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DATALAB BROWN BAG SEMINAR, ZHAW 30.05.2018

BAYESIAN NETWORKS LEARNING IN A NUTSHELL

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OUTLINE

- Motivational examples
- Elements of graph theory/probability theory
- Bayesian Network Learning
  - Constraint-based algorithms
  - Score-and-search
- Causal versus acausal thinking
- Real-data applications using R

Credit Card Fraud Detection Using Bayesian and Neural Networks

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Abstract

This paper discuss process of learning,
tection by means ble to correctly clas-
of digitalization, seen before as fraud-
great importance t ome features of that
two machine learr s as follows: first we
ing under uncertai main of credit card
and 4 we briefly ex-

experiment	±10% false pos	±15% false pos
ANN-fig 2(a)	60% true pos	70% true pos
ANN-fig 2(a)	47% true pos	58% true pos
ANN-fig 2(c)	60% true pos	70% true pos
BBN-fig 2(e)	68% true pos	74% true pos
BBN-fig 2(g)	68% true pos	74% true pos

Table 1: This table compares the results achieved with ANN and BBN, for a false positive rate of respectively 10% and 15%.

MOTIVATIONAL EXAMPLE: VETERINARY EPIDEMIOLOGY DATA VISUALISATION

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Contents lists available at SciVerse ScienceDirect

Preventive Veterinary Medicine

journal homepage: www.elsevier.com/locate/prevetmed

Using Bayesian networks to explore the role of weather as a potential determinant of disease in pigs

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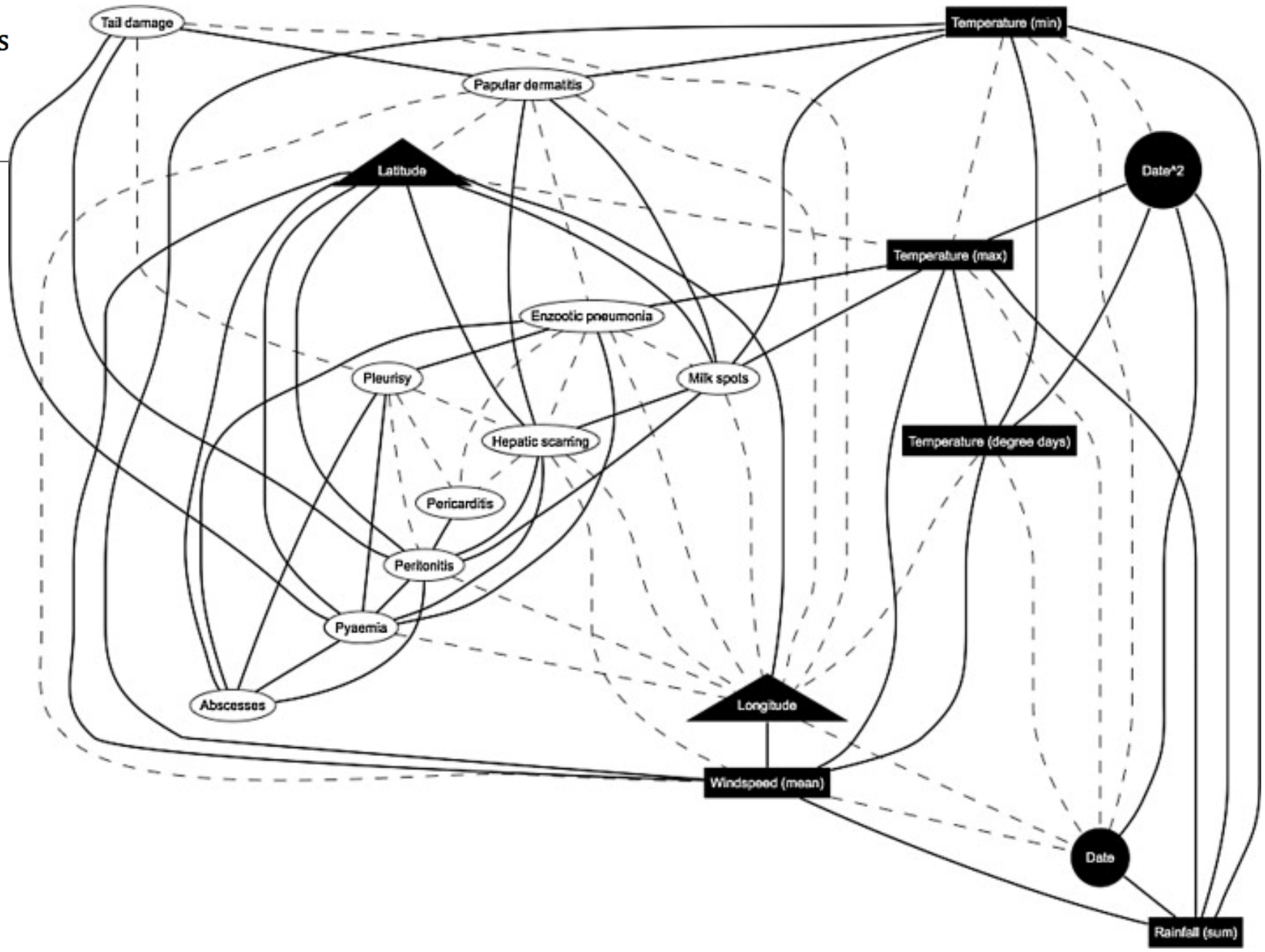

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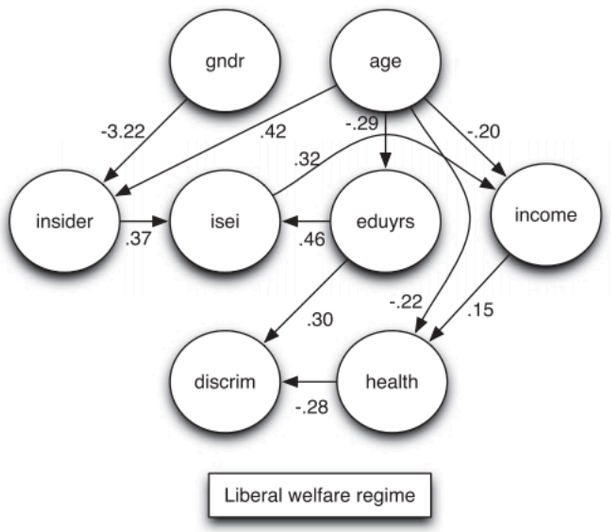
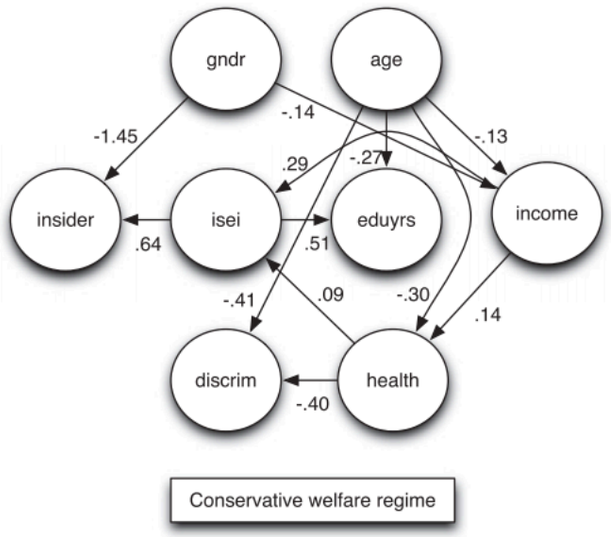
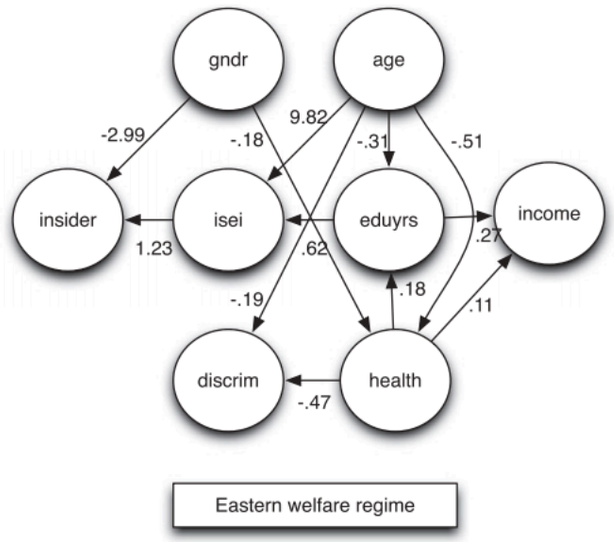
Discovering complex interrelationships between socioeconomic status and health in Europe: A case study applying Bayesian Networks

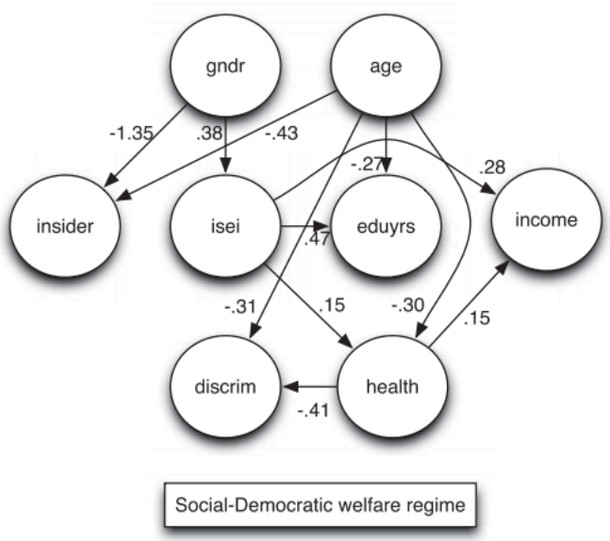
Javier Alvarez-Galvez [a, b, *]

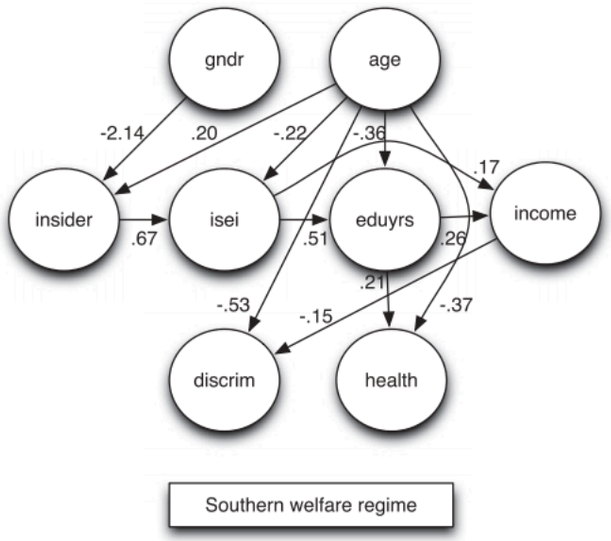
[a] *Loyola University Andalusia, Department of International Studies, Campus de Palmas Altas, Faculty of Political Sciences and Law, Seville 41014, Spain*
[b] *Complutense University of Madrid, Department of Sociology IV (Research Methodology and Communication Theory), Campus de Somosaguas, Faculty of Political*











Description of the variables:

1. GNDR: Gender (0= male; 1=female).
2. AGE: Age of respondent.
3. INSIDER: Insiderness (0=outsider; 1=insider).
4. ISEI: International Socio-Economic Index of occupational status.
5. EDUYRS: Years of education.
6. INCOME: Household total net income.
7. DISCRIM: Self-Perceived Discrimination (SPD) (1=discrim.).
8. HEALTH: Self-Rated Health (SRH).

