Bayesian Networks - II : Parameter and structure learning

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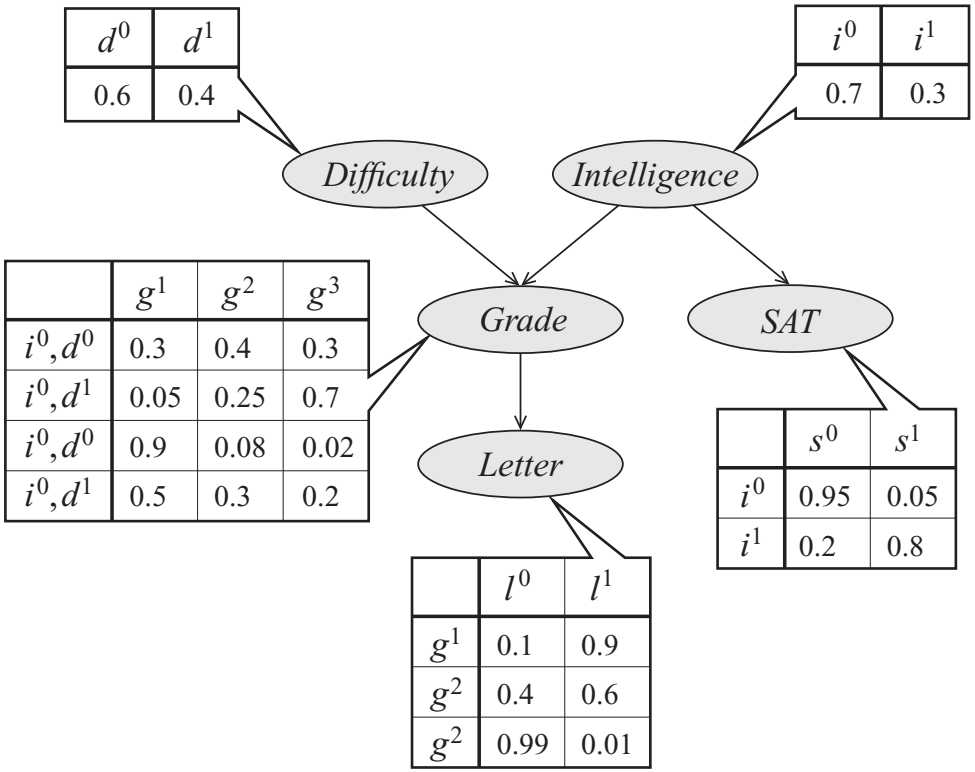
One model... but two learning tasks

BN = graph G and set of CPDs Θ

- parameter learning / G given
- structure learning



d^0	d^1
0.6	0.4

i^0	i^1
0.7	0.3

	g^1	g^2	g^3
i^0, d^0	0.3	0.4	0.3
i^0, d^1	0.05	0.25	0.7
i^0, d^0	0.9	0.08	0.02
i^0, d^1	0.5	0.3	0.2

