covdepGE versus competitor

Data generation

The extraneous covariate is created as the union of three disjoint intervals with nearly adjacent endpoints. Within each interval, the individuals' covariate values are equally spaced.

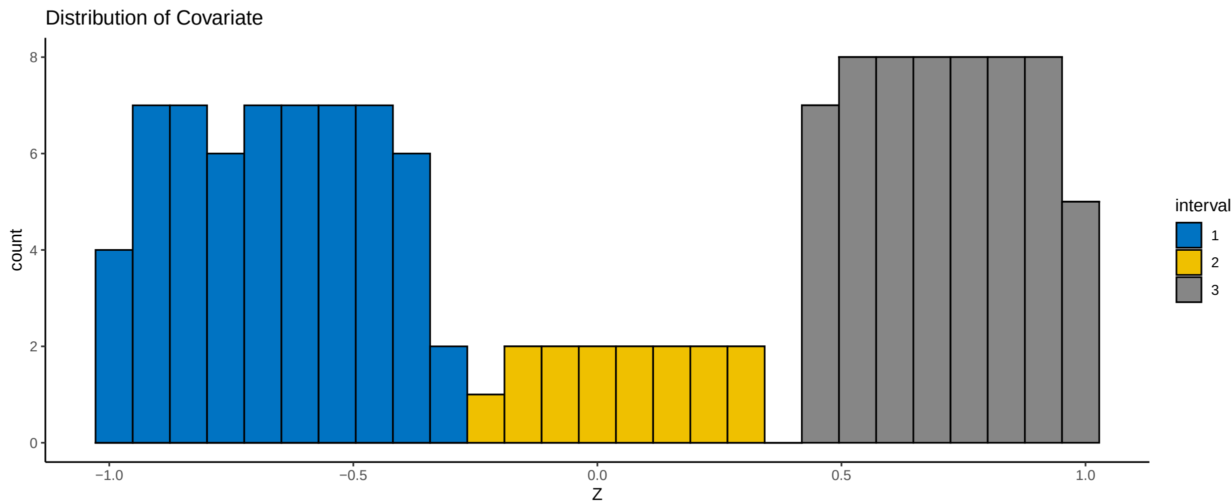
The second interval is the sparse part of the covariate space.

```
library(ggplot2)
library(ggpubr)
library(covdepGE)
library(mclust)
```

```
## Package 'mclust' version 5.4.9
## Type 'citation("mclust")' for citing this R package in publications.
```

```
library(varbvs)

set.seed(1)

# create covariate for individuals in each of the three intervals

# define the dimensions of the data
n1 <- 60
n2 <- 15
n3 <- 60
n <- sum(n1, n2, n3)
p <- 4

# define the limits of the intervals
limits1 <- c(-0.99, -0.331)
limits2 <- c(-0.229, 0.329)
limits3 <- c(0.431, 0.99)

# define the covariate values within each interval
z1 <- seq(limits1[1], limits1[2], length = n1)
z2 <- seq(limits2[1], limits2[2], length = n2)
z3 <- seq(limits3[1], limits3[2], length = n3)
Z <- matrix(c(z1, z2, z3), n, 1)

# visualize the covariate
cov_df <- cbind.data.frame(rbind(cbind(1, z = z1), cbind(2, z = z2), cbind(3, z = z3)),
    1:n)
names(cov_df) <- c("interval", "Z", "individual_index")
cov_df$interval <- factor(cov_df$interval)
```

```r
ggplot(cov_df, aes(Z, fill = interval)) + geom_histogram(color = "black", bins = n%/%5) +
    theme_classic() + ggsci::scale_fill_jco() + labs(title = "Distribution of Covariate")
```




```r
# individual index by interval
ind_idx <- tapply(cov_df$individual_index, cov_df$interval, function(indices) paste0(min(indices),
    ",...,", max(indices)))
data.frame(interval = names(ind_idx), individual_indices = ind_idx)
```