Networks score goodness of fit (log marginal likelihood):
Liberal welfare-state (N=16,591): -90117.89
Social-Democratic-welfare state (N=29,120): -192477.4
Conservative welfare-state (N=58,184): -319176.2
Southern welfare-state (N=37,247): -136176.5
Eastern welfare-state (N=43,846): -135422.5

Fig. 1. Bayesian networks describing interrelationships between SES and health in five European welfare states.

BAYESIAN NETWORKS IN THE MACHINE LEARNING WORLD

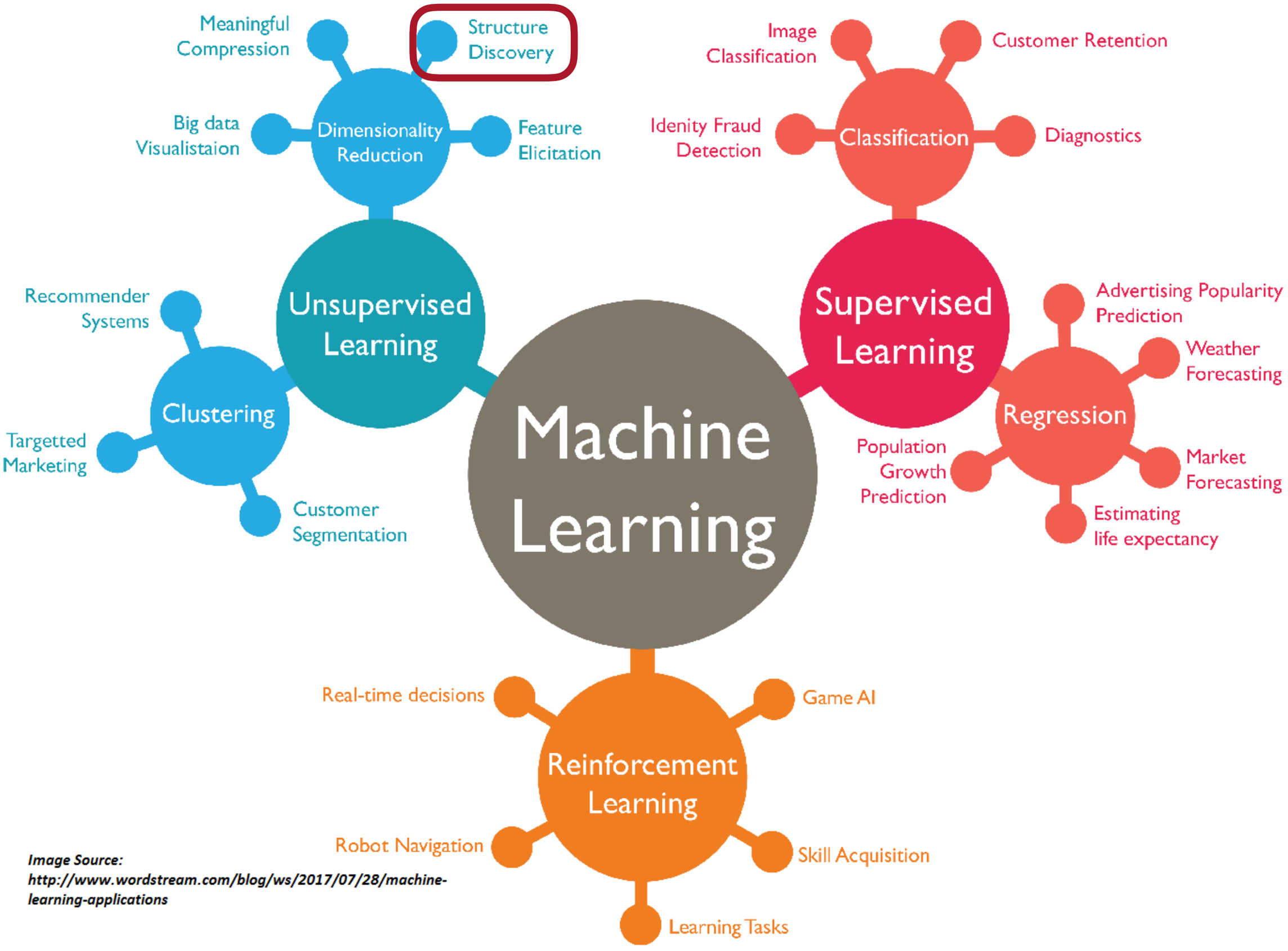


Image Source:
http://www.wordstream.com/blog/ws/2017/07/28/machine-learning-applications

WHAT IS A BAYESIAN NETWORK?

Bayesian Networks are defined by two elements:

Network structure:

Directed Acyclic Graph (DAG): G = (V, A)

in which each node vi ∈ V corresponds to a random variable Xi

Probability distribution:

Probability distribution X with parameters Θ, which can be factorised into smaller local probability distributions according to the arcs aij ∈ A present in the graph.

A BN encodes the factorisation of the joint distribution

$$P(\mathbf{X}) = \prod_{j=1}^{n} P(X_j \mid \mathbf{Pa}_j, \Theta_j), \text{ where } \mathbf{Pa}_j \text{ is the set of parents of } X_j$$

SOME ELEMENTS OF PROBABILITY THEORY

The conditional probability of A given B is: $$P(A \mid B) = \frac{P(A, B)}{P(B)}$$

Bayes theorem: $$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}$$

Let A, B and C non intersecting subsets of nodes in a DAG G

A is conditionally independent of B given C if: $A \perp\!\!\!\perp_P B | C$

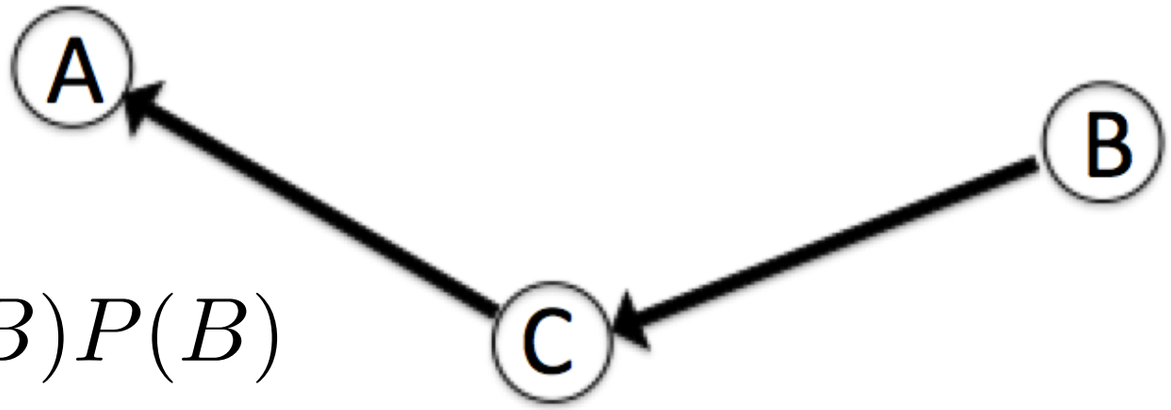
$$P(A, B \mid C) = P(A \mid C)P(B \mid C)$$

