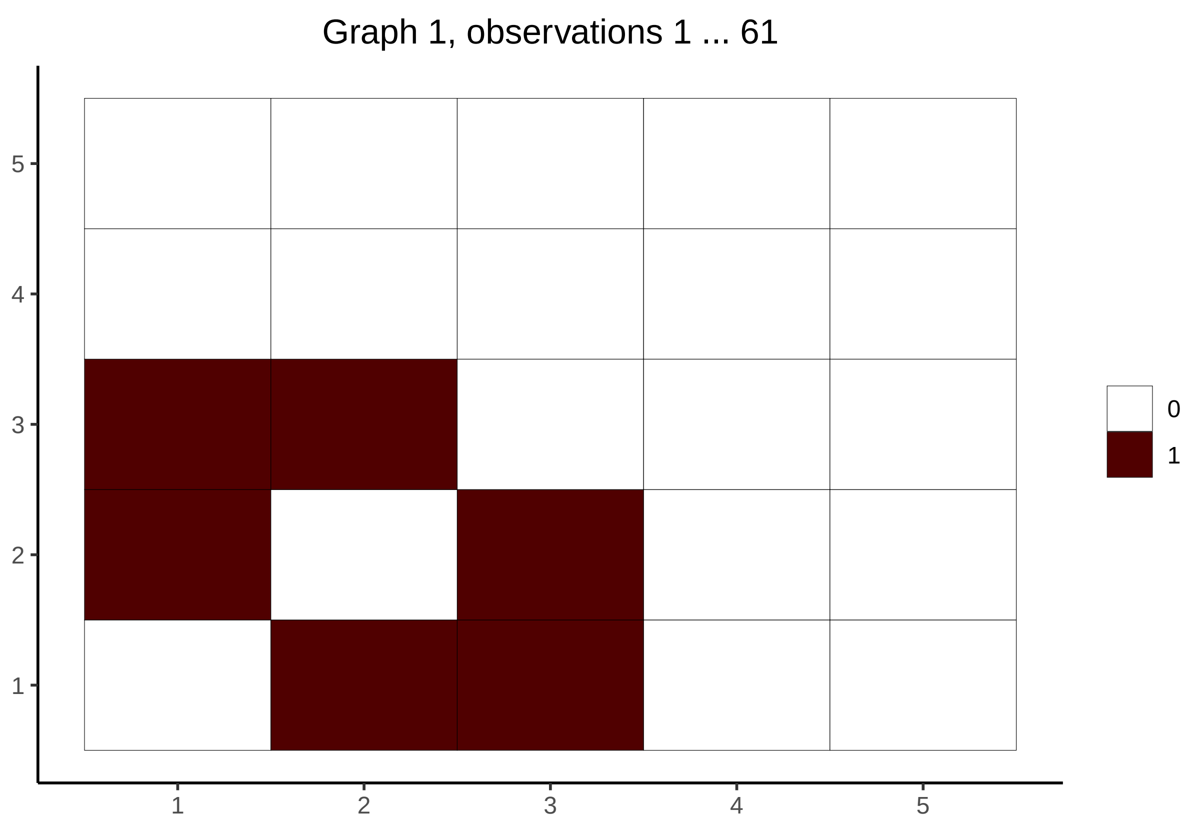
```
out_hetGGM$Opt_lambda
```

```
## [1] 1.0 0.2 5.0
```

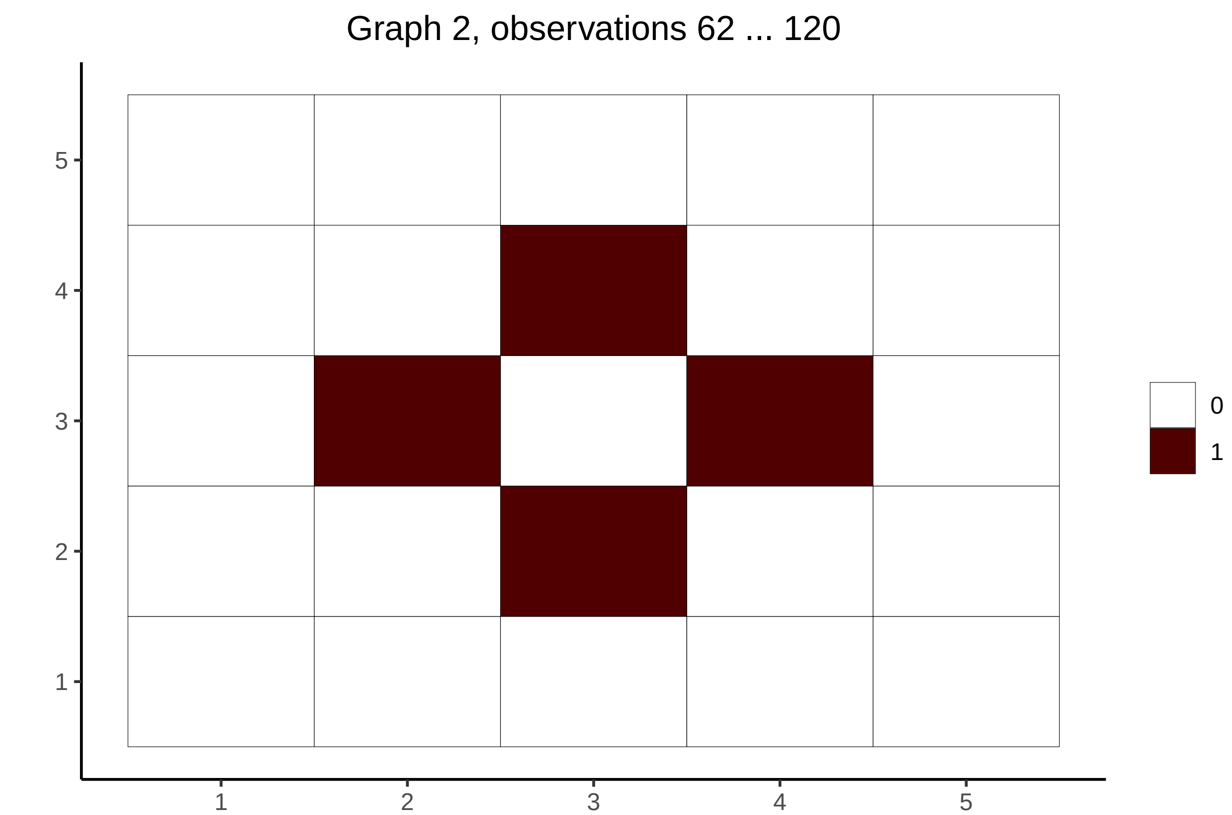
```
# get the optimal graphs and best hyperparameters
best_hyp <- out_hetGGM$Opt_num
ggm_prec <- out_hetGGM$Theta_hat.list[[best_hyp]]
ggm_inds <- out_hetGGM$member.list[[best_hyp]]
ggm_graphs <- (ggm_prec != 0) * 1 - replicate(dim(ggm_prec)[3], diag(ncol(data$X)))
graphs_arr <- ggm_graphs[ , , ggm_inds]
graphs <- vector("list", dim(graphs_arr)[3])
for (j in 1:length(graphs)) graphs[[j]] <- graphs_arr[ , , j]

# get the unique graphs and find which observations they correspond to
unique_graphs <- unique(graphs)
unique_sum <- vector("list", length(unique_graphs))
names(unique_sum) <- paste0("graph", 1:length(unique_graphs))

# iterate over each of the unique graphs
for (j in 1:length(unique_graphs)){