	s^0	s^1
i^0	0.95	0.05
i^1	0.2	0.8

	l^0	l^1
g^1	0.1	0.9
g^2	0.4	0.6
g^2	0.99	0.01

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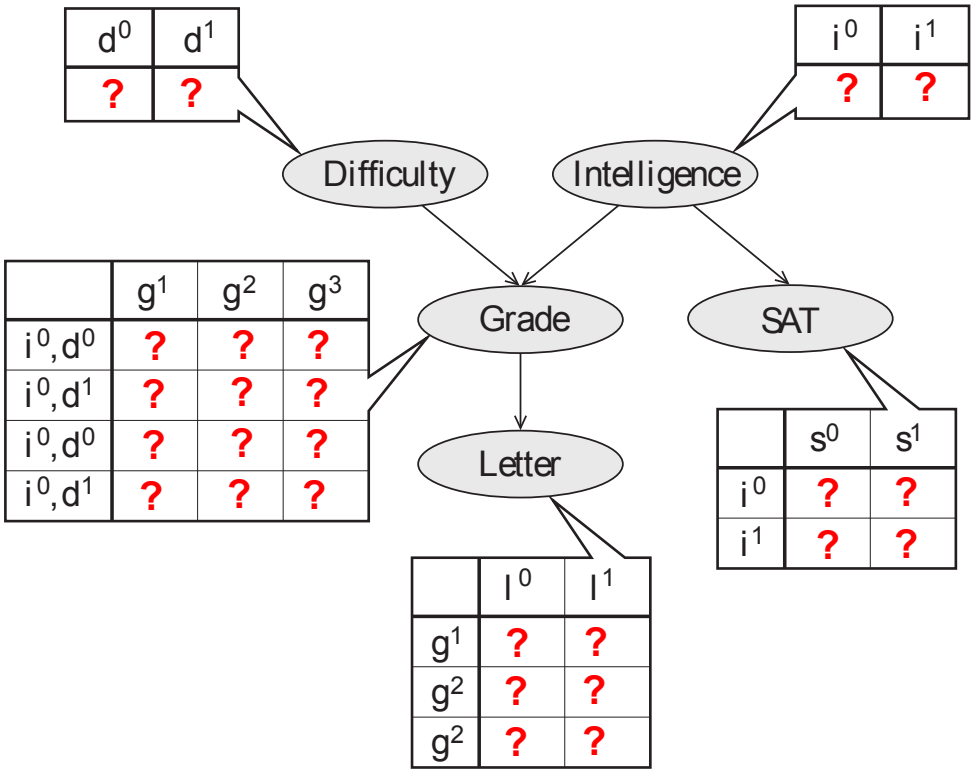

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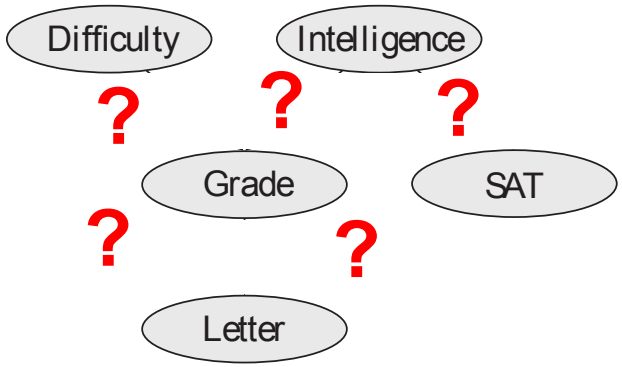


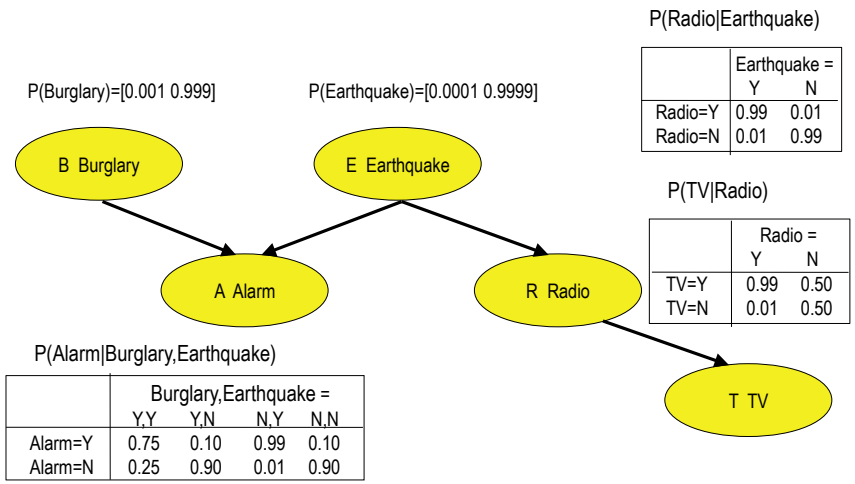
BN dimension

Definition

number of independent parameters needed to describe all the CPDs related to one BN.