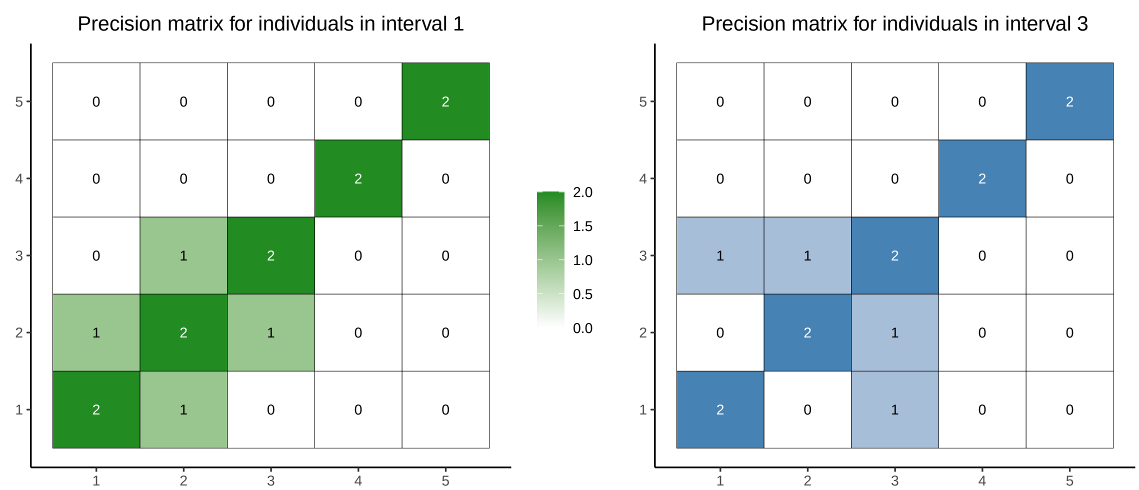
```
##   interval individual_indices
## 1        1           1,...,60
## 2        2          61,...,75
## 3        3         76,...,135
```

All of the individuals in interval 1 have the same precision matrix, as do all of the individuals in interval 3. The first individual in interval 2 has the same precision matrix as those in interval 1.

As the individual index in interval 2 increases, the precision matrix continuously shifts from the precision matrix in interval 1 to the precision matrix in interval 3 such that the last individual in interval 2 has the same precision matrix as the individuals in interval 3.

