

Project 1 Bayesian Networks and Gene Regulation

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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:

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

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 $A \perp B|C$

Consider $A \perp B|C$, we'll have $P(A, B|C) = P(A|C)P(B|C)$.

From the BN and by applying Bayes theorem we can derive that:

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

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 $A \rightarrow E \rightarrow G$.

Alternatively it can also be proved by meticulously simplifying the total probability (since d-separation is not introduced yet):

$$\begin{aligned}
 P(D|A, B, C, E, F, G) &= \frac{P(A, B, C, D, E, F, G)}{P(A, B, C, E, F, G)} \\
 &= \frac{\cancel{P(A)}\cancel{P(B)}\cancel{P(F)}P(D|B, F)\cancel{P(E|A)}P(G|D, E)P(C|D)}{\sum_D \cancel{P(A)}\cancel{P(B)}\cancel{P(F)}P(D|B, F)\cancel{P(E|A)}P(G|D, E)P(C|D)} \\
 &= \frac{P(D|B, F)P(G|D, E)P(C|D)}{\sum_D P(D|B, F)P(G|D, E)P(C|D)}
 \end{aligned}$$

It's clear that the total probability depends only on $MB(D)$. Hence we have $P(D|A, B, C, E, F, G) = P(D|MB(D))$

Problem 3: Learning Bayesian networks from protein data

Package and Dataset Preparation

```
set.seed(42)
```

```
# download dataset
```

```
df <- read.csv(file="https://raw.githubusercontent.com/felixleopoldo/benchpress/master/resources/data/m")
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)

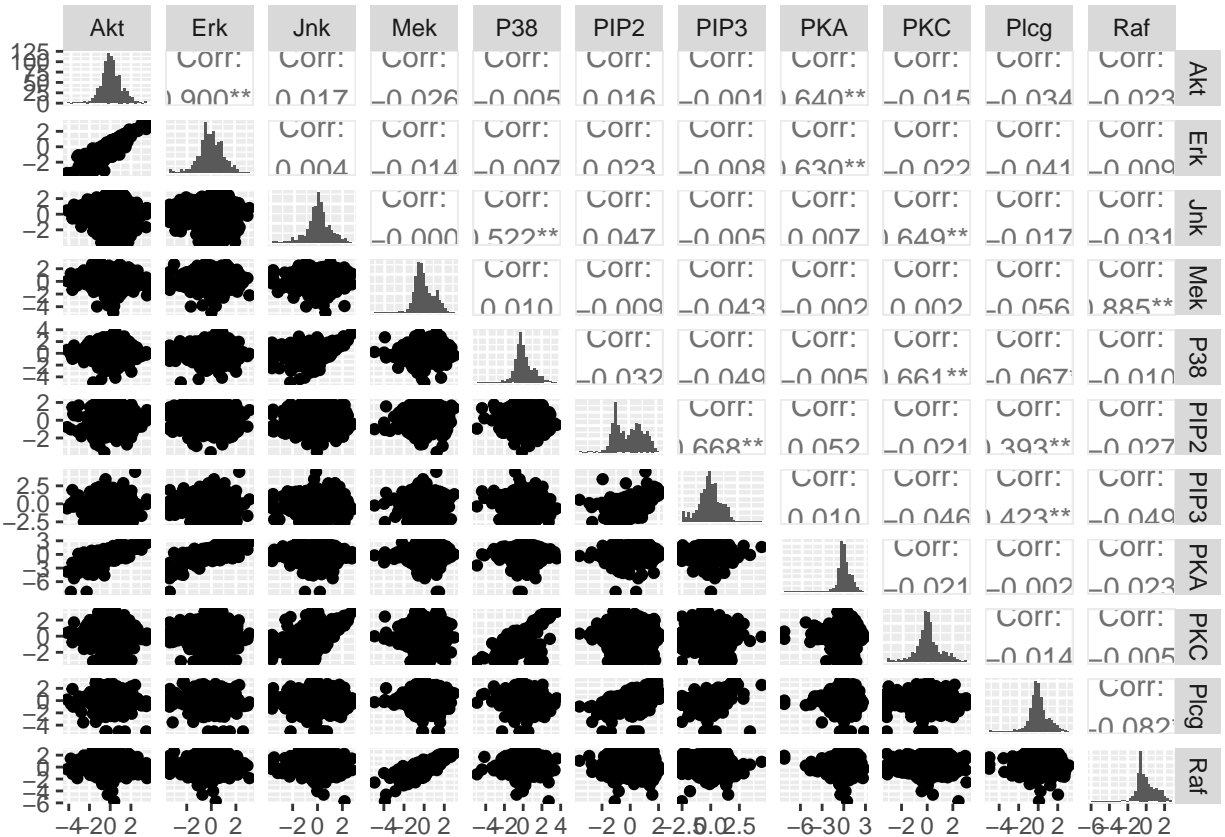
Number of variables (n): 11 Number of observations (N): 902

```
dim(df)
```

```
## [1] 902 11
```

Visualization of the transformed data using ggpairs function.