Examples

- $Dim(B) = 1+1+4+2+2$
- empty graph : $Dim(B_0) = ?$
- completely connected graph : $Dim(B_c) = ?$



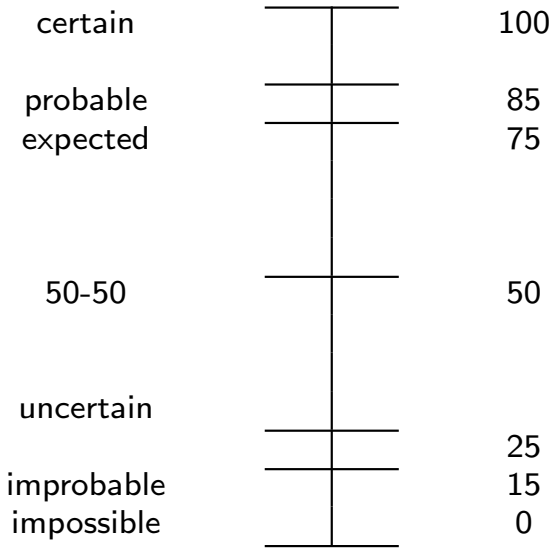
Knowledge acquisition

How to determine the structure by interacting with experts ?

- Identifying variables of interest
- Controlling the model dimension : variable cardinality + intermediate variables

How to determine the conditional distributions without data ?

- First find one cooperative expert
- Use some specific tools for determining numerical values without asking for it [Drusdel, 2001]



Example

Let's assume that success in an exam results in a grade between A and C that may depend on many other variables (difficulty of the subject, level of the student, time spent revising, etc.) and may influence other variables.

- Propose about 5 discrete relevant variables (and the values they can take). *Tip: restrict your variables to no more than 2 or 3 possible values.*
- Propose a BN (structure and parameters) modelling this problem, using these variables, justifying the choice of the structure and the values of the conditional probabilities. *Tip: to avoid having a variable with too many parents, do not hesitate to add intermediate variables.*
- implement your model in pyAgrum, and show by careful choice of examples that exam success increases as observable variables become more and more favourable.

Simplify some CPDs

Noisy OR model [Pearl, 1986]

- $P(Y|X_1 \dots X_n)$ (boolean variables) $= 2^n$ values !
- Let suppose that
  - we can estimate each $p_i = P(y|\bar{x}_1, \bar{x}_2, ..., x_i, ..., \bar{x}_n)$
  - there is no mutual effect between X_i variables and Y.
- so
  - if one X_i is true, then Y is almost true (with probability p_i)
  - is several X_i are true, then

$$P(y|\mathcal{X}) = 1 - \prod_{i/X_i \in \mathcal{X}_p} (1 - p_i)$$

where $\mathcal{X}_p$ is the set of X_i equal to true.

Simplify some CPDs

Noisy OR model [Pearl, 1986]

- extension when Y is true when no cause is present (*leaky noisy-OR gate*) [Henrion, 1989]
- extension to multi-valued variables (*generalized noisy-OR gate*)

- this simplification can also be used for learning less parameters from data....

Example

Parameter learning with complete data

Parameter learning — complete data $\mathcal{D}$

- estimation of CPD parameters from $\mathcal{D}$
- usual statistical approach = *max. of likelihood (ML)*

$$\hat{\theta}^{ML} = \text{argmax } P(\mathcal{D}|\theta)$$

- probability of an event = frequency of this event in data

Maximum of likelihood (ML)

$$\hat{P}(X_i = x_k | Pa(X_i) = x_j) = \hat{\theta}^{ML}_{i,j,k} = \frac{N_{i,j,k}}{\sum_k N_{i,j,k}}$$

$N_{i,j,k}$ = nb of occurences of $\{X_i = x_k \text{ and } Pa(X_i) = x_j\}$

Parameter learning with complete data

Demonstration

Parameter learning with complete data

Other approach

- one Bayesian approach = *max. a posteriori (MAP)*

$$\hat{\theta}^{MAP} = \text{argmax } P(\theta|\mathcal{D}) = \text{argmax } P(\mathcal{D}|\theta)P(\theta)$$

- need to define an a priori distribution $P(\theta)$
- *conjugated* distribution associated to X distribution
- if $P(X)$ multinomial, associated $P(\theta)$ = Dirichlet :

$$P(\theta) \propto \prod_{i=1}^{n} \prod_{j=1}^{q_i} \prod_{k=1}^{r_i} (\theta_{i,j,k})^{\alpha_{i,j,k}-1}$$

where $\alpha_{i,j,k}$ are the cœfficients of Dirichlet distribution associated to parameter $\theta_{i,j,k}$

