SMCB Project 1

February 24, 2023

Problem 1: Conditional independence and BNs

(a)

$A \perp B|C$ holds, but $A \perp B$ does not hold.

Proof for $A \perp B|C$

From the BN, we know that

$$P(A, B, C) = P(A|C)P(B|C)P(C)$$

To prove that $A \perp B|C$, we need to show that $P(A, B|C) = P(A|C)P(B|C)$.

$$\begin{aligned}
P(A, B|C) &= \frac{P(A, B, C)}{P(C)} \\
&= \frac{P(A|C)P(B|C)P(C)}{P(C)} \\
&= P(A|C)P(B|C)
\end{aligned}$$

Disproof for $A \perp B$

Consider $P(A, B) = \sum_C P(A, B, C)$. From the BN, we have:

$$\begin{aligned}
P(A, B) &= \sum_C P(A, B, C) \\
&= \sum_C P(A|C)P(B|C)P(C) \\
&= \sum_C \frac{P(C|A)P(A)}{P(C)} \frac{P(C|B)P(B)}{P(C)} P(C) \\
&= P(A)P(B) \sum_C \frac{P(C|A)P(C|B)}{P(C)} \\
&\neq P(A)P(B) && \text{(usually)}
\end{aligned}$$

Hence, in general $A \perp B$ does not hold for this Bayesian network.

(b)

$A \perp B|C$ does not hold, but $A \perp B$ holds

Disproof for $A \perp B|C$

Proof for $A \perp B$

From the BN, we know that

$$P(A, B, C) = P(A)P(B)P(C|A, B)$$

We know from Bayes theorem that $P(A, B, C) = P(C|A, B)P(A, B)$.

Hence we have:

$$P(C|A, B)P(A)P(B) = P(C|A, B)P(A, B)$$

i.e., $P(A, B) = P(A)P(B)$. We have consequently proven that $A \perp B$.

Problem 2: Markov blanket

The Markov blanket $MB(D)$ is $\{B, C, E, F, G\}$, where B and F are the parents of D, C and G are the children of D, and E is the co-parent of D.

To prove that the conditional probability of $P(X_k|X_{n \neq k})$ is equivalent to $P(X_k|MB(X_k))$, we can prove that $\forall X_j$ where $j \in [1, n], j \neq k$, if $X_j \notin MB(X_k)$, then $X_j \perp X_k|MB(X_k)$.

For this specific question, we need to prove that $A \perp D|MB(D)$. It is obvious that $A \perp D|MB(D)$ because A and D are d-separated given $MB(D)$ since $E \in MB(D)$ is on the (only) path from A to D and E is in a cascade structure $A \rightarrow E \rightarrow G$.