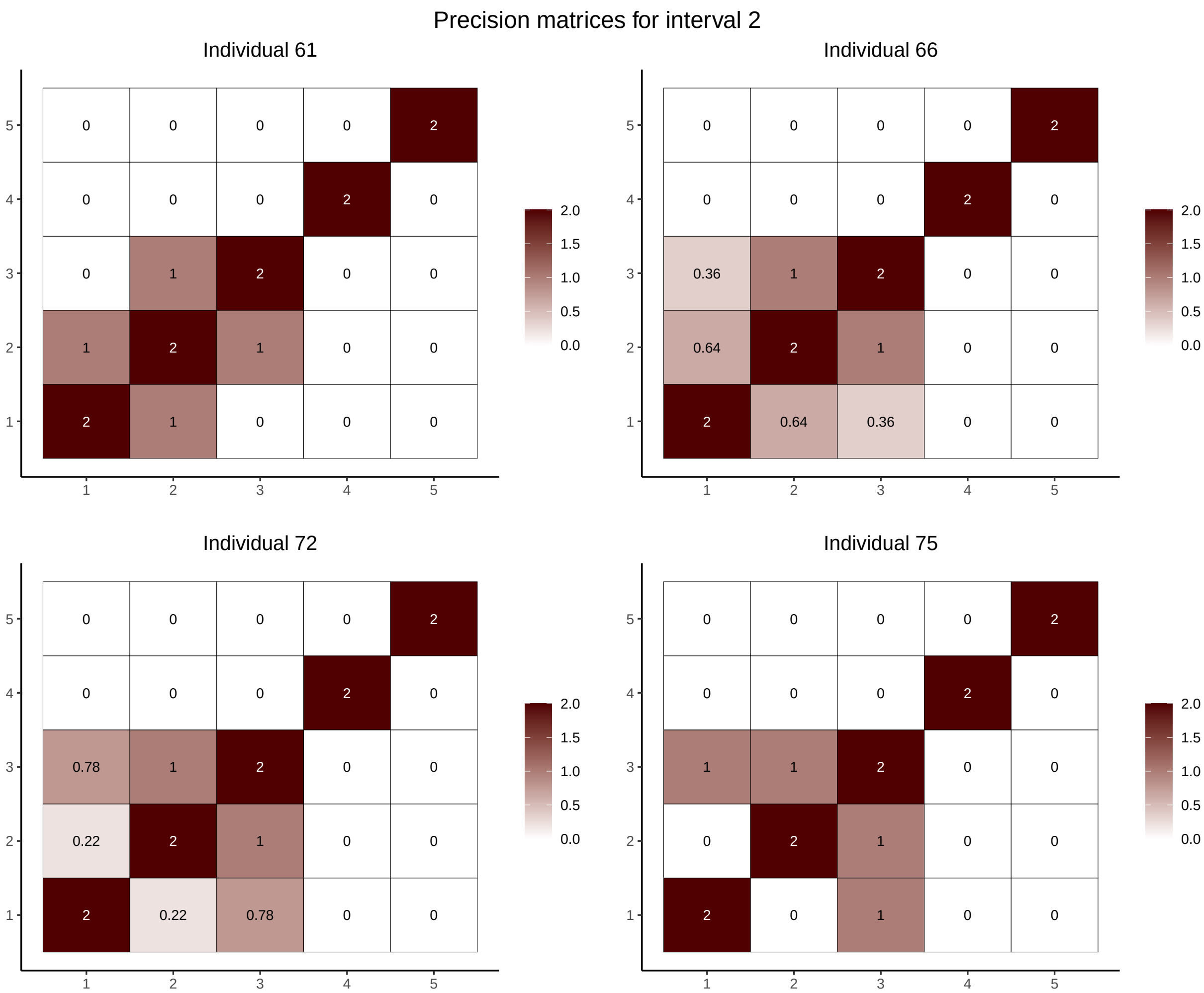
```r
# create precision matrices

# the shared part of the structure for all three intervals is a 2 on the
# diagonal and a 1 in the (2, 3) position
common_str <- diag(p + 1)
common_str[2, 3] <- 1

# define constants for the structure of interval 2
const1 <- 0.23
const2 <- 0.56

# interval 2 has two different linear functions of Z in the (1, 2) position and
# (1, 3) positions; define structures for each of these components
int2_str12 <- int2_str13 <- matrix(0, p + 1, p + 1)
int2_str12[1, 2] <- int2_str13[1, 3] <- 1
```

```r
# define the precision matrices for each of the individuals in interval 2
int2_prec <- lapply(z2, function(z) common_str + ((1 - (z + const1)/const2) * int2_str12) +
    ((z + const1)/const2 * int2_str13))

# interval 1 has a 1 in the (1, 2) and interval 3 has a 1 in the (1, 3)
# position; define structures for each of these components
int1_str12 <- int3_str13 <- matrix(0, p + 1, p + 1)
int1_str12[1, 2] <- int3_str13[1, 3] <- 1

# define the precision matrices for each of the individuals in interval 1 and
# interval 3
int1_prec <- rep(list(common_str + int1_str12), n1)
int3_prec <- rep(list(common_str + int3_str13), n3)

# put all of the precision matrices into one list
prec_mats <- c(int1_prec, int2_prec, int3_prec)

# symmetrize the precision matrices
prec_mats <- lapply(prec_mats, function(mat) t(mat) + mat)

# visualize the precision matrices for each interval

# all of the individuals in interval 1 and 3 have the same precision matrix
int1_g <- gg_adjMat(prec_mats[[1]], color1 = "forestgreen") + ggtitle("Precision matrix for individuals
int3_g <- gg_adjMat(prec_mats[[n1 + n2 + 1]], color1 = "steelblue") + ggtitle("Precision matrix for indi

ggarrange(int1_g, int3_g)
```




```r
# the first individual in interval 2 has the same precision matrix as the
# individuals in interval 1; as the subject index grows, the (1, 3)/ (3, 1)
# entry changes from 0 to 1 and the (1, 2)/ (2, 1) entry changes from 1 to 0.
# The last individual has the same precision matrix as the individuals in
# interval 3
int2_g_inds <- n1 + c(1, 2 * n2%/%5, 4 * n2%/%5, n2)
int2_graphs <- lapply(int2_g_inds, function(indv_idx) gg_adjMat(prec_mats[[indv_idx]]) +
    labs(title = paste0("Individual ", indv_idx)))
```

```r
annotate_figure(ggarrange(plotlist = int2_graphs), top = text_grob("Precision matrices for interval 2",
    size = 15))
```




```r
# invert the precision matrices to get the covariance matrices
cov_mats <- lapply(prec_mats, solve)

# generate the data using the covariance matrices
data_mat <- t(sapply(cov_mats, MASS::mvrnorm, n = 1, mu = rep(0, p + 1)))
```

Covariate dependent graph estimation

```r
# use varbvs to get the hyperparameter sigma
sigmasq <- sapply(1:(p + 1), function(col_ind) mean(varbvs(data_mat[, -col_ind],
    Z, data_mat[, col_ind], verbose = F)$sigma))
sigmasq
```

```
## [1] 0.7251686 0.6471107 0.6433086 0.4229079 0.4621893
```

```r
mean(sigmasq)
```

```
## [1] 0.580137
```

```r
# estimate the covariance structure dependent of the covariate
out_dep <- covdepGE(data_mat,
                    Z, # extraneous covariates
                    sigmasq = mean(sigmasq), # hyperparameter residual variance
                    var_min = 1e-3, # smallest sigmabeta_sq grid value
                    var_max = 5, # largest sigmabeta_sq grid value
                    n_sigma = 50, # length of the sigmabeta_sq grid
                    pi_vec = 0.1, # prior inclusion probability
                    tolerance = 1e-10, # variational parameter exit condition 1
                    max_iter = 1e3, # variational parameter exit condition 2
                    print_time = T)
```