ELEMENT OF GRAPH THEORY

Let A, B and C non intersecting subsets of nodes in a DAG G

A is conditionally independent of B given C if: $A \perp\!\!\!\perp_P B | C$

$$P(A, B \mid C) = P(A \mid C)P(B \mid C)$$



$$P(A, B, C) = P(A \mid C)P(C \mid B)P(B)$$

$$P(A, B \mid C) = \frac{P(A \mid C)P(C \mid B)P(B)}{P(C)}$$

$$= \frac{P(A \mid C)P(B, C)}{P(C)}$$

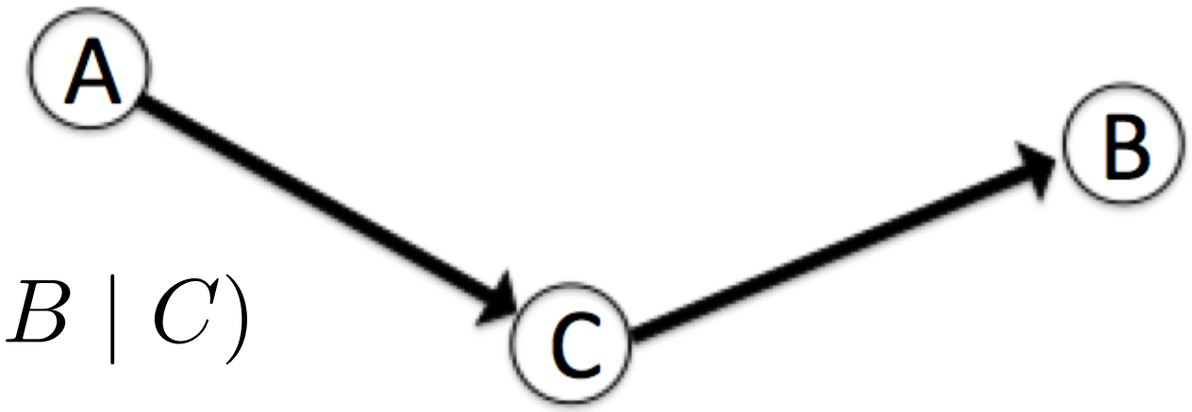
$$= P(A \mid C)P(B \mid C)$$

ELEMENT OF GRAPH THEORY

Let A, B and C non intersecting subsets of nodes in a DAG G

A is conditionally independent of B given C if: $A \perp\!\!\!\perp_P B | C$

$$P(A, B \mid C) = P(A \mid C)P(B \mid C)$$



$$P(A, B, C) = P(A)P(C \mid A)P(B \mid C)$$

$$P(A, B \mid C) = \frac{P(A)P(C \mid A)P(B \mid C)}{P(C)}$$

$$= \frac{P(A, C)P(B \mid C)}{P(C)}$$

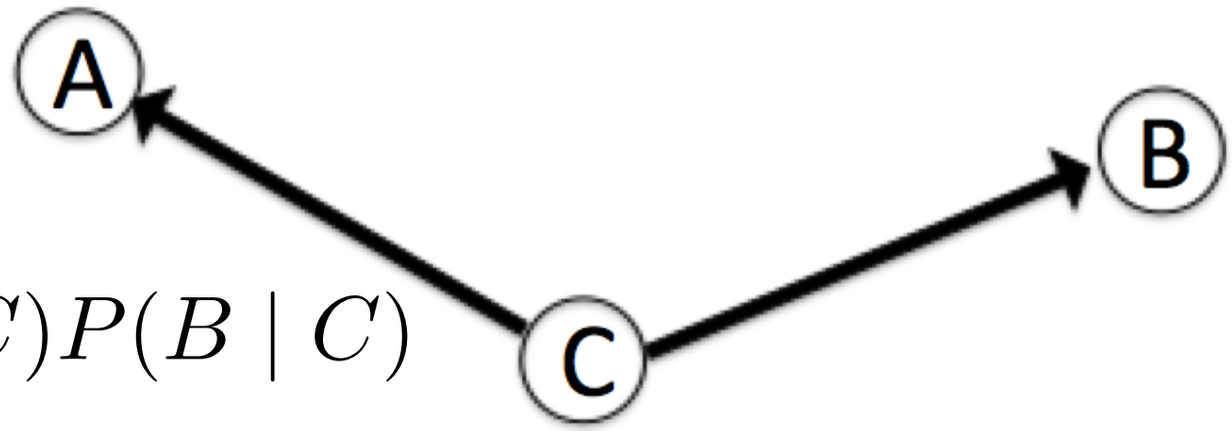
$$= P(A \mid C)P(B \mid C)$$

ELEMENT OF GRAPH THEORY

Let A, B and C non intersecting subsets of nodes in a DAG G

A is conditionally independent of B given C if: $A \perp\!\!\!\perp_P B | C$

$$P(A, B \mid C) = P(A \mid C)P(B \mid C)$$



$$P(A, B, C) = P(C)P(A \mid C)P(B \mid C)$$

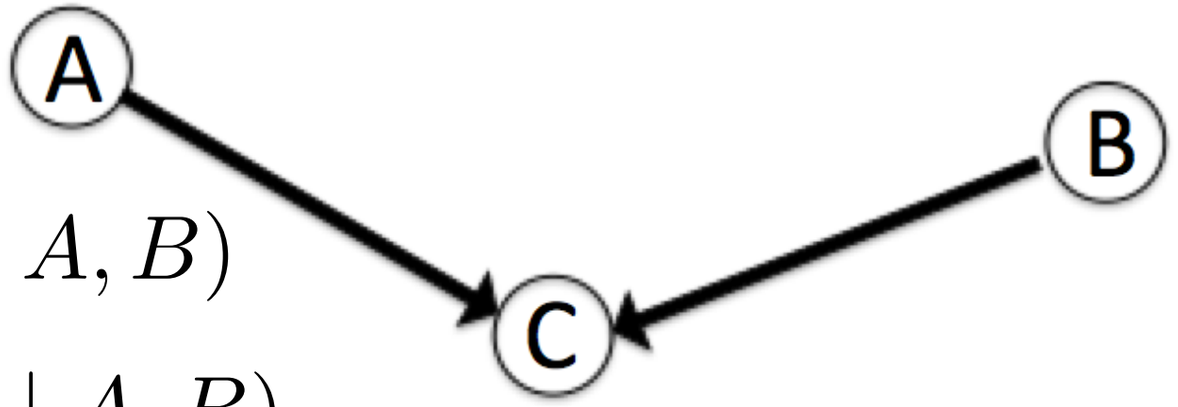
$$P(A, B \mid C) = \frac{P(C)P(A \mid C)P(B \mid C)}{P(C)}$$

$$= P(A \mid C)P(B \mid C)$$

Let A, B and C non intersecting subsets of nodes in a DAG G

A is conditionally independent of B given C if: $A \perp\!\!\!\perp_P B|C$

$$P(A, B \mid C) = P(A \mid C)P(B \mid C)$$



$$P(A, B, C) = P(A)P(B)P(C \mid A, B)$$

$$P(A, B \mid C) = \frac{P(A)P(B)P(C \mid A, B)}{P(C)}$$

$$= \frac{P(A)P(B)P(A, B, C)}{P(A)P(B)P(C)}$$

$$= P(A, B \mid C)$$

$A \not\perp\!\!\!\perp_P B|C$

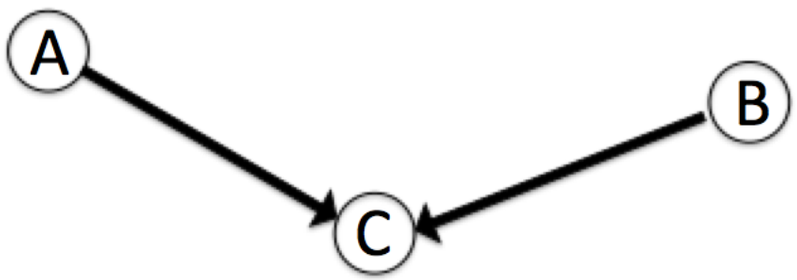
ELEMENT OF GRAPH THEORY

Let A, B and C non intersecting subsets of nodes in a DAG G

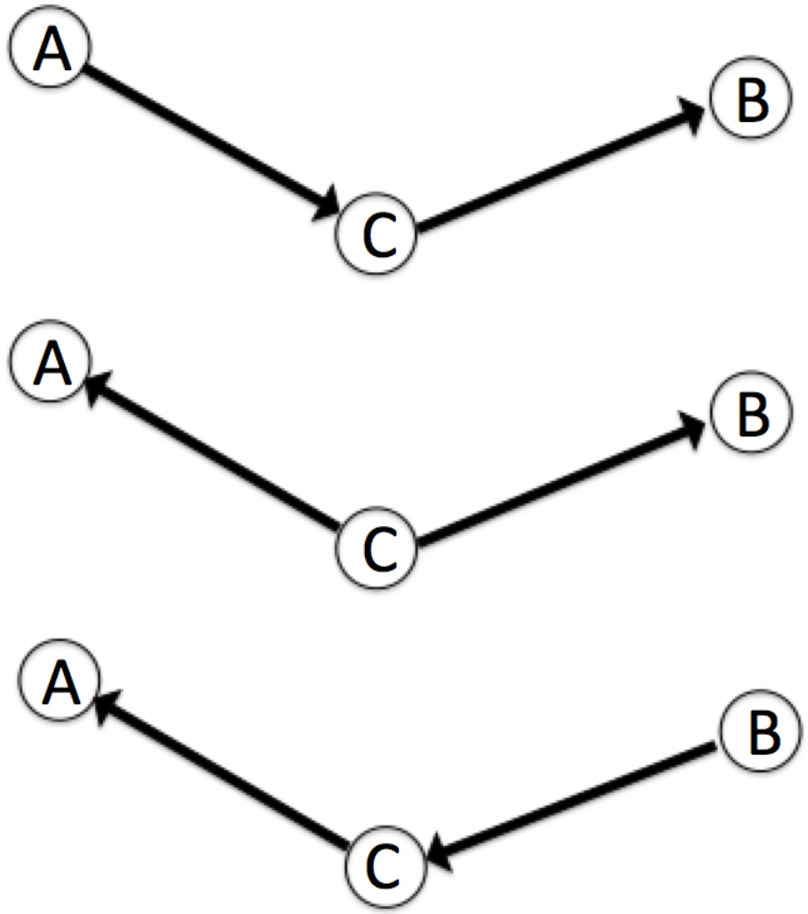
A is conditionally independent of B given C if: $A \perp\!\!\!\perp_P B|C$

$$P(A, B \mid C) = P(A \mid C)P(B \mid C)$$

$A \not\perp\!\!\!\perp_P B|C$



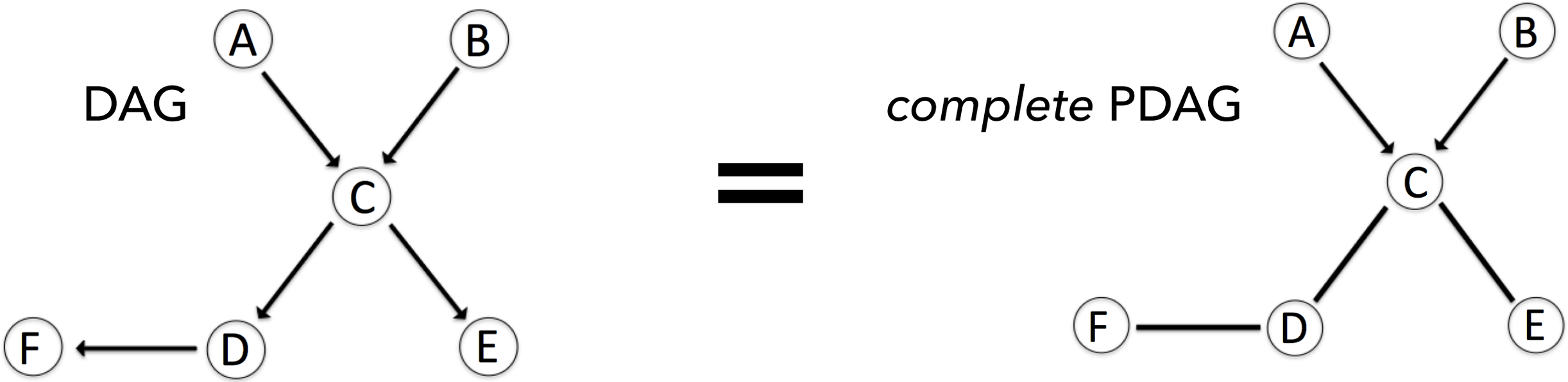
$A \perp\!\!\!\perp_P B|C$



LEARNING BAYESIAN NETWORKS

- In a practical perspective, for observational data, if learning algorithms rely on probabilistic learning algorithm. Then one can learn up to the Markov equivalence class.

- Markov equivalence class are the set of DAGs that have the same skeleton and v-structure.



A path from A to B is blocked if it contains a node s.t. either

- the arrows on the path meet either head-to-tail or tail-to-tail at the node, and the node is in the set C, or
- the arrows meet head-to-head at the node, and neither the node, nor any of its descendants, are C.