  # fix the unique graph
  graph <- unique_graphs[[j]]

  # find indices of the observations corresponding to this graph
  graph_inds <- which(sapply(graphs, identical, graph))

  # split up the contiguous subsequences of these indices
```

```
  cont_inds <- split(sort(graph_inds), cumsum(c(1, diff(sort(graph_inds)) != 1)))

  # create a character summary for each of the contiguous sequences
  inds_sum <- sapply(cont_inds, function(idx_seq) ifelse(length(
    idx_seq) > 3, paste0(min(idx_seq), " ... ", max(idx_seq)),
    paste0(idx_seq, collapse = ", ")))

  # combine the summary
  inds_sum <- paste0(inds_sum, collapse = ",")

  # add the graph, indices, and summary to the unique graphs summary list
  unique_sum[[j]] <- list(graph = graph, indices = graph_inds,
                          ind_sum = inds_sum)
}

# visualize each of the unique graphs
lapply(1:length(unique_sum), function(j) matViz(unique_sum[[j]]$graph)
         + labs(title = stringr::str_wrap(paste0("Graph ", j, ", observations ",
                                                  unique_sum[[j]]$ind_sum), 75)))
```

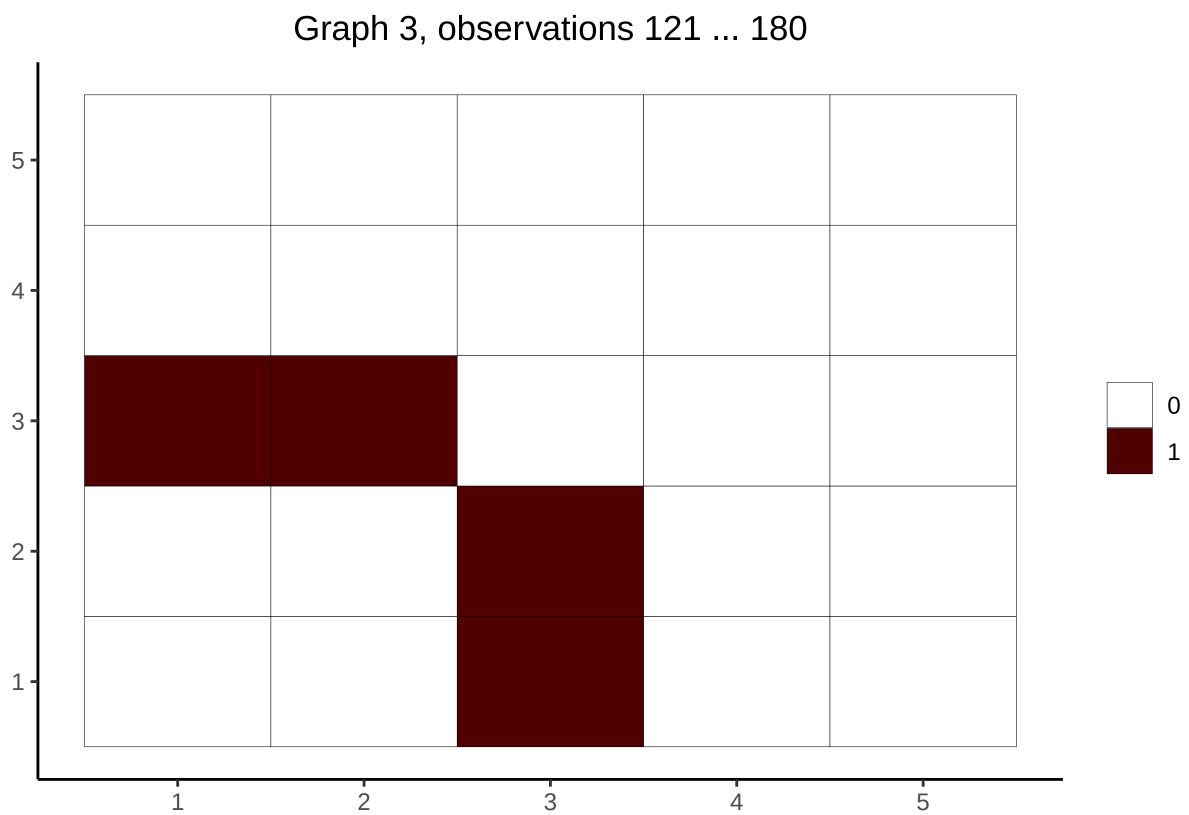
```
## [[1]]
```




```
##
## [[2]]
```




```
##
## [[3]]
```




```
# calculate number of correctly detected edges
correct1 <- sum(graphs_arr == trueGraphs & trueGraphs == 1, na.rm = T)

# calculate number of correctly detected non-edges
correct0 <- sum(graphs_arr == trueGraphs & trueGraphs == 0, na.rm = T)

# display sensitivity and specificity
sens <- correct1 / num_true1
spec <- correct0 / num_true0
cat("\nSensitivity:", round(sens, 3))
```

```
##
## Sensitivity: 0.719
```

```
cat("\nSpecificity:", round(spec, 3))
```

```
##
## Specificity: 0.914
```