Parameter learning with complete data

Maximum a Posteriori (MAP)

$$\hat{P}(X_i = x_k | Pa(X_i) = x_j) = \hat{\theta}^{MAP}_{i,j,k} = \frac{N_{i,j,k} + \alpha_{i,j,k} - 1}{\sum_k (N_{i,j,k} + \alpha_{i,j,k} - 1)}$$

Another bayesian approach

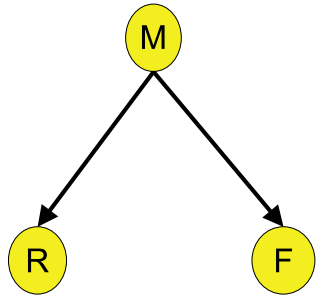
- *expectation a posteriori (EAP)* : Computation of the expectation of $\theta_{i,j,k}$ instead of the max. value

$$\hat{P}(X_i = x_k | Pa(X_i) = x_j) = \hat{\theta}^{EAP}_{i,j,k} = \frac{N_{i,j,k} + \alpha_{i,j,k}}{\sum_k (N_{i,j,k} + \alpha_{i,j,k})}$$

ML Example

$$\hat{P}(M = m_0) = 6/15 = 0.4$$
$$\hat{P}(M = m_1) = 8/15 = 0.53$$
$$\hat{P}(M = m_2) = 1/15 = 0.07$$

$$\hat{P}(F = OK|M = m_0) = 1/6 = 0.17$$
$$\hat{P}(F = BAD|M = m_0) = 5/6 = 0.83$$
etc ...



M	F	R
m_0	BAD	O
m_0	BAD	O
m_0	BAD	O
m_0	BAD	O
m_0	BAD	N
m_0	OK	O
m_1	BAD	O
m_1	BAD	N
m_1	OK	O
m_1	OK	N
m_1	OK	O
m_1	OK	N
m_1	OK	O
m_1	OK	N
m_2	OK	N

Problem

$\hat{P}(F = BAD|M = m_2) = 0/1$
because this configuration is not present in the (small) dataset

EAP Example

- we have to give some a priori coefficients for each $\theta_{i,j,k}$
- $\approx$ pseudo counts corresponding to N^* virtual measurements
- examples
  - Dirichlet coefficients associated to M $= [50 \quad 50 \quad 0]$

$$\begin{aligned}\hat{P}(M = m_0) &= (6 + 50)/(15 + 100) = 0.487\\ \hat{P}(M = m_1) &= (8 + 50)/(15 + 100) = 0.5043\\ \hat{P}(M = m_2) &= (1 + 0)/(15 + 100) = 0.0087\end{aligned}$$

M	F	R
m_0	BAD	O
m_0	BAD	O
m_0	BAD	O
m_0	BAD	O
m_0	BAD	N
m_0	OK	O
m_1	BAD	O
m_1	BAD	N
m_1	OK	O
m_1	OK	N
m_1	OK	O
m_1	OK	N
m_1	OK	O
m_1	OK	N
m_2	OK	N

  - Dirichlet coefficients associated to $(F|M = m_i) = [9 \quad 1]$

$$\hat{P}(F = BAD|M = m_2) = (0 + 1)/(1 + 10) = 0.09$$

Parameter learning with incomplete data

several types of incomplete data [Rubin, 1976]

- MCAR : *Missing Completely At Random*
  - data loss = completely random phenomenon
  - how to estimate ML or MAP ?
    - Complete / Available Case Analysis ...
- MAR : *Missing At Random*
  - probability one data is lost depends on some known variables
  - how to estimate ML or MAP ?
    - *Expectation Maximisation* ...
- NMAR : *Not Missing At Random*
  - probability one data is lost depends on some external unknown variables
  - need to improve the model by identifying and adding these variables

Complete / Available Case Analysis

Complete Case Analysis

- extract samples completely observed from the incomplete dataset
- advantage : we come back to complete dataset situation
- inconvenient : important missing rate $\Rightarrow$ few complete samples

Available Case Analysis

- principle : we don't need to observe C to estimate the CPD $P(A|B)$ parameters
- for $P(A|B)$ estimation, extract samples for which A and B are observed
- advantage : we come back to complete dataset situation

Complete / Available Case Analysis

Complete Case Analysis

Available Case Analysis

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Expectation Maximisation Algorithm

Very general algorithm [Dempster, 1977]