```
ggpairs(df, diag = list(continuous = "barDiag"))
```



Randomly split the data into 80% training 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)
```

(b)

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

```
BN <- iterativeMCMC(scorepar=train_scorepar, verbose=FALSE)
```

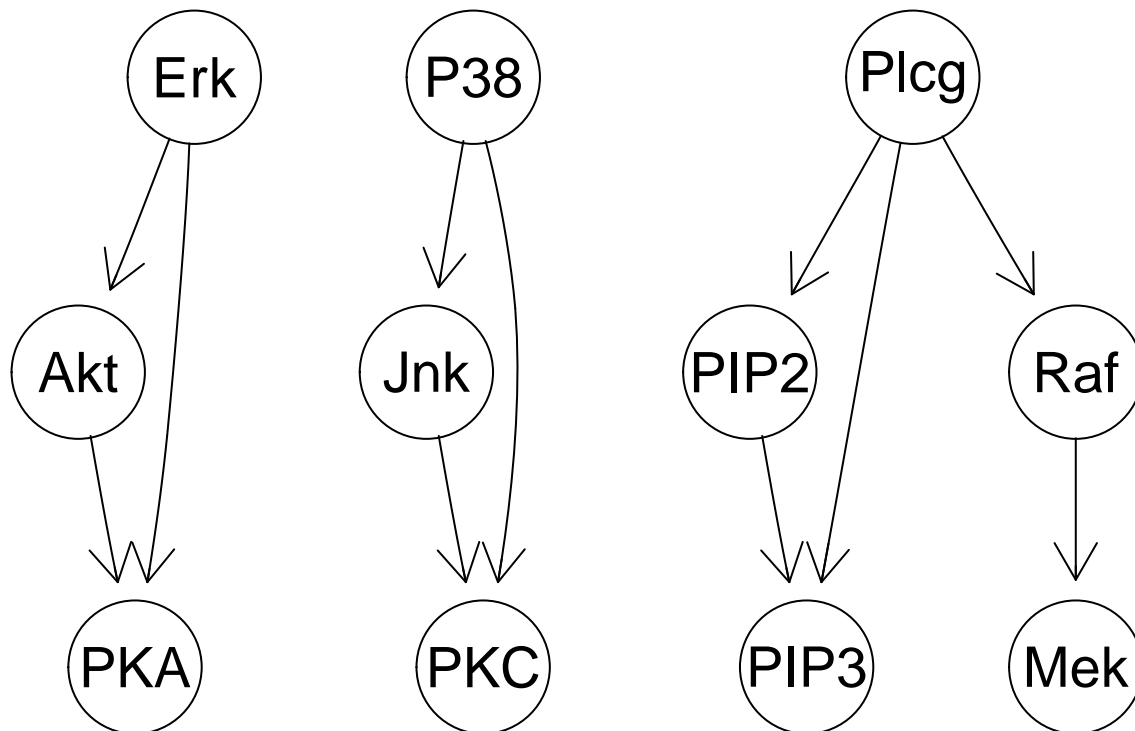
```
summary(BN)
```

```
## object of class 'iterativeMCMC'
##
## Results:
## maximum score DAG with 11 nodes and 11 edges:
## maximum DAG score= -9395.297
##
## algorithm: iterative order MCMC
## number of search space expansion steps: 1
```

```
## number of edges in the initial search space: 22
## number of added edges: 0
## total number of MCMC iterations: 25000
## total number of MCMC sampling steps (length of trace): 1001
## number of MCMC iterations per expansion step: 25000
## number of MCMC sampling steps per expansion step: 1001
## initial search space: PC
## sample/MAP: MAP
##
## Additional output:
```

Plot the DAG.

```
par(mfrow=c(1, 1))
plot(graphAM(as.matrix(BN$DAG), edgemode = "directed"))
```



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

```
sum(scoreagainstDAG(scorepar = train_scorepar, BN$DAG, test_data))
```

```
## [1] -2234.434
```

(c)

The following code blocks run 10 iterations for each experiments.

```
res <- data.frame(matrix(vector(mode = 'numeric', length = 10), ncol=5, nrow=2))
colnames(res) <- c(1, 2, 3, 4, 5)
rownames(res) <- c("ecount", "logscore")
```

```

am_list <- 10^(c(-5, -3, -1, 1, 2))

num_cores <- detectCores()
registerDoParallel(num_cores)
index <- 1
foreach (am=am_list) %do% {
  # by default doRNG uses "L'Ecuyer-CMRG" so should be fine
  v <- foreach (i=1:10, .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)
    )
    BN <- BiDAG::iterativeMCMC(scorepar=train_scorepar)
    ecount <- sum(BN$DAG)
    log_score <- sum(BiDAG::scoreagainstDAG(train_scorepar, BN$DAG, test_data))
    return(c(ecount=ecount, log_score=log_score))
  }
  avg <- colMeans(v)
  res[1, index] <- avg[1]
  res[2, index] <- avg[2]
  index <- index + 1
}
stopImplicitCluster()

colnames(res) <- am_list
print(res)

```

```

##           1e-05      0.001      0.1      10      100
## ecount      7.000      7.000      9.100     13.400     15.800
## logscore -2352.435 -2347.451 -2367.043 -2326.321 -2366.537

```

It seems that as am increase, the average number of edges also increases.

The log score seems to have an optimum at am=1 for the parameters we tested.

The final graph from the whole dataset is visualized in the following code block.

```

scorepar <- BiDAG::scoreparameters(scoretype="bge", df, bgepar=list(am=1, aw=NULL))
BN <- BiDAG::iterativeMCMC(scorepar=scorepar, verbose=FALSE)
par(mfrow=c(1,1))
plot(graphAM(as.matrix(BN$DAG), edgemode = "directed"))

```