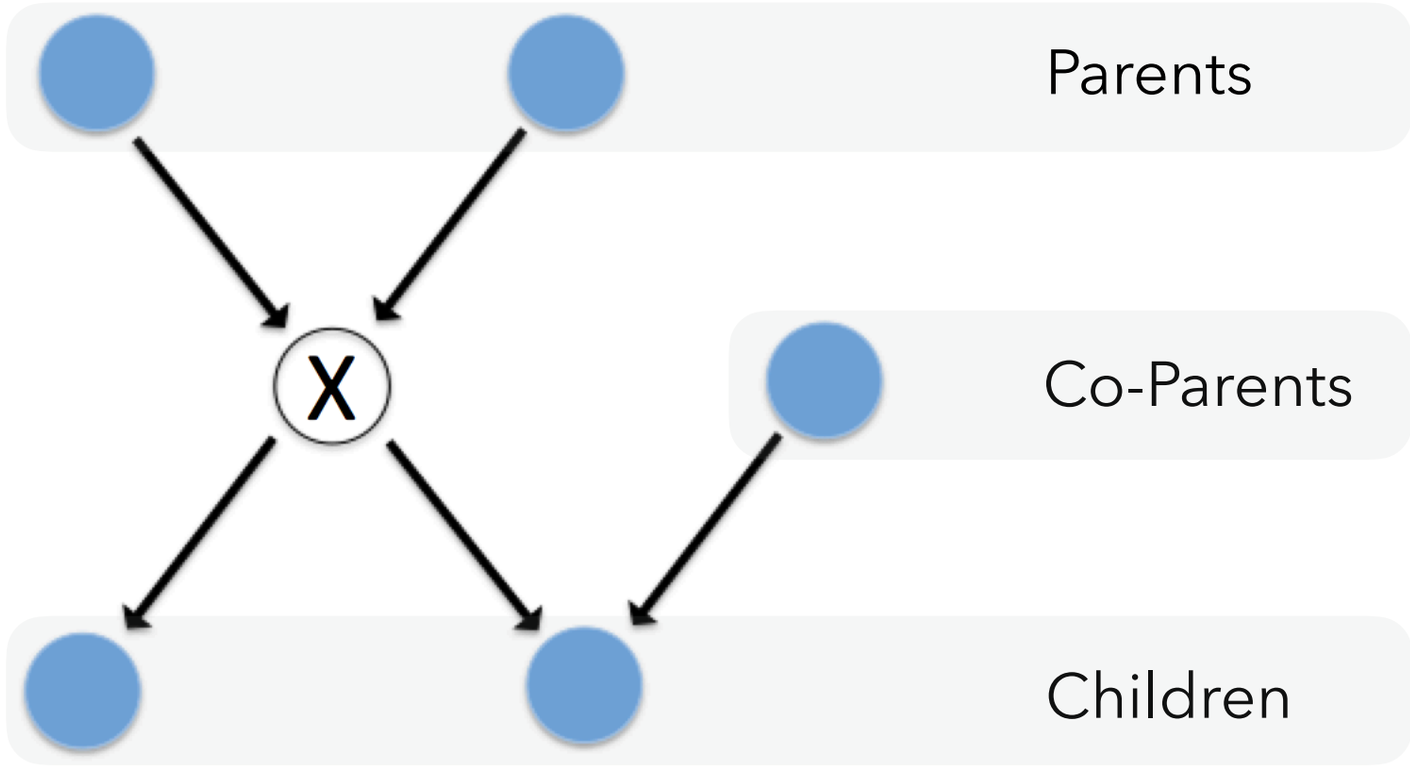
If all paths from A to B are blocked, A is said to be d-separated from B by C.

Theorem (Verma & Pearl, 1988): A is d-separated from B by C if, and only if, the joint distribution over all variables in the graph satisfies:

$$A \perp\!\!\!\perp_G B | C$$

Link between statistical statement (conditionally independent) and a graph propriety (d-separation)

The Markov Blanket of a node is the set of parents, co-parents and children.



$$P(X_k \mid X_n, k \neq n) = P(X_k \mid X_{\mathrm{MB}(k)}), \forall k$$

The Markov Blanket of a node is the set of nodes that shields the index node from the rest of the network

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$$\mathcal{M} = (\mathcal{S}, \theta_{\mathcal{M}})$$

Model selection

Structure learning

Parameter estimation

Parameter learning

$$P(\mathcal{M}|\mathcal{D}) = \underbrace{P(\theta_{\mathcal{M}}, \mathcal{S}|\mathcal{D})}_{\text{model learning}} = \underbrace{P(\theta_{\mathcal{M}}|\mathcal{S}, \mathcal{D})}_{\text{parameter learning}} \underbrace{P(\mathcal{S}|\mathcal{D})}_{\text{structure learning}}$$

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	Fully Observed data	Missing data/hidden variables
Known graph structure	Easy Sample statistics	EM algorithm Gradient ascent Variational inference Doable
Unknown graph structure	Doable **Search-and-score** **PC algorithm**	Hard Structural EM

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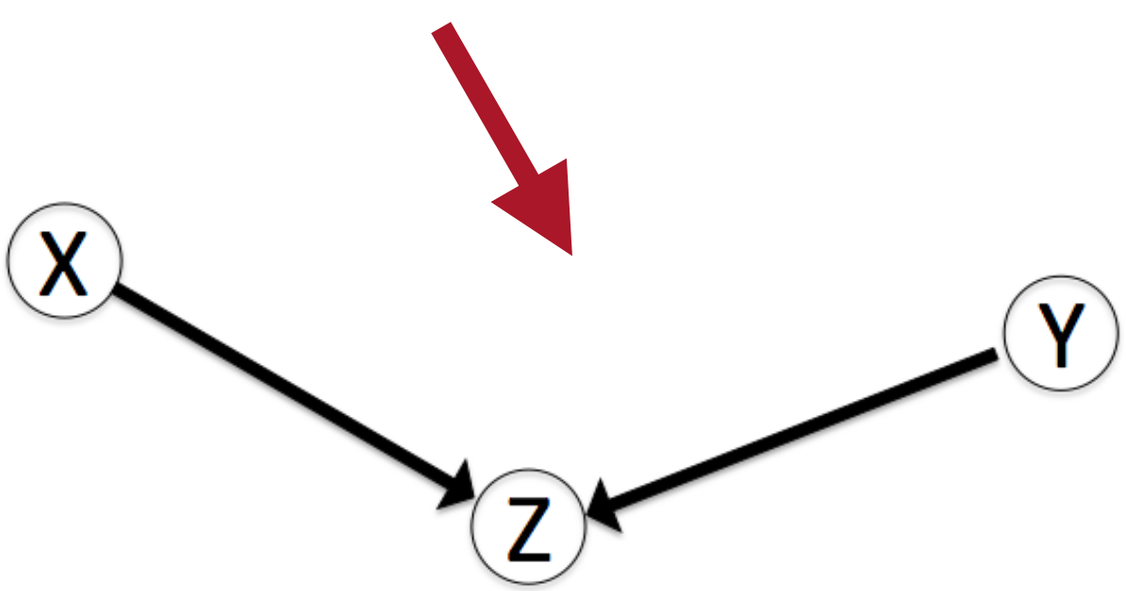
Constraint based algorithms

$$P_{X \perp\!\!\!\perp Y|Z} < \alpha$$

$$X \perp\!\!\!\perp_{\mathcal{S}} Y|Z = X \perp Y|Z$$



Search-and-score algorithms

Maximum a posteriori score

$$G^* = \underset{G}{\operatorname{argmax}}\ f(\mathcal{D}, G, n, \dots)$$

Example of scoring functions:

- Bayesian versus ML scores
  - log marginal likelihood
  - Bayesian-Dirichlet (BDeu,BDs,BDe)
  - Bayesian Information Criterion (BIC)

Constraint-based algorithms

- *Inductive Causation* (IC): (Verma and Pearl, 1991)
  - Provides a framework for learning the structure of Bayesian networks using conditional independence tests in three steps
  - A major problem of the IC algorithm is that the first two steps cannot be applied to any real-world problem due to computational complexity …
- *PC*: first practical application of the IC algorithm (Spirtes et al., 2001)
  - backward selection procedure from the saturated graph
- *Grow-Shrink* (GS) (Margaritis, 2003)
  - Simple forward selection MB detection approach
- *Incremental Association* (IAMB): (Tsamardinos et al., 2003)
  - two-phase selection scheme based on a forward selection followed by a backward selection of the MB

LEARNING BAYESIAN NETWORKS

- Constraint-based methods require a Markov and faithfulness assumption
- Conditional independencies in the distribution exactly equal the ones encoded in the DAG via d-separation

$$A \perp\!\!\!\perp_G B|C \overset{\text{Markov}}{\underset{\text{Faithful}}{\rightleftarrows}} A \perp\!\!\!\perp_P B|C$$

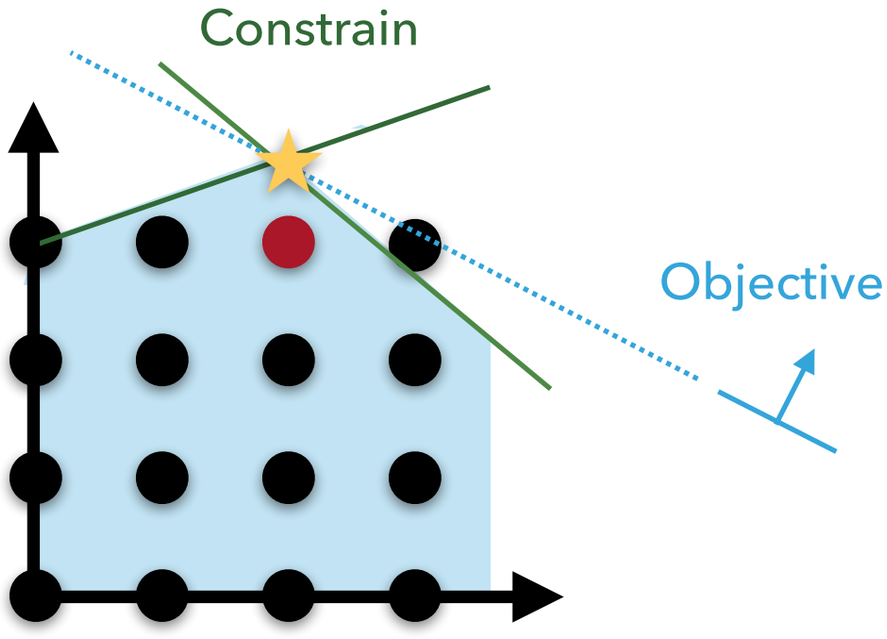
- Causal sufficiency: no unmeasured common causes

In a pratical perspective:

- Testing mixture of data?
- Testing assumptions?

Score-and-search algorithms

- *Heuristic approaches / Greedy search*
  - Hill-climbing (with possibly random restarts/stochastics …)
  - Tabu search (Glover, 1986)
  - Simulated annealing (Kirkpatrick et al, 1983)
  - Plus an entire zoo of methods …
- *Exact search*
  - Exact node ordering (Koivisto et al. , 2004)
  - Learning with cutting planes (Cussens, 2012)



Scores

- Decomposability!
- Discrete BNs:
  - Bayesian-Dirichlet: BDeu (Heckerman et al. ,1995)
- Score equivalence for additive regression framework:
  - Bayesian based scores: not always score equivalent due to the prior!
  - Information theoretic scores: BIC asymptotically score equivalent

Counter example

- Maximum likelihood estimator … return fully connected BN!

In a practical perspective:

- Scoring mixture of data?
- Score equivalence!