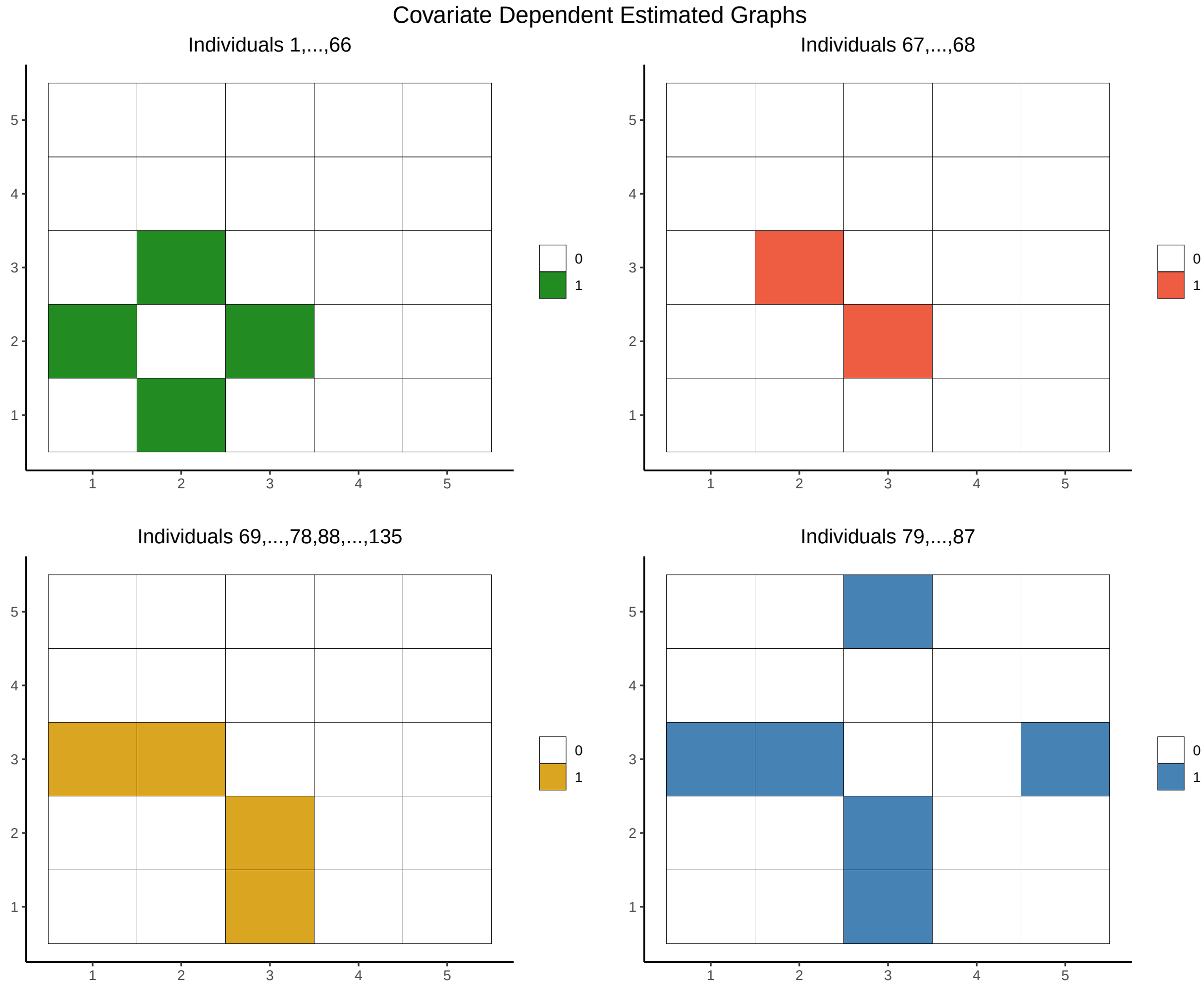
```
## Warning in covdepGE(data_mat, Z, sigmasq = mean(sigmasq), var_min = 0.001, : For
## 2/5 responses, the selected value of sigmabeta_sq was on the grid boundary. See
## return value ELBO for details
```

```
## Time difference of 3.8202 secs
```

```r
# find the unique graphs and the individuals belonging to each
unique_graphs <- unique(out_dep$graphs)
length(unique_graphs)
```

```
## [1] 4
```

```r
indiv_graphs <- lapply(1:length(unique_graphs), function(graph_ind) which(sapply(out_dep$graphs,
    identical, unique_graphs[[graph_ind]])))
indiv_graphs_sum <- sapply(indiv_graphs, function(indv_idx) paste0(lapply(split(indv_idx,
    cumsum(c(1, diff(indv_idx) != 1))), function(idx_seq) paste0(min(idx_seq), ",...,",
    max(idx_seq))), collapse = ","))

# visualize each of the unique graphs
colors <- c("forestgreen", "tomato2", "goldenrod", "steelblue")
graph_viz <- lapply(1:length(unique_graphs), function(graph_ind) gg_adjMat(unique_graphs[[graph_ind]],
    color1 = colors[[graph_ind]]) + labs(title = paste0("Individuals ", indiv_graphs_sum[graph_ind])))
annotate_figure(ggarrange(plotlist = graph_viz), top = text_grob("Covariate Dependent Estimated Graphs"
    size = 15))
```



Covariate independent graph estimation

Gaussian Mixture Model clustering will first be applied to the extraneous covariate. The number of clusters is selected by optimizing BIC.