- parameter estimation with incomplete data

Principle

- iterative algorithm
  - parameter initialization $\theta^{(0)}$
  - E estimate missing data distribution from current model $\theta^{(t)}$
    - = compute $P(X_{\text{missing}}|X_{\text{observed}})$ in current BN
    - = use probabilistic inference
  - M estimate again $\theta^{(t+1)}$ from this new "completed" dataset
    - by using ML, MAP, or EAP approach

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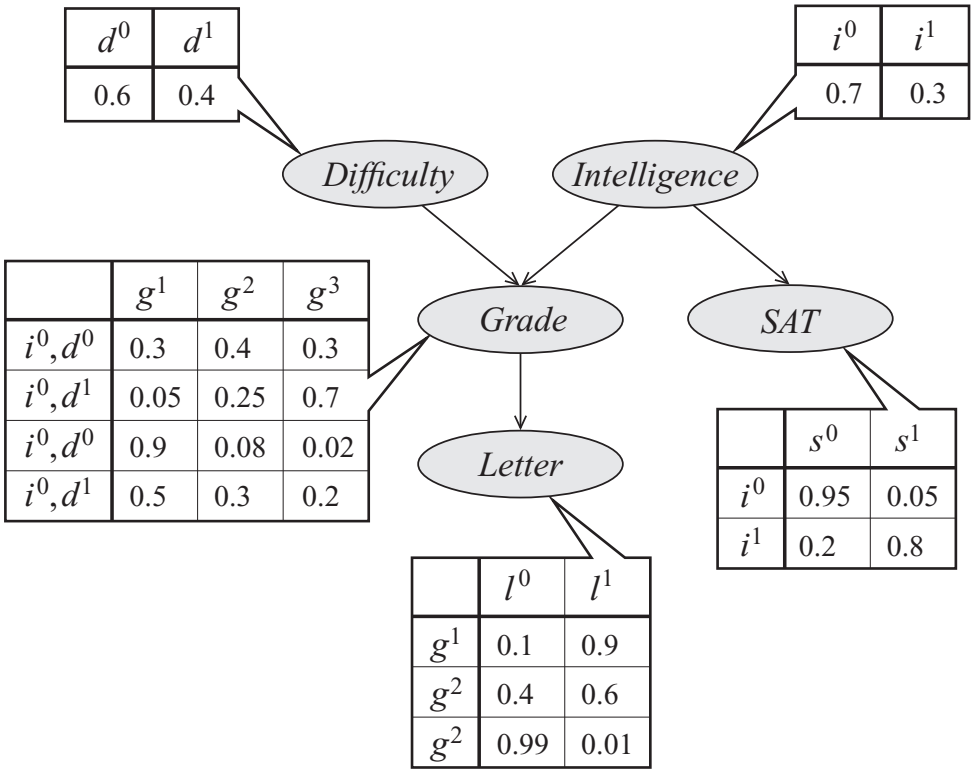

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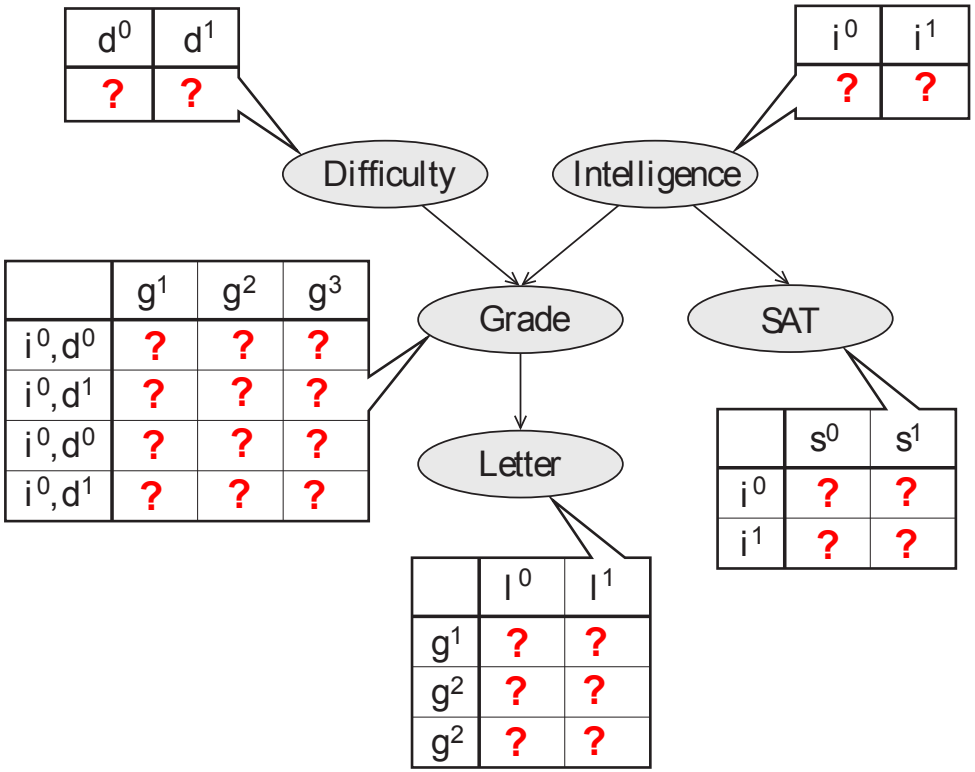