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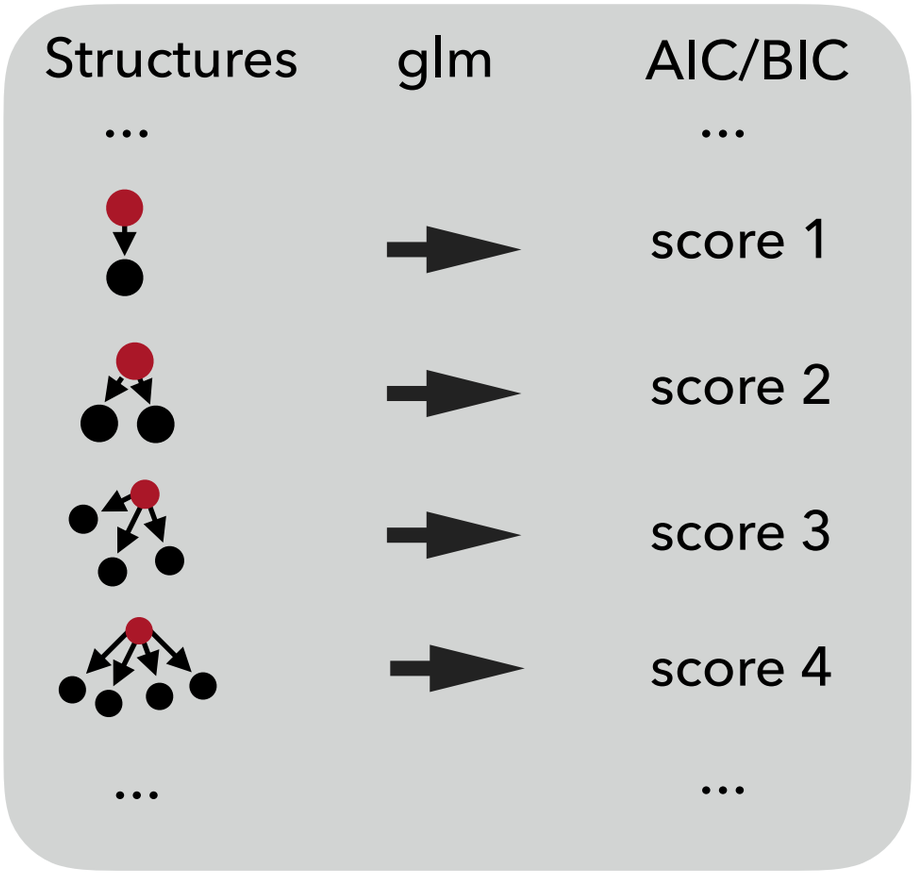
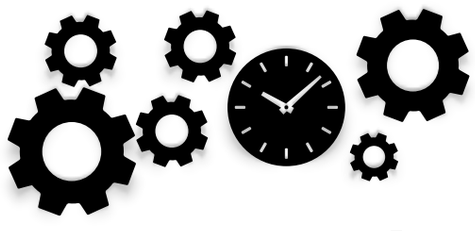
Search and score algorithm

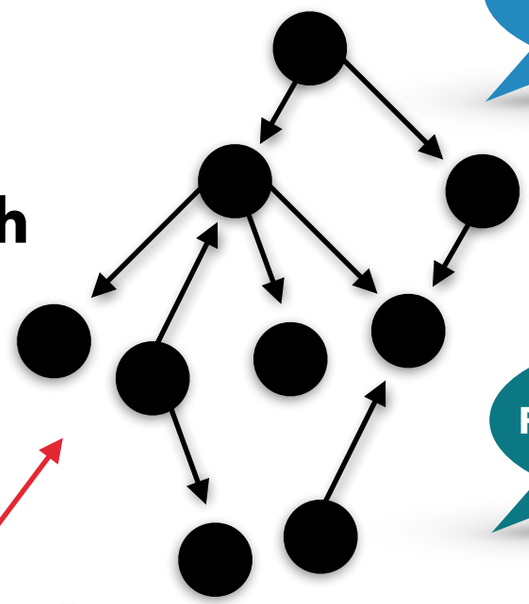


Exact or heuristic search



Causality!

Ban/Retain structures



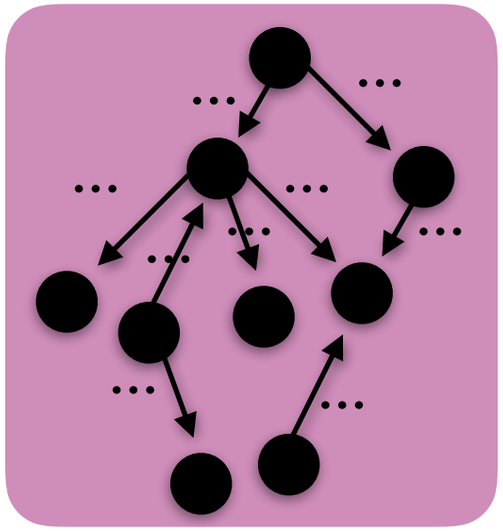
Adjustment

Random effect

Bayesian network with highest posterior probability

Parameter estimation

- compute marginal posterior density
- regression estimate



Using R

buildscorecache()

mostprobable()

fitabn()

CAUSAL THINKING VERSUS ACAUSAL THINKING

- Strong assumptions … but common in statistics, no?
- *"It seems that if conditional independence judgements are byproducts of stored causal relationships, then tapping and representing those relationships directly would be a more natural and more reliable way of expressing what we know or believe about the world. This is indeed the philosophy behind causal Bayesian networks."* (Pearl, 2009)

- The do-calculus
  - Interventions
  - In epidemiology: Randomised Controlled Trial
- So … BN is a nice framework to treat causal and causal thinking

R CODE: SOFTWARE IMPLEMENTATION

Popular R packages (available on CRAN)

bnlearn

- Learning via constraint-based and score-based algorithms (many!)

pcalg

- Robust estimation of CPDAG via the PC-Algorithm

deal

- Learning BNs with mixed (discrete and continuous) variables

catnet

- Discrete BNs using likelihood-based criteria

abn

- Learning BNs with mixed (discrete, continuous, Poisson) variables
- Score based methods: Bayesian and frequentist estimation
- Exact and heuristic search

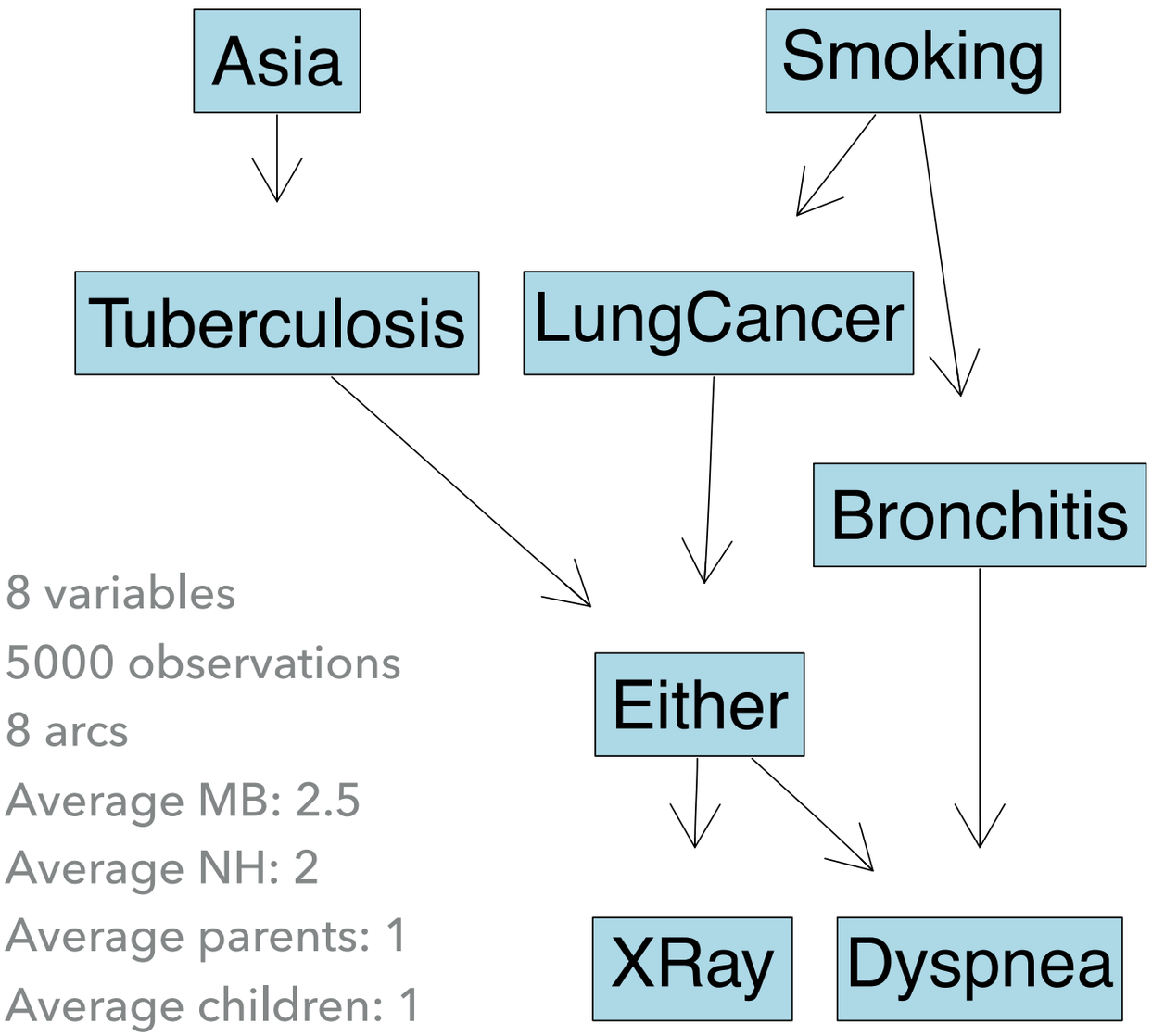
Disclaimer: I am author and maintainer of the abn R package. I will use it for the example part.