Problem 3

Package and Dataset Preparation

```
## Warning: package(s) not installed when version(s) same as or greater than current; use
##   `force = TRUE` to re-install: 'graph' 'Rgraphviz' 'RBGL'
```

```r
list.of.packages <- c("GGally", "BiDAG", "igraph")
new.packages <- list.of.packages[!(list.of.packages %in% installed.packages()[,"Package"])]
if(length(new.packages)) install.packages(new.packages)
```

```r
library(GGally)
```

```
## Warning: package 'GGally' was built under R version 4.2.2

## Loading required package: ggplot2

## Warning: package 'ggplot2' was built under R version 4.2.2

## Registered S3 method overwritten by 'GGally':
##   method from
##   +.gg   ggplot2
```

```r
library(BiDAG)
```

```
## Warning: package 'BiDAG' was built under R version 4.2.2
```

```r
library(igraph)
```

```
## Warning: package 'igraph' was built under R version 4.2.2
```

```
##
## Attaching package: 'igraph'

## The following objects are masked from 'package:stats':
##
##     decompose, spectrum

## The following object is masked from 'package:base':
##
##     union
```

```r
set.seed(2023)
```

```r
# download da
df <- read.csv(file="https://raw.githubusercontent.com/felixleopoldo/benchpress/master/resources/data/my
head(df)
```

```
##           Akt        Erk        Jnk         Mek         P38       PIP2
## 1 -0.63433612 -0.1117883 -0.3707515 -0.58558428 -0.06458972  0.6818205
## 2 -3.04091029 -2.5379116  1.0548648 -0.08291055 -0.10231212  1.6658269
## 3 -0.10795269 -0.7494918  0.7096003  0.86363654 -0.23355736 -1.1057101
## 4 -0.05846518  0.3253933  1.1038411 -1.69765652 -0.18079485  1.3026594
## 5  0.32095996  0.5678002  0.6809554 -0.22157981 -0.11327037  0.1823161
## 6 -0.25409240 -0.2603138 -1.6322745 -1.61663169  0.92638128 -1.3078990
##          PIP3         PKA        PKC       Plcg        Raf
## 1 -0.32402294 -0.04326735 -0.6878319 -0.3955337 -0.5148379
## 2  1.18130472 -4.07209170  0.2993658  0.6777917 -0.1101130
## 3  0.09555701 -0.43897960 -0.1565200 -0.2206535  0.6457071
## 4  1.36106920 -0.12200029  0.1600811  0.9960279 -1.6614249
## 5 -0.08623616 -0.74481674 -0.2974304 -0.7794014 -0.3258126
## 6  0.23050612 -0.11188567 -0.6522629 -0.9392948 -0.8496813
```

(a)

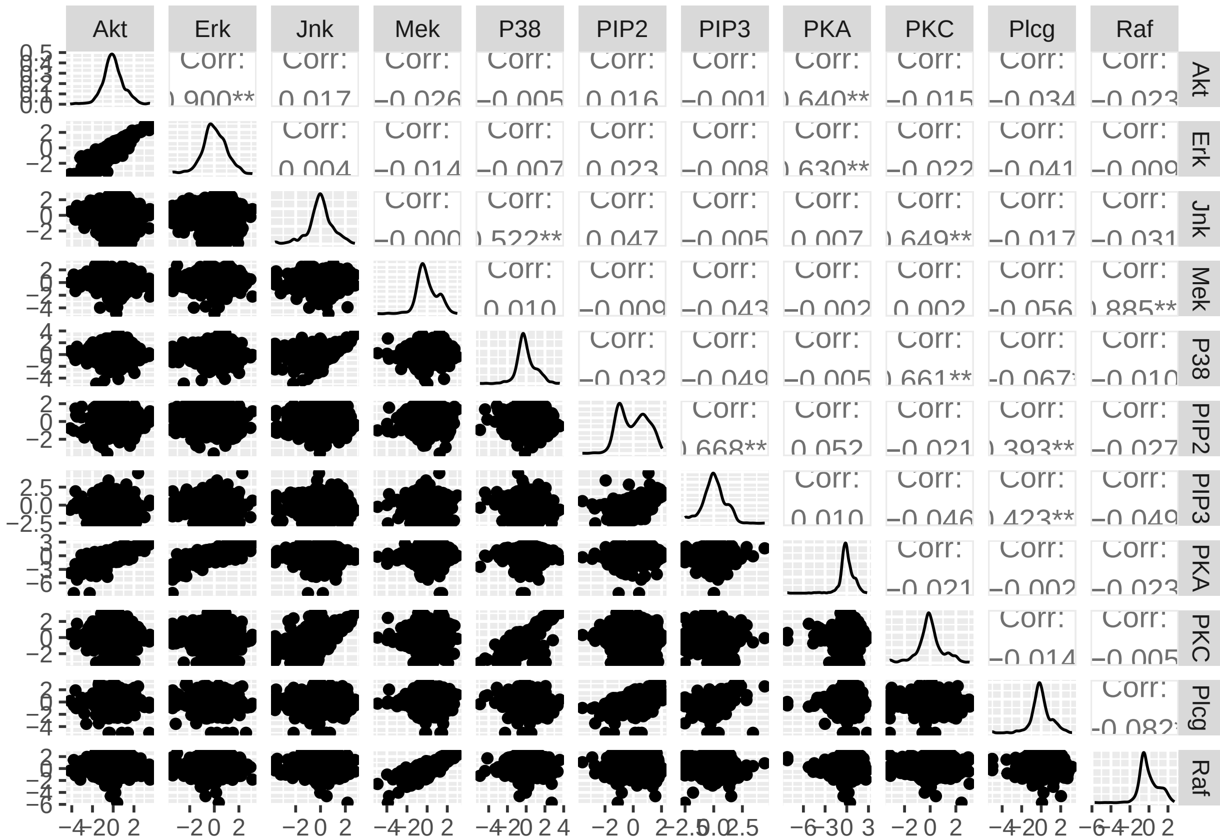
Number of variables (n): 11 Number of observations (N): 902

```r
str(df)
```

```
## 'data.frame':    902 obs. of  11 variables:
##  $ Akt : num  -0.6343 -3.0409 -0.108 -0.0585 0.321 ...
##  $ Erk : num  -0.112 -2.538 -0.749 0.325 0.568 ...
##  $ Jnk : num  -0.371 1.055 0.71 1.104 0.681 ...
##  $ Mek : num  -0.5856 -0.0829 0.8636 -1.6977 -0.2216 ...
##  $ P38 : num  -0.0646 -0.1023 -0.2336 -0.1808 -0.1133 ...
##  $ PIP2: num  0.682 1.666 -1.106 1.303 0.182 ...
##  $ PIP3: num  -0.324 1.1813 0.0956 1.3611 -0.0862 ...
##  $ PKA : num  -0.0433 -4.0721 -0.439 -0.122 -0.7448 ...
##  $ PKC : num  -0.688 0.299 -0.157 0.16 -0.297 ...
##  $ Plcg: num  -0.396 0.678 -0.221 0.996 -0.779 ...
##  $ Raf : num  -0.515 -0.11 0.646 -1.661 -0.326 ...
```