For all of the individuals within each of the clusters identified by GMM, the shared graph will be estimated by applying `covdepGE` using a constant value for the extraneous covariate. Using a constant value for the extraneous covariate will result in the same estimate for all individuals within each cluster.

```
# estimate the dependence structure independent of the covariate

# apply Gaussian Mixture model clustering; selects number of clusters based on
# the model that results in the best BIC
gmm <- Mclust(Z)

# find accuracy of the clustering
fossil::rand.index(gmm$classification, as.numeric(cov_df$interval))
```

```
## [1] 0.9838585
```

```r
# find number of clusters in final clustering
(num_clusters <- length(unique(gmm$classification)))
```

```
## [1] 3
```

```r
out_indep <- vector("list", num_clusters)

# iterate over each of the clusters identified by GMM
for (k in 1:num_clusters){

  # fix the datapoints in the k-th cluster
  data_mat_k <- data_mat[gmm$classification == k, ]

  # use varbvs to get the hyperparameter sigma
  sigmasq_k <- sapply(1:(p + 1), function (col_ind) mean(varbvs(data_mat_k[ , -col_ind], NULL, data_mat_

  # apply the GGM using covdepGE with constant Z, save the resulting graph
  out_indep[[k]] <- covdepGE(data_mat_k,
                             rep(0, nrow(data_mat_k)), # extraneous covariates
                             sigmasq = mean(sigmasq_k), # hyperparameter residual variance
                             var_min = 1e-3, # smallest sigmabeta_sq grid value
                             var_max = 5, # largest sigmabeta_sq grid value
                             n_sigma = 50, # length of the sigmabeta_sq grid
                             pi_vec = 0.1, # prior inclusion probability
                             tolerance = 1e-10, # variational parameter exit condition 1
                             max_iter = 1e3, # variational parameter exit condition 2
                             print_time = T,
                             kde = F, # whether to use kde to calculate bandwidths
                             scale = F # whether to scale the extraneous covariates
                             )

}
```

```
## Warning in covdepGE(data_mat_k, rep(0, nrow(data_mat_k)), sigmasq =
## mean(sigmasq_k), : For 2/5 responses, the selected value of sigmabeta_sq was on
## the grid boundary. See return value ELBO for details
```

```
## Time difference of 0.584743 secs
```