R CODE: EXAMPLE ASIA

Proposed by Lauritzen et al.,1988 and provided by Scutari, 2009

"Shortness-of-breath (dyspnoea) may be due to tuberculosis, lung cancer or bronchitis, or none of them, or more than one of them. A recent visit to Asia increases the chances of tuberculosis, while smoking is known to be a risk factor for both lung cancer and bronchitis. The results of a single chest X-ray do not discriminate between lung cancer and tuberculosis, as neither does the presence or absence of dyspnoea."

```
##defining distributions
dist = list(Asia = "binomial",
            Smoking = "binomial",
            Tuberculosis = "binomial",
            LungCancer = "binomial",
            Bronchitis = "binomial",
            Either = "binomial",
            XRay = "binomial",
            Dyspnea = "binomial")

#plot BN
plotabn(dag.m = ~Asia|Tuberculosis +
            Tuberculosis|Either +
            Either|XRay:Dyspnea +
            Smoking|Bronchitis:LungCancer +
            LungCancer|Either +
            Bronchitis|Dyspnea,
          data.dists = dist,
          edgedir = "cp",
          fontsize.node = 30,
          edge.arrowwise = 3)
```

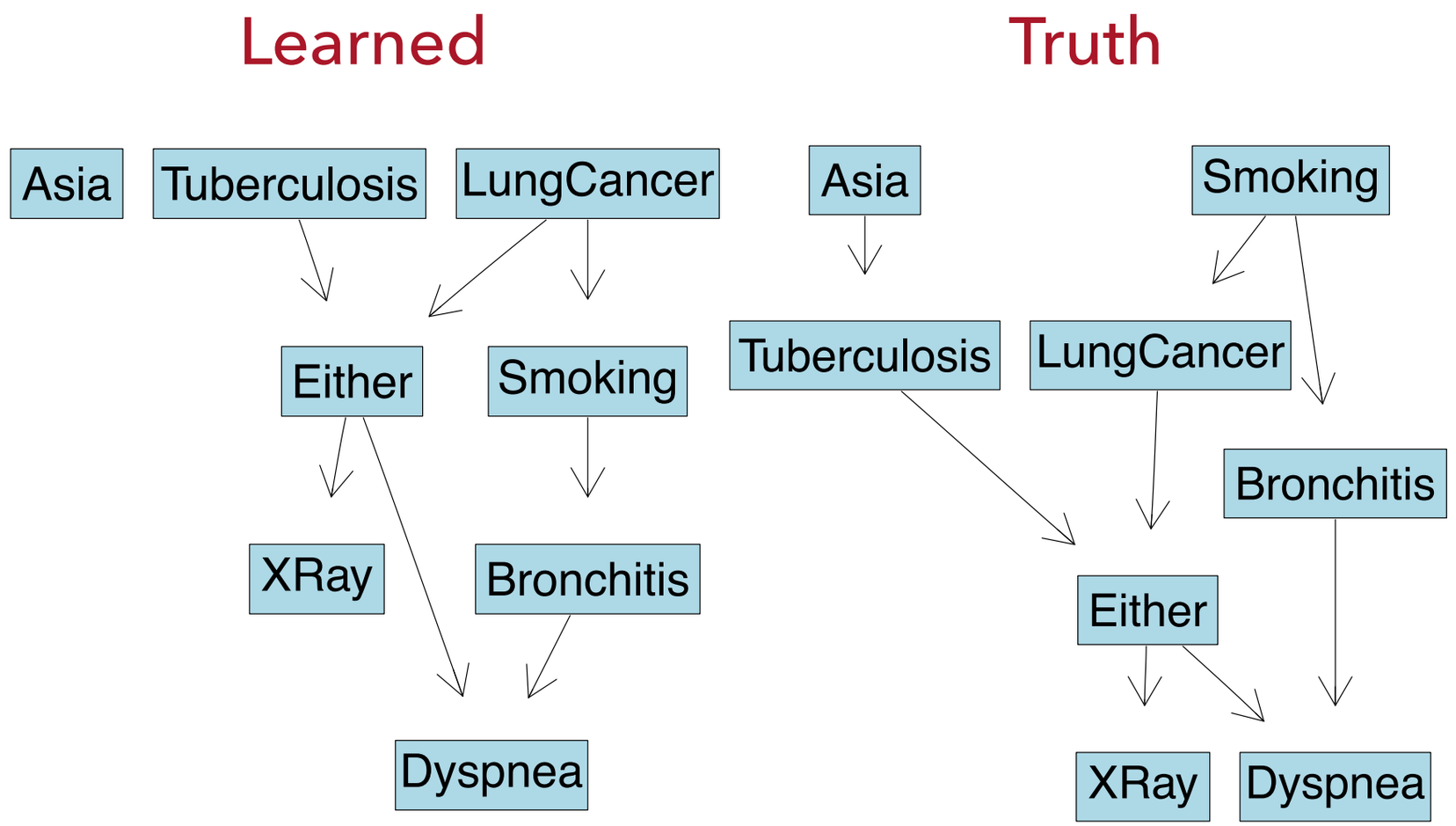


8 variables
5000 observations
8 arcs
Average MB: 2.5
Average NH: 2
Average parents: 1
Average children: 1

ASIA: SCORE BASED ALGORITHM

```
##============================
##score based algorithm
##============================

#loglikelihood score
bsc.compute <- buildscorecache(data.df = asia,
                               data.dists = dist,
                               max.parents = 2)

dag <- mostprobable(score.cache = bsc.compute)
plotabn(dag.m = dag,data.dists = dist, fontsize.node = 30, edge.arrc
```

```
> compareDag(ref = t(dag.adj),
+            test = dag)
$TPR
[1] 0.75

$FPR
[1] 0.01785714

$Accuracy
[1] 0.953125

$FDR
[1] 0.2857143

$`G-measure`
[1] 0.8017837

$`F1-score`
[1] 44.8

$PPV
[1] 0.8571429

$FOR
[1] 0.2857143

$`Hamming-distance`
[1] 3
```



ASIA: KNOWN NETWORK

```
fitabn(dag.m = ~Asia|Tuberculosis+
         Tuberculosis|Either +
         Either|XRay:Dyspnea +
         Smoking|Bronchitis:LungCancer +
         LungCancer|Either +
         Bronchitis|Dyspnea,data.df = asia,data.dists = dist)$modes
```

```
$Asia
 Asia|(Intercept) Asia|Tuberculosis
        -4.811200           1.765763

$Smoking
Smoking|(Intercept)  Smoking|LungCancer  Smoking|Bronchitis
          -1.027065            2.356988            1.807460

$Tuberculosis
Tuberculosis|(Intercept)      Tuberculosis|Either
                -12.22120                 10.21823

$LungCancer
LungCancer|(Intercept)      LungCancer|Either
             -12.07565              14.18547

$Bronchitis
Bronchitis|(Intercept)     Bronchitis|Dyspnea
             -1.388644               3.200393

$Either
Either|(Intercept)        Either|XRay     Either|Dyspnea
         -8.656348           8.259773           1.538789

$XRay
XRay|(Intercept)
       -2.052496

$Dyspnea
Dyspnea|(Intercept)
         -0.1201444
```

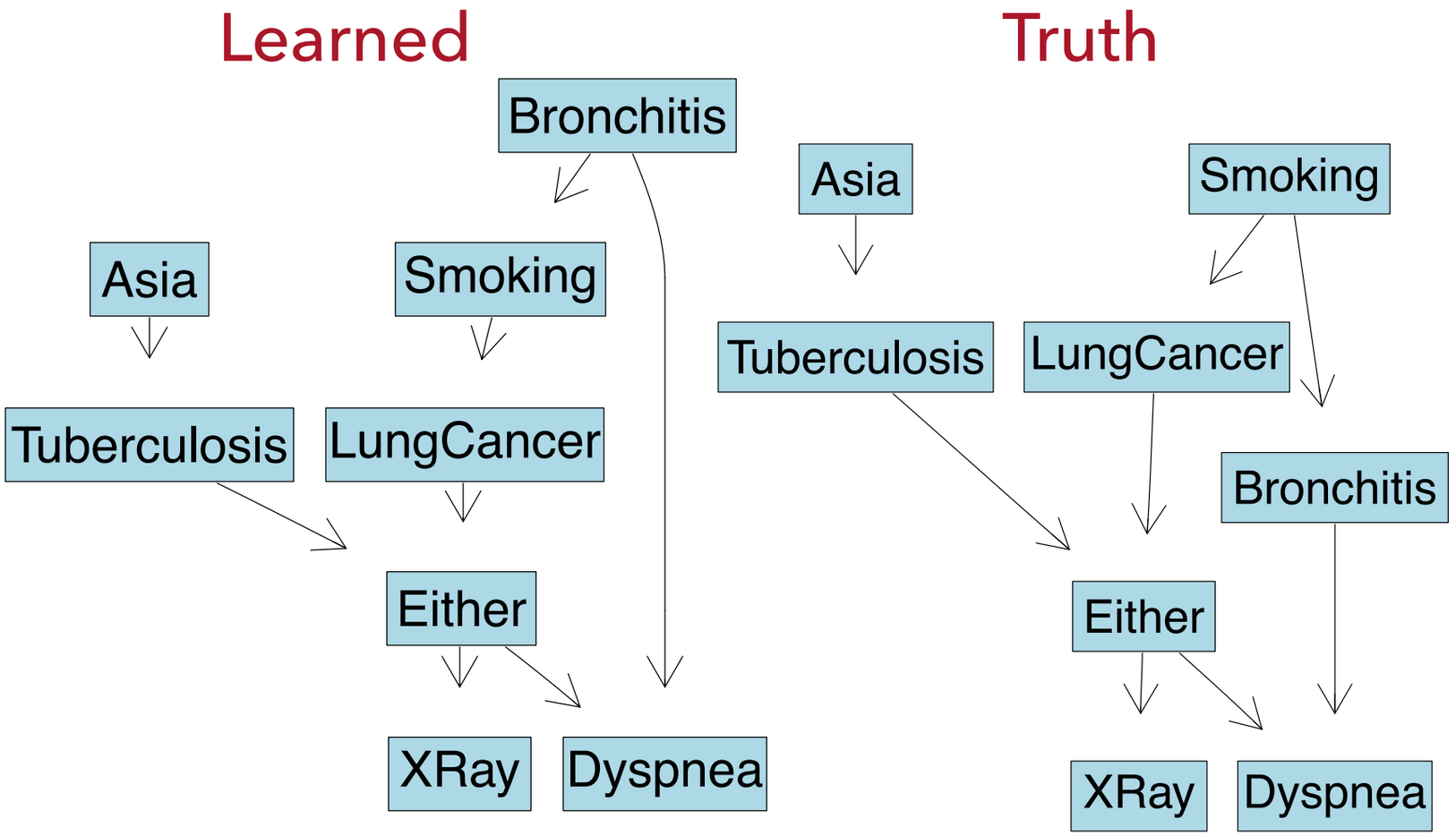
```
fitabn.mle(dag.m = dag.adj,data.df = asia,data.dists = dist)$coef
```

```
$Asia
     Asia|intercept Tuberculosis
[1,]      -4.811371     1.766849

$Smoking
     Smoking|intercept LungCancer Bronchitis
[1,]         -1.027075   2.357079   1.807472

$Tuberculosis
     Tuberculosis|intercept   Either
[1,]              -8.517393 6.516139

$LungCancer
     LungCancer|intercept   Either
[1,]             -8.517393 10.62598

$Bronchitis
     Bronchitis|intercept  Dyspnea
[1,]            -1.388655 3.200415

$Either
     Either|intercept     XRay  Dyspnea
[1,]        -8.665128 8.268402 1.539146

$XRay
     XRay|intercept
[1,]        -2.0525

$Dyspnea
     Dyspnea|intercept
[1,]        -0.1201443
```