Visualization of the transformed data using `ggpairs` function.

```r
ggpairs(df)
```



Randomly split the data into 80% traning data and 20% test data.

```
train_data_size <- floor(0.8*nrow(df))
picked <- sample(seq_len(nrow(df)), size=train_data_size)
train_data <- df[picked, ]
test_data  <- df[-picked,]
```

Initialize the parameters using the function `BiDAG::scoreparameters` with the training data and the Bayesian Gaussian equivalent (BGe) score.

```
train_scorepar <- BiDAG::scoreparameters(scoretype="bge", train_data)
test_scorepar <- BiDAG::scoreparameters(scoretype="bge", test_data)
```

(b)

Learn a Bayesian network using the `BiDAG::iterativeMCMC` function.

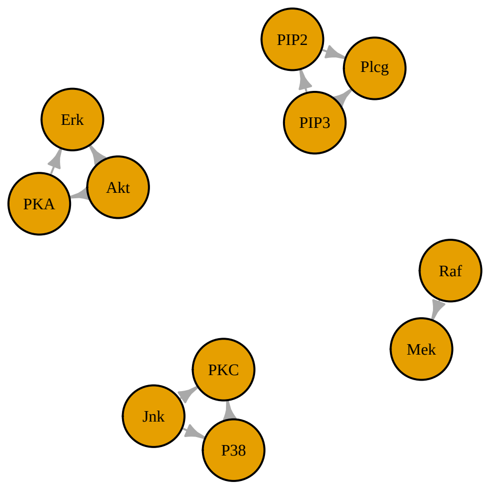
```
BN <- BiDAG::iterativeMCMC(scorepar=train_scorepar)
```

```
## maximum parent set size is 2
## core space defined, score table are being computed
## score tables completed, iterative MCMC is running
```

Plot the DAG.

```
DAG <- BiDAG::getDAG(BN)
g <- igraph::graph.adjacency(DAG, mode="directed")
test.layout <- layout_nicely(g)
igraph::plot.igraph(g,
```

```
                    edge.arrow.size=.5,
                    vertex.size=30,
                    vertex.label.cex=.5,
                    vertex.label.color="black",
                    layout=test.layout
)
```