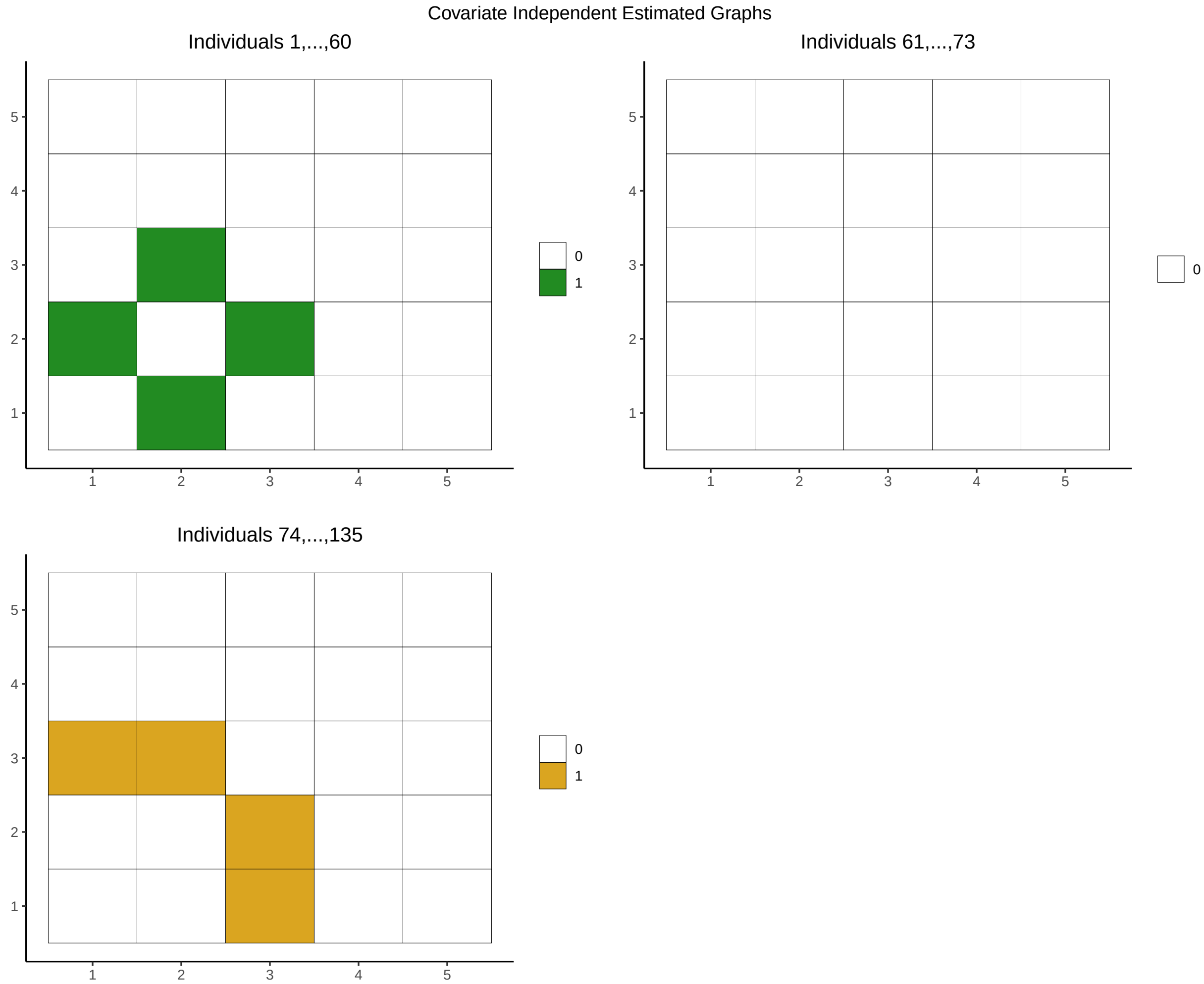
```
## Warning in covdepGE(data_mat_k, rep(0, nrow(data_mat_k)), sigmasq =
## mean(sigmasq_k), : For 1/5 responses, the selected value of sigmabeta_sq was on
## the grid boundary. See return value ELBO for details
```

```
## Time difference of 0.03685904 secs
```

```
## Warning in covdepGE(data_mat_k, rep(0, nrow(data_mat_k)), sigmasq =
## mean(sigmasq_k), : For 2/5 responses, the selected value of sigmabeta_sq was on
## the grid boundary. See return value ELBO for details
```

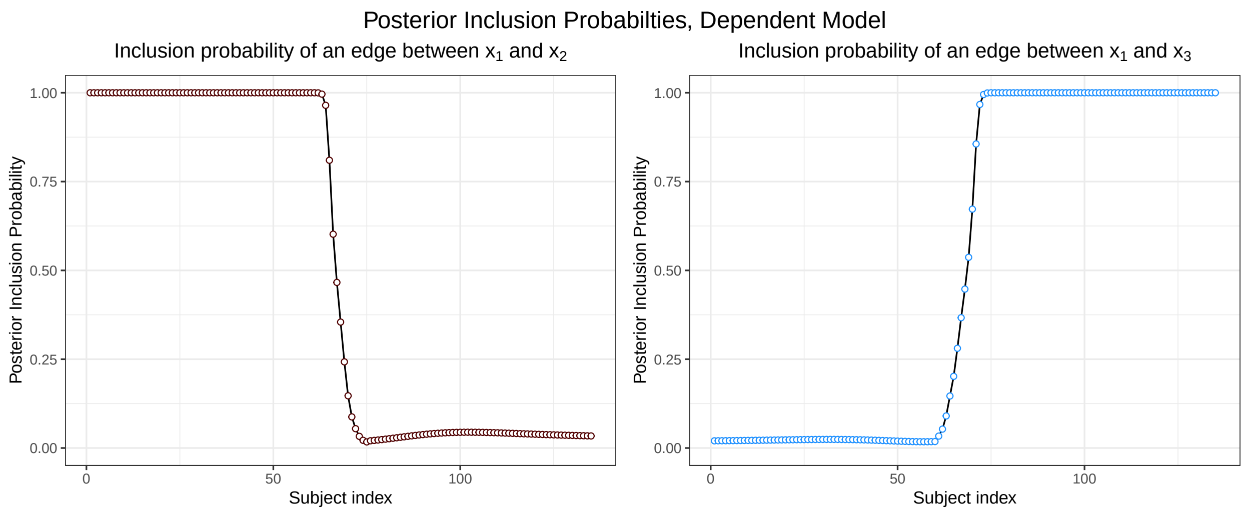
```
## Time difference of 0.581507 secs
```

```r
# get the graphs and pip matrices for each cluster
pip_mats <- sapply(out_indep, function(out) unique(out$inclusion_probs))
adj_mats <- sapply(out_indep, function(out) unique(out$graphs))
if (length(pip_mats) != num_clusters | length(adj_mats) != num_clusters) {
    stop("Too many graphs")
}

# find the individuals in each of the clusters
clust_inds <- lapply(1:num_clusters, function(cl_ind) which(gmm$classification ==
    cl_ind))
clust_inds_sum <- sapply(clust_inds, function(clust) paste0(lapply(split(clust, cumsum(c(1,
    diff(clust) != 1))), function(idx_seq) paste0(min(idx_seq), ",...,", max(idx_seq))),
    collapse = ","))

# create a list of n graphs according to the independent estimate for each
# cluster and the gmm cluster assignment for each individual
indep_graphs <- sapply(1:n, function(ind_idx) adj_mats[gmm$classification[ind_idx]])

# create a list of n posterior inclusion probabilities
indep_pip <- sapply(1:n, function(ind_idx) pip_mats[gmm$classification[ind_idx]])

# visualize the resulting graphs
cl_gr_viz <- lapply(1:num_clusters, function(cl_ind) gg_adjMat(adj_mats[[cl_ind]],
    color1 = colors[[cl_ind]]) + labs(title = paste0("Individuals ", clust_inds_sum[cl_ind])))
cl_gr_vis <- rep(list(ggplot() + theme_void()), 4)
cl_gr_vis[1:length(cl_gr_viz)] <- cl_gr_viz
annotate_figure(ggarrange(plotlist = cl_gr_vis), top = text_grob("Covariate Independent Estimated Graph
```