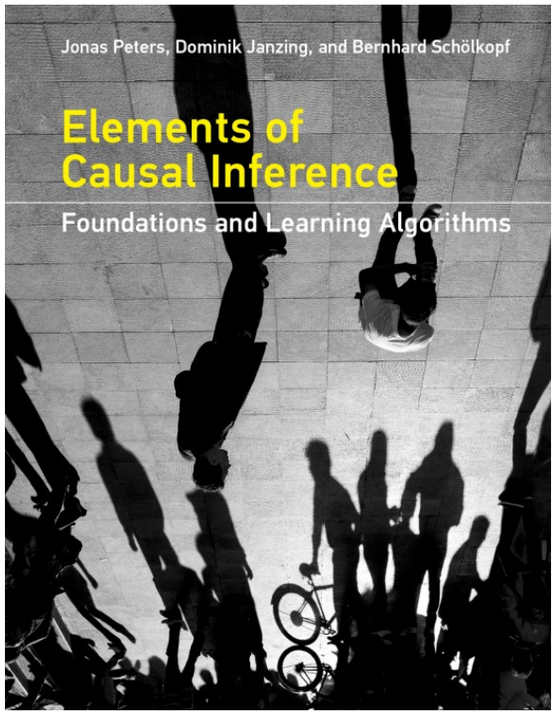
ASIA: EXTERNAL KNOWLEDGE

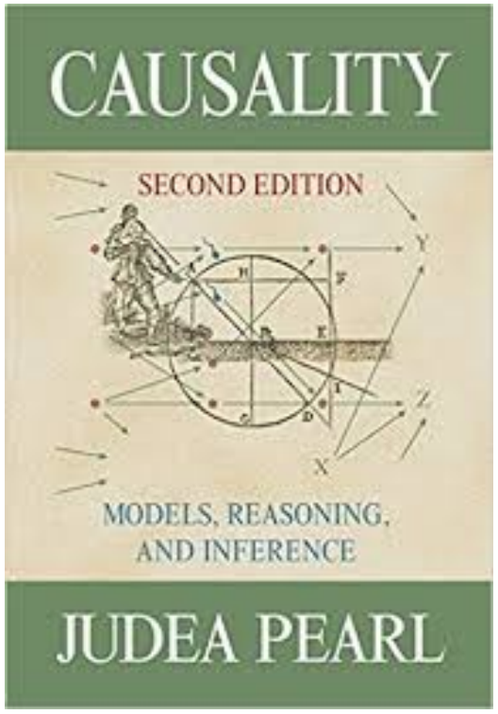
```
##============================
##external knowledge
##============================

##recent visit to Asia increases risk of tuberculosis
bsc.compute <- buildscorecache.mle(data.df = asia,
                                   data.dists = dist,
                                   max.parents = 2,
                                   dag.retained = ~Tuberculosis|Asia)

dag <- mostprobable(score.cache = bsc.compute,score = "bic")
plotabn(dag.m = dag,data.dists = dist, fontsize.node = 30, edge.arro
```

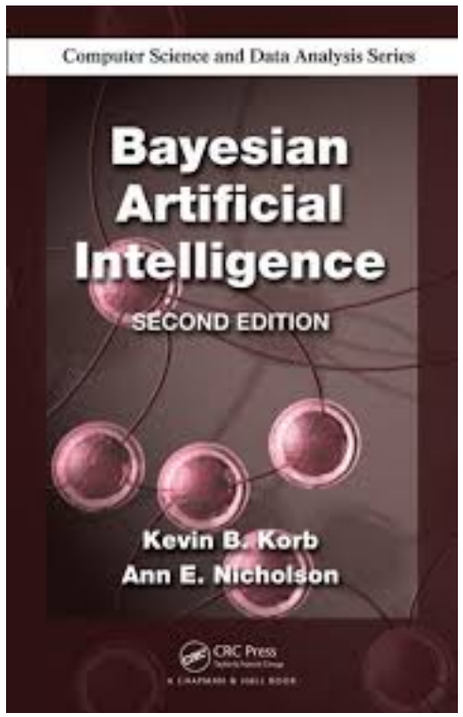
```
> compareDag(ref = t(dag.adj),
+            test = (dag))
$TPR
[1] 0.875

$FPR
[1] 0.01785714

$Accuracy
[1] 0.96875

$FDR
[1] 0.125

$`G-measure`
[1] 0.875

$`F1-score`
[1] 56

$PPV
[1] 0.875

$FOR
[1] 0.125

$`Hamming-distance`
[1] 2
```