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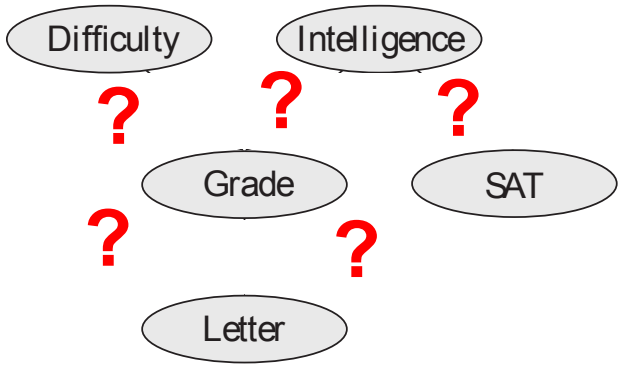

Structure learning is a complex task

What is the number of DAGs with 3 nodes ?

Structure learning is a complex task

Size of the "solution" space

- the number of possible DAGs with n variables is super-exponential w.r.t n [Robinson, 1977]

$$NS(n) = \begin{cases} 1 & , \quad n = 0 \text{ or } 1 \\ \sum_{i=1}^{n} (-1)^{i+1} \binom{n}{i} 2^{i(n-1)} NS(n-i), & n > 1 \end{cases}$$

$$NS(4) = 543$$
$$NS(5) = 29281$$
$$NS(10) = 4.2 \times 10^{18}$$

- an exhaustive search is impossible !

One thousand millenniums $= 3.2 \times 10^{13}$ seconds

Structure learning algorithms

How to search a good BN ?

- constraint-based methods
  BN = independence model
  $\Rightarrow$ find CI in data in order to build the DAG
- score-based methods
  BN = probabilistic model that must fit data as well as possible
  $\Rightarrow$ search the DAG space in order to maximize a scoring/fitness function
- hybrid methods

Score-based methods

How to search a good BN ?

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Notion of score

General principle : Occam razor

- *Pluralitas non est ponenda sine neccesitate*
  plurality should not be posited without necessity
- *Frustra fit per plura quod potest fieri per pauciora*
  It is pointless to do with more what can be done with fewer

= Parcimony principle : find a model

- fitting the data $\mathcal{D}$: likelihood : $\boxed{L(\mathcal{D}|\theta, B)}$
- the simplest possible : dimension of B : $\boxed{Dim(B)}$

Score examples

AIC and BIC

- compromise between likelihood and complexity
- application of AIC [Akaïke, 1970] and BIC [Schwartz, 1978]

$$S_{AIC}(B, \mathcal{D}) = \log L(\mathcal{D}|\theta^{MV}, B) - Dim(B)$$

$$S_{BIC}(B, \mathcal{D}) = \log L(\mathcal{D}|\theta^{MV}, B) - \frac{1}{2} Dim(B) \log N$$