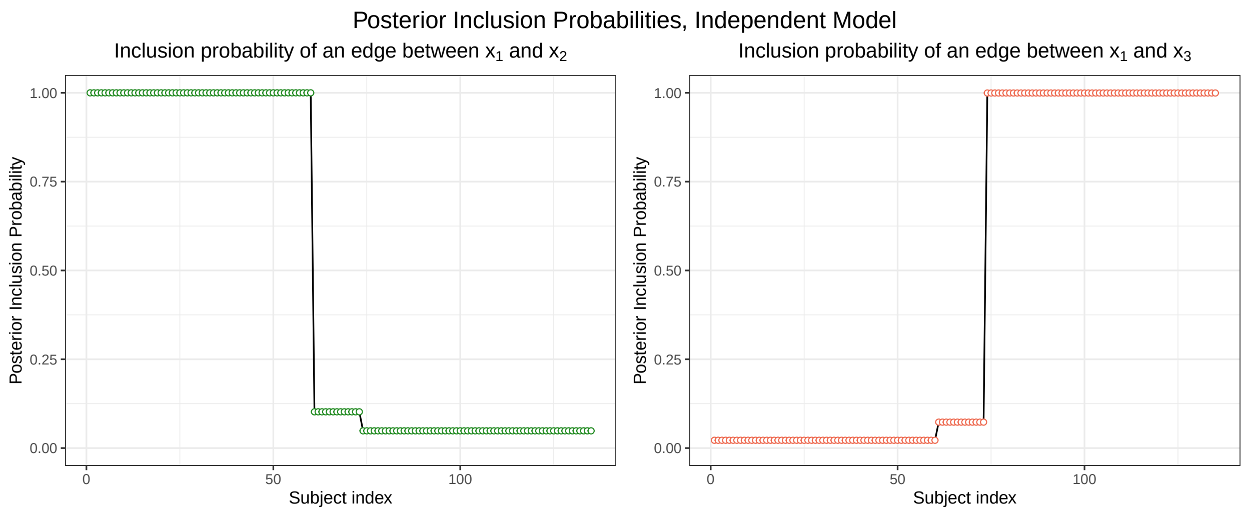


Performance Analysis

```
# analyze results

# visualize the posterior inclusion probabilties for both models
annotate_figure(ggarrange(gg_inclusionCurve(out_dep, 1, 2), gg_inclusionCurve(out_dep,
    1, 3, point_color = "dodgerblue")), top = text_grob("Posterior Inclusion Probabilties, Dependent Mod
    size = 15))
```




```
out_dep_copy <- out_dep
out_dep_copy$inclusion_probs <- indep_pip
annotate_figure(ggarrange(gg_inclusionCurve(out_dep_copy, 1, 2, point_color = "forestgreen"),
    gg_inclusionCurve(out_dep_copy, 1, 3, point_color = "coral2")), top = text_grob("Posterior Inclusio
    size = 15))
```