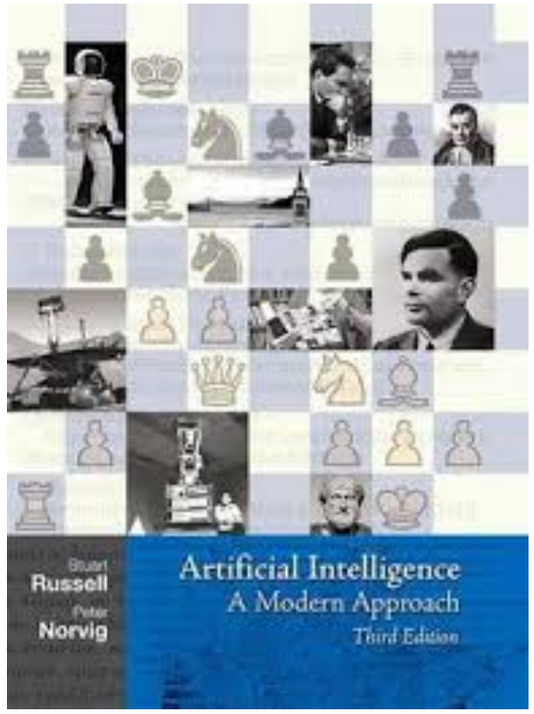


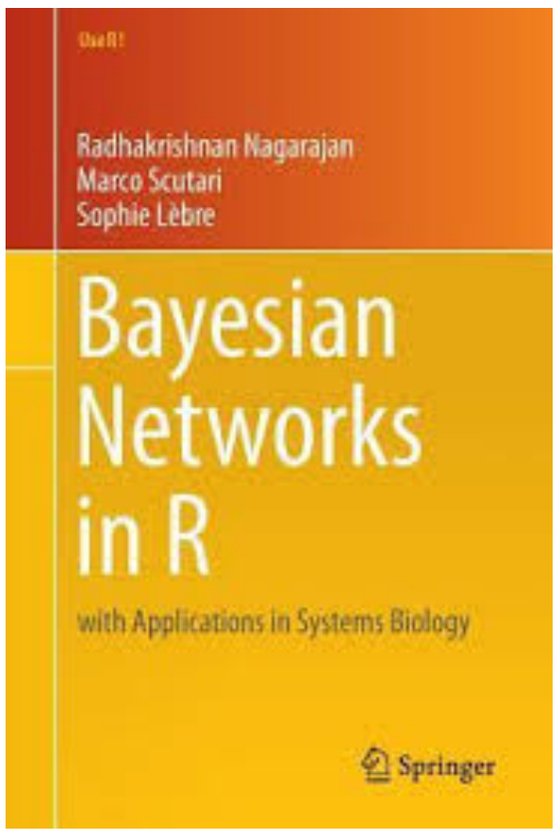
SELECTED BIBLIOGRAPHY

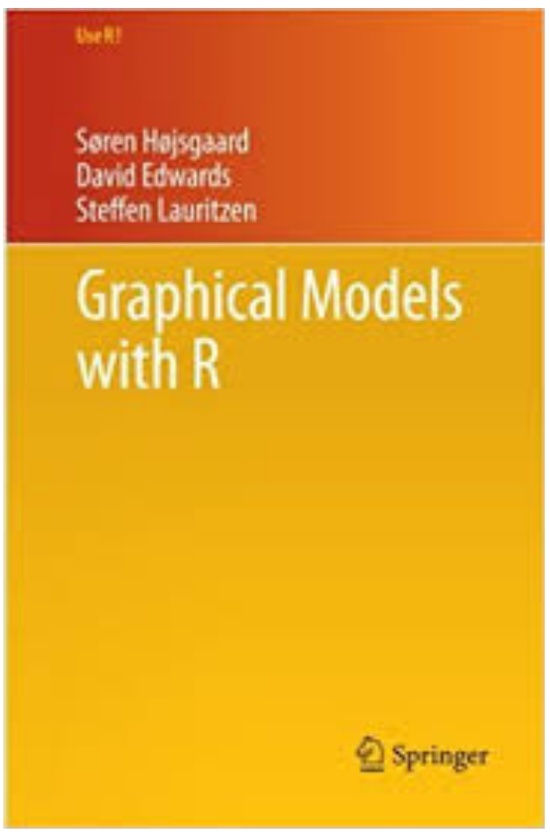


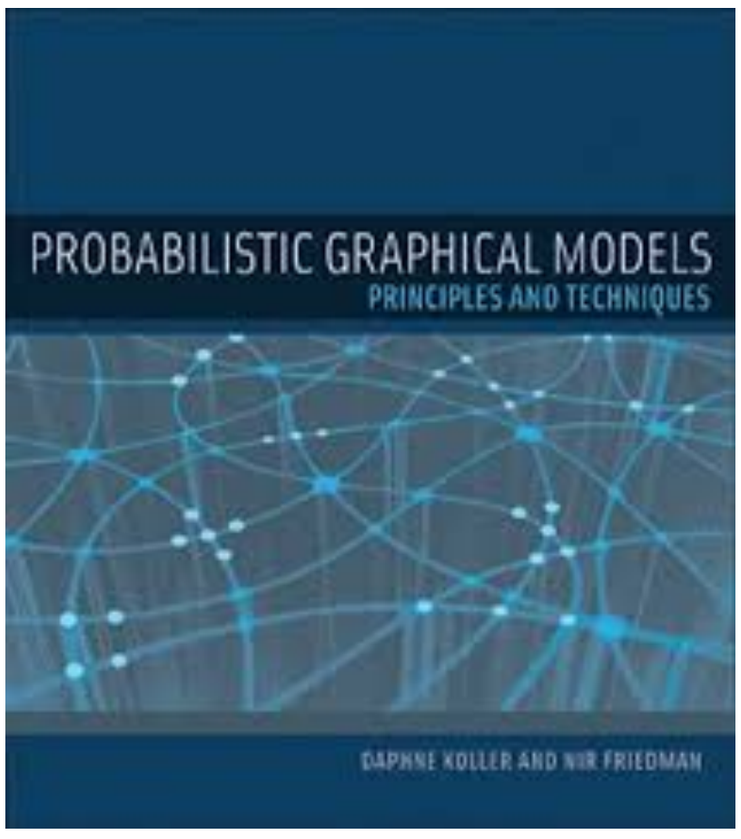












Thank you for your attention

xkcd.com

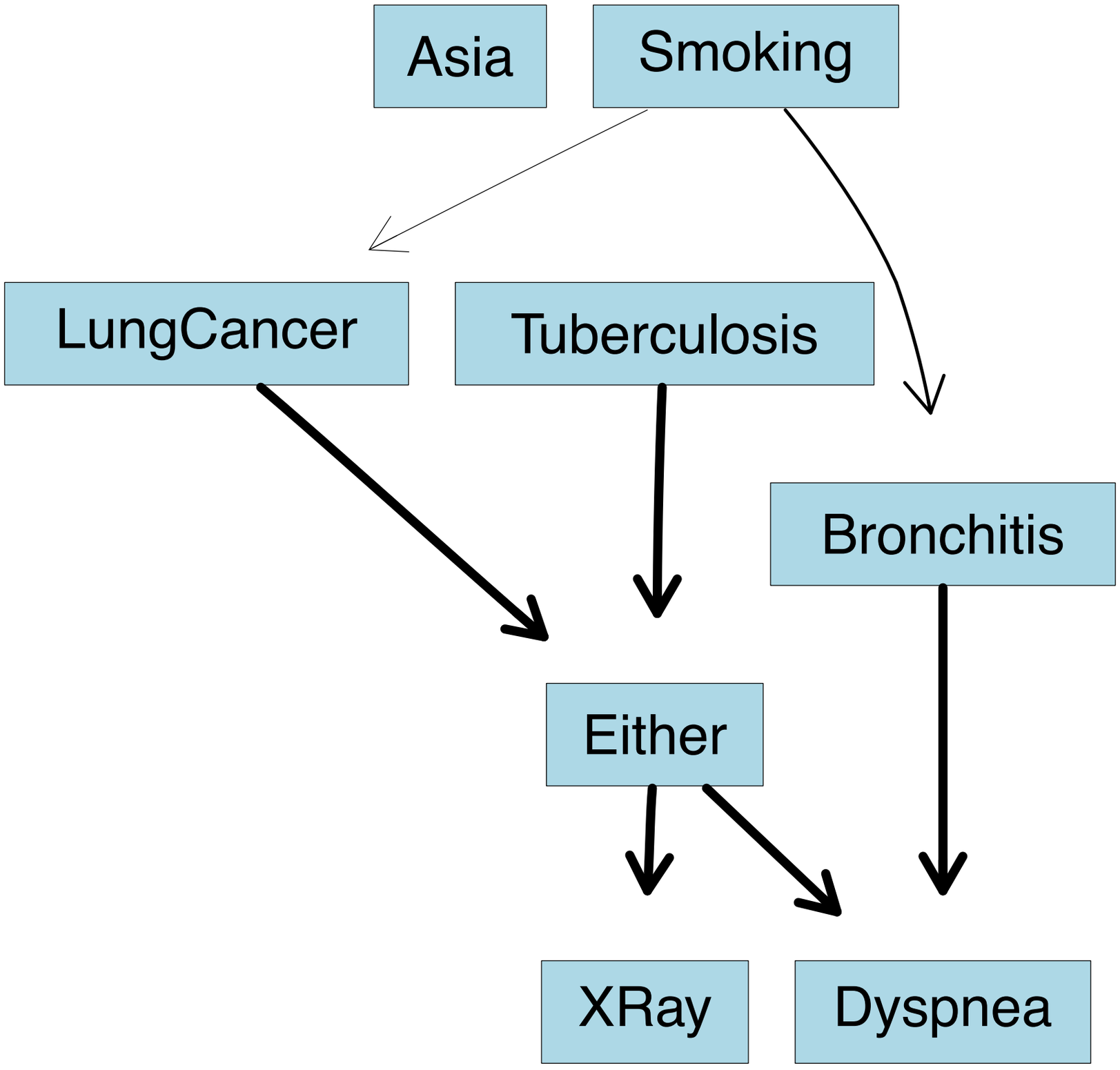
Backup slides

ASIA: BOOTSTRAPPING

University of Zurich[UZH]

```
library(doParallel)
library(foreach)

cl <- makeCluster(2)
registerDoParallel(cl)

set.seed(1120)
nboot <- 200
nvars <- dim(asia)[2]
nobs <- dim(asia)[1]
bootstrap.dag <- array(data = NA,dim = c(nvars, nvars, nboot))

start_time <- Sys.time()
bootstrap.dag <- foreach(i = 1:nboot,.packages = c("mlabn", "abn")) %dopar% {
  mycache.computed.mle <- buildscorecache.mle(data.df = asia[sample(x = 1:nobs,size = 0.8*nobs,replace = FALSE),],
                                              data.dists = dist,
                                              max.parents = 2,
                                              dry.run = FALSE,
                                              maxit = 1000,
                                              tol = 1e-11)

  dag <- mostprobable(score.cache = mycache.computed.mle, score = "bic")}
compute_time <- Sys.time()-start_time

##analysis
df.boot <- array(data = unlist(bootstrap.dag), dim = c(8, 8, 200))

dag<-apply(df.boot, 1:2, mean)

#dag.mdl<-dag.before

colnames(dag) <- rownames(dag) <- names(dist)

dag.boot.50 <- dag
dag.boot.50[dag>0.5] <- 1
dag.boot.50[dag<=0.5] <- 0

dag[dag<=0.5] <- 0

colnames(dag.boot.50) <- rownames(dag.boot.50) <- names(dist)

plotabn(dag.m = t(dag.boot.50),data.dists = dist,fontsize.node = 30,arc.strength = 10*dag,digit.precision = 2,edge.arrowwise = 3)
```

ASIA: BOOTSTRAPPING

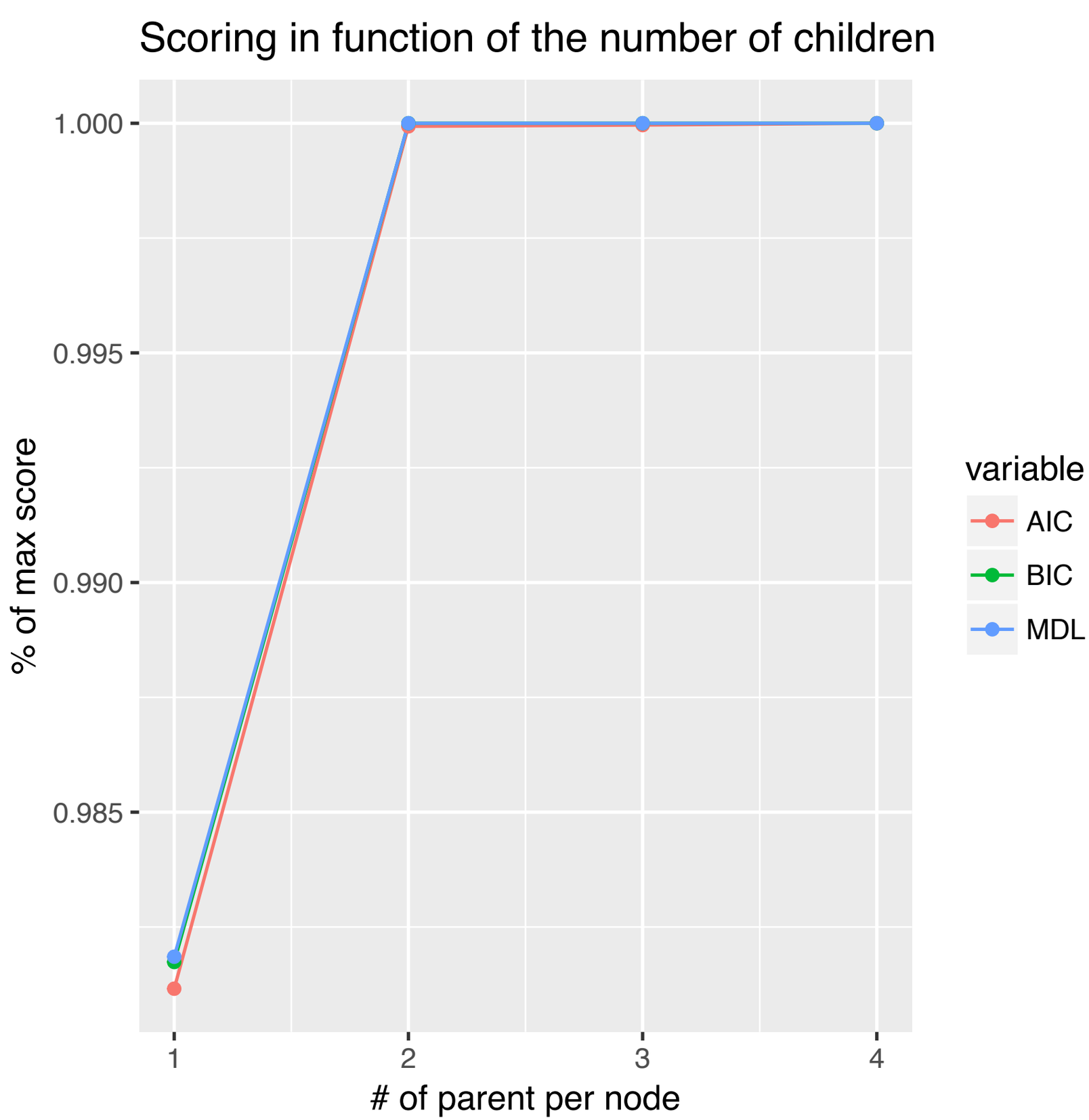


ASIA: HOW MANY PARENT ARE NEEDED?

University of Zurich[UZH]

```
res.mlik <- NULL
res.aic <- NULL
res.bic <- NULL
res.mdl <- NULL

for(i in 1:4){
  mycache.computed.mle <- buildscorecache.mle(data.df = asia,
                                              data.dists = dist,
                                              max.parents = i,
                                              dry.run = FALSE,
                                              maxit = 1000,
                                              tol = 1e-11)

  dag <- mostprobable(score.cache = mycache.computed.mle,score = "aic")
  res.aic <- rbind(res.aic,fitabn.mle(dag.m = dag,data.df = mycache.computed.mle$data.df,data.dists = dist)$aic)
  dag <- mostprobable(score.cache = mycache.computed.mle,score = "bic")
  res.bic <- rbind(res.bic,fitabn.mle(dag.m = dag,data.df = mycache.computed.mle$data.df,data.dists = dist)$bic)
  dag<-mostprobable(score.cache = mycache.computed.mle,score = "mdl")
  res.mdl <- rbind(res.mdl,fitabn.mle(dag.m = dag,data.df = mycache.computed.mle$data.df,data.dists = dist)$mdl)
}

library(ggplot2)
library(reshape)
scoring <- data.frame(AIC = max(-res.aic)/-res.aic, BIC = max(-res.bic)/-res.bic, MDL = max(-res.mdl)/-res.mdl, 1:4)

scoring.long <- melt(scoring, id.vars="X1.4")

ggplot(data = scoring.long, aes(x=X1.4, y=(value), group=variable, color=variable)) +
  geom_line() +
  geom_point() +
  ggtitle("Scoring in function of the number of children", subtitle = NULL) +
  xlab("# of parent per node") +
  ylab("% of max score") +
  scale_x_continuous(breaks=c(1,2,3,4,5,6,7))
```

ASIA: HOW MANY PARENT ARE NEEDED?



ASIA: CONSTRAINT-BASED LEARNING

```
##============================
## constraint-based algorithm
##============================

bn.gs <- gs(asia)
plot(bn.gs)

bn.iamb <- iamb(asia)
plot(bn.iamb)
```