Evaluate the log score of the test data agaisnt the estimated DAG using `BiDAG::scoreagainstDAG`.

```
log_score <- BiDAG::scoreagainstDAG(scorepar=test_scorepar, incidence=DAG)
mean(log_score)
```

```
## [1] -12.42144
```

(c)

```
res <- data.frame(matrix(ncol=5, nrow=2))
colnames(res) <- c(1, 2, 3, 4, 5)
rownames(res) <- c("ecount", "logscore")
```

```
procedure <- function(am, index=1) {
    picked <- sample(seq_len(nrow(df)), size=train_data_size)
    train_data <- df[picked, ]
    test_data  <- df[-picked,]
    train_scorepar <- BiDAG::scoreparameters(
        scoretype="bge",
        train_data,
```

```r
        bgepar=list(am=am, aw=NULL)
    )
    BN <- BiDAG::iterativeMCMC(scorepar=train_scorepar)
    return(BN)
}
```

```r
list.of.packages <- c("foreach", "doParallel", "doRNG")
new.packages <- list.of.packages[!(list.of.packages %in% installed.packages()[,"Package"])]
if(length(new.packages)) install.packages(new.packages)
```

```r
library(foreach)
```

```
## Warning: package 'foreach' was built under R version 4.2.2
```

```r
library(doParallel)
```

```
## Warning: package 'doParallel' was built under R version 4.2.2

## Loading required package: iterators

## Warning: package 'iterators' was built under R version 4.2.2

## Loading required package: parallel
```

```r
library(doRNG)
```

```
## Warning: package 'doRNG' was built under R version 4.2.2

## Loading required package: rngtools

## Warning: package 'rngtools' was built under R version 4.2.2
```

```r
library(parallel)
```

```r
num_cores <- detectCores()
registerDoParallel(num_cores)
index <- 1
# foreach (am=c(1e-3, 1e-1, 1e0, 1e1, 1e2)) %do% {
#     v <- foreach (i=1:100, .combine=rbind) %dorng% {
#         picked <- sample(seq_len(nrow(df)), size=train_data_size)
#         train_data <- df[picked, ]
#         test_data  <- df[-picked,]
#         train_scorepar <- BiDAG::scoreparameters(
#             scoretype="bge", train_data,
#             bgepar=list(am=am, aw=NULL)
#         )
#         test_scorepar <- BiDAG::scoreparameters(
#             scoretype="bge", test_data,
#             bgepar=list(am=am, aw=NULL)
#         )
#         BN <- BiDAG::iterativeMCMC(scorepar=train_scorepar)
#         DAG <- BiDAG::getDAG(BN)
#         g <- igraph::graph.adjacency(DAG, mode="directed")
#         ecount <- igraph::ecount(g)
#         log_score <- BiDAG::scoreagainstDAG(
#             scorepar=test_scorepar,
#             incidence=DAG
#         )
#         avg_log_score <- mean(log_score)
```

```
#         return(c(ecount=ecount, log_score=avg_log_score))
#     }
#     avg <- colMeans(v)
#     res[1, index] <- avg[1]
#     res[2, index] <- avg[2]
#     index <- index + 1
# }
stopImplicitCluster()
print(res)
```

```
##           1  2  3  4  5
## ecount   NA NA NA NA NA
## logscore NA NA NA NA NA
```

```
scorepar <- BiDAG::scoreparameters(scoretype="bge", df, bgepar=list(am=1e-1, aw=NULL))
BN <- BiDAG::iterativeMCMC(scorepar=scorepar)
```

```
## maximum parent set size is 3
## core space defined, score table are being computed
## score tables completed, iterative MCMC is running
```

```
DAG <- BiDAG::getDAG(BN)
g <- igraph::graph.adjacency(DAG, mode="directed")
igraph::plot.igraph(g)
```