Bayesian scores : BD, BDe, BDeu

- $S_{BD}(B, \mathcal{D}) = P(B, \mathcal{D})$ [Cooper et Herskovits, 1992]
- $BDe = BD + \textit{score equivalence}$ [Heckerman, 1994]

$$S_{BD}(B, \mathcal{D}) = P(B) \prod_{i=1}^{n} \prod_{j=1}^{q_i} \frac{\Gamma(\alpha_{ij})}{\Gamma(N_{ij} + \alpha_{ij})} \prod_{k=1}^{r_i} \frac{\Gamma(N_{ijk} + \alpha_{ijk})}{\Gamma(\alpha_{ijk})}$$

Score properties

Two important properties

Decomposability

$$(Global)Score(B, \mathcal{D}) = \sum_{i=1}^{n} (local)score(X_i, pa_i)$$

Score equivalence

If two BN B_1 and B_2 are Markov equivalent then
$S(B_1, \mathcal{D}) = S(B_2, \mathcal{D})$

Example

Empty graph G_0

- estimate CPDs $P(X_1)$ and $P(X_2)$ (with ML approach)
- log-likelihood of G_0 ? AIC score ?

Complete graph G_c

- estimate CPDs $P(X_1)$ and $P(X_2|X_1)$ (with ML approach)
- log-likelihood of G_c ? AIC score ?

What is the best graph according to likelihood ? according to AIC ?

X_1	X_2
Y	N
Y	Y
Y	Y
Y	Y
N	N
N	Y
N	Y
N	Y

Heuristic exploration of search space

Search space and heuristics

- space $\mathcal{B}$
  - restriction to tree space : Chow&Liu, MWST
  - DAG with node ordering : K2 algorithm
  - greedy search
  - genetic algorithms, ...
- space $\mathcal{E}$
  - greedy equivalence search

Restriction to tree space

Principle

- what is the best tree connecting all the nodes,
  i.e. maximizing a weight defined for each possible edge ?

Answer : maximal weighted spanning tree (MWST)

- [Chow and Liu, 1968] : weight = mutual information :

$$W(X_A, X_B) = \sum_{a,b} \frac{N_{ab}}{N} \log \frac{N_{ab} N}{N_{a.} N_{.b}}$$

- [Heckerman, 1994] : any local score local :

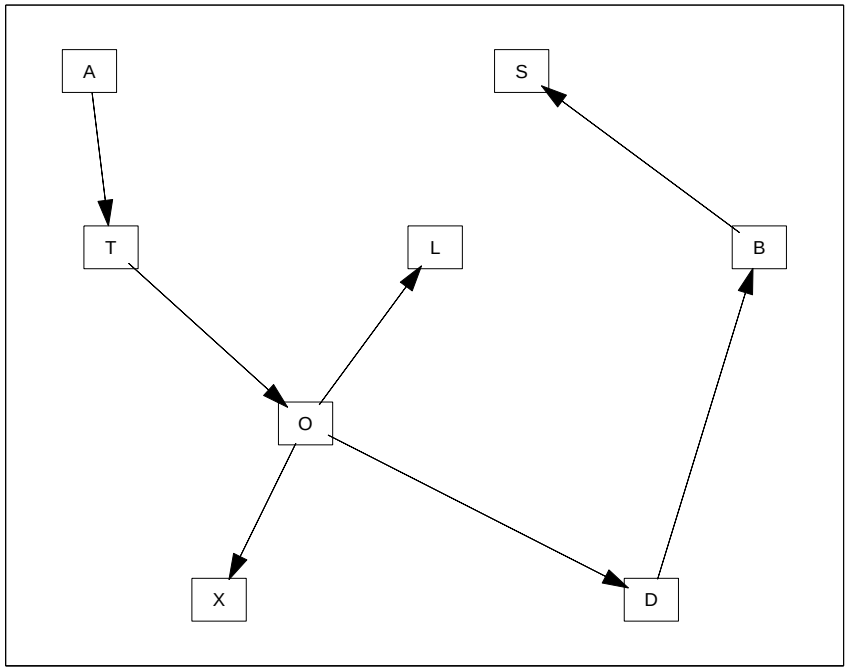
$$W(X_A, X_B) = score(X_A, Pa(X_A) = X_B) - score(X_A, \emptyset)$$

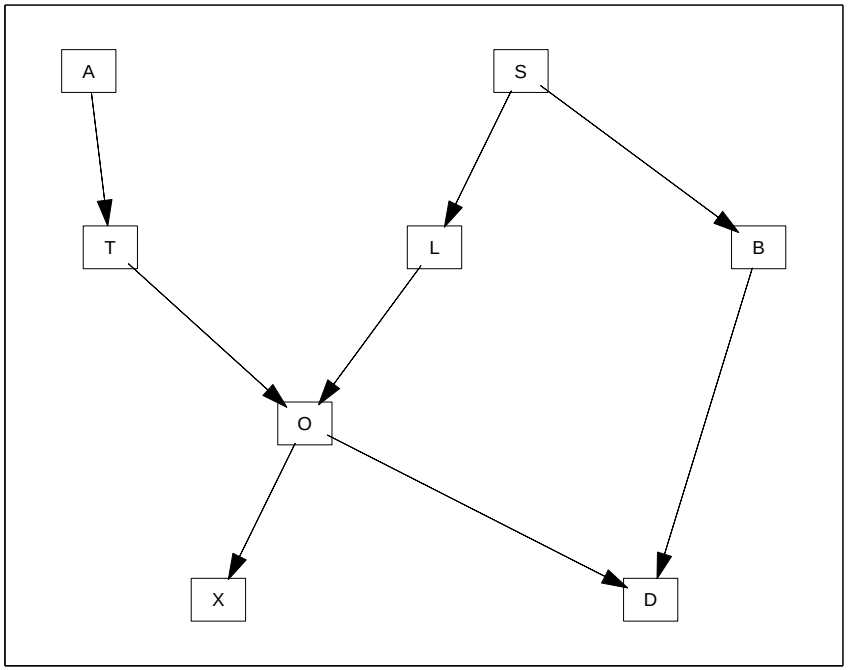
Restriction to tree space

Remarks

- MWST returns an undirected tree
- this undirected tree = CPDAG of all the directed tree with this skeleton
- obtain a directed tree by (randomly) choosing one root and orienting the edges with a depth first search over this tree

Example : obtained DAG vs. target one





MWST can not discover cycles neither V-structures (tree space !)

Example

local score $s(X_i; Pa_i = X_j)$

$X_i \setminus Pa_i$	X_1	X_2	X_3	X_4	X_5
X_1	5	15	13	7	10
X_2	16	6	13	7	10
X_3	11	10	3	6	9
X_4	6	5	7	4	4.5
X_5	15	14	16	10.5	10

diagonal contains $s(X_i; Pa_i = \emptyset)$.

What is the corresponding MWST and its score ?

Heuristic exploration of search space

Search space and heuristics

- space $\mathcal{B}$
  - restriction to tree space : Chow&Liu, MWST
  - DAG with node ordering : K2 algorithm
  - greedy search
  - genetic algorithms, ...
- space $\mathcal{E}$
  - greedy equivalence search

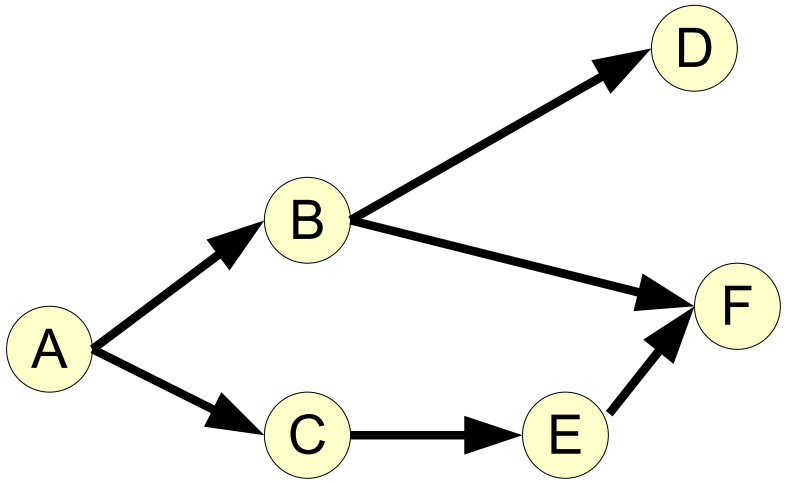
Greedy search

Principle

- exploration of the search space with traversal operators
  - add edge
  - invert edge
  - delete edge
- and respect the DAG definition (no cycle)