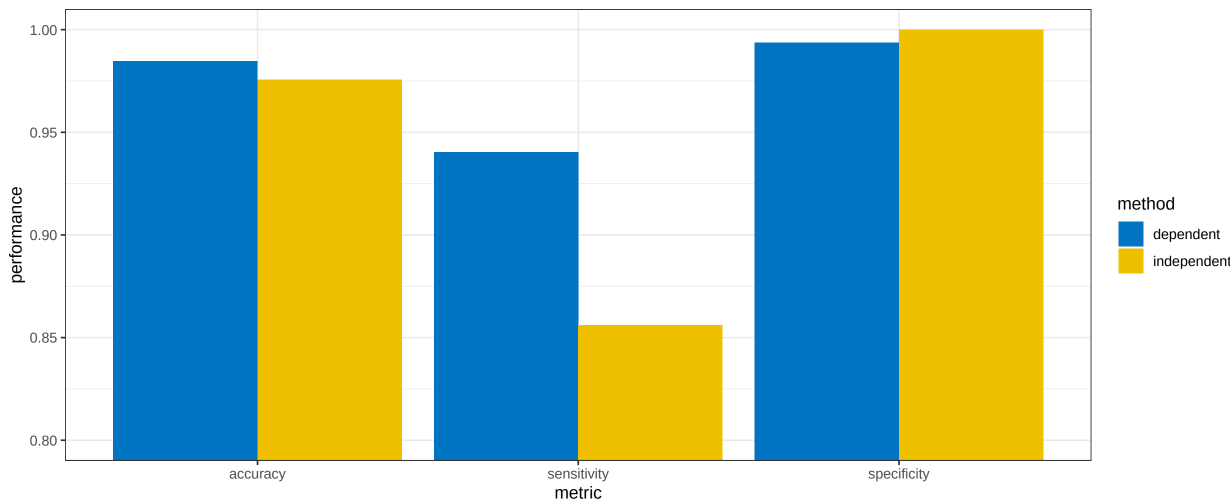



```
# find sensitivity, specificity, and accuracy for each method

# find the true graph for each individual
true_graphs <- lapply(prec_mats, function(mat) ((mat - diag(diag(mat))) != 0) * 1)

# find the total number of entries in all of the graphs
true_gr_vector <- unlist(true_graphs)
num_entries <- length(true_gr_vector)
# num_entries == n * (p + 1)^2

# find the total number of 1's and 0's in all the graphs
tot1 <- sum(true_gr_vector)
tot0 <- sum(-true_gr_vector + 1)
# tot1 + tot0 == num_entries
```

```r
# create a list of lists; the j-th value in the outer list is a list with three
# values: the true, estimated (covariate dependent), and estimated (covariate
# independent) graphs for the j-th individual
true_est_graphs <- lapply(1:n, function(ind_idx) list(true = true_graphs[[ind_idx]],
    est_dep = out_dep$graphs[[ind_idx]], est_indep = indep_graphs[[ind_idx]]))

# find the number of true positives for each method
TP_dep <- sum(sapply(1:n, function(ind_idx) sum((true_est_graphs[[ind_idx]]$true ==
    1) & (true_est_graphs[[ind_idx]]$est_dep == 1))))
TP_indep <- sum(sapply(1:n, function(ind_idx) sum((true_est_graphs[[ind_idx]]$true ==
    1) & (true_est_graphs[[ind_idx]]$est_indep == 1))))

# find the number of true negatives for each method
TN_dep <- sum(sapply(1:n, function(ind_idx) sum((true_est_graphs[[ind_idx]]$true ==
    0) & (true_est_graphs[[ind_idx]]$est_dep == 0))))
TN_indep <- sum(sapply(1:n, function(ind_idx) sum((true_est_graphs[[ind_idx]]$true ==
    0) & (true_est_graphs[[ind_idx]]$est_indep == 0))))

# find sensitivity, specificity, and accuracy for each method
sensitivity_dep <- TP_dep/tot1
sensitivity_indep <- TP_indep/tot1

specificity_dep <- TN_dep/tot0
specificity_indep <- TN_indep/tot0

accuracy_dep <- (TN_dep + TP_dep)/num_entries
accuracy_indep <- (TN_indep + TP_indep)/num_entries

# visualize performance
(perf_res_df <- data.frame(performance = c(sensitivity_dep, sensitivity_indep, specificity_dep,
    specificity_indep, accuracy_dep, accuracy_indep), method = rep(c("dependent",
    "independent"), 3), metric = rep(c("sensitivity", "specificity", "accuracy"),
    each = 2)))
```

```
##   performance      method      metric
## 1   0.9403509   dependent sensitivity
## 2   0.8561404 independent sensitivity
## 3   0.9935829   dependent specificity
## 4   1.0000000 independent specificity
## 5   0.9845926   dependent    accuracy
## 6   0.9757037 independent    accuracy
```

```r
y_lower <- floor(min(perf_res_df$performance) * 10)/10
ggplot(perf_res_df, aes(metric, performance, fill = method)) + geom_bar(stat = "identity",
    position = position_dodge()) + coord_cartesian(ylim = c(y_lower, 1)) + theme_bw() +
    ggsci::scale_fill_jco()
```


1.00
0.95
0.90
0.85
0.80
performance
accuracy
sensitivity
specificity
metric
method
dependent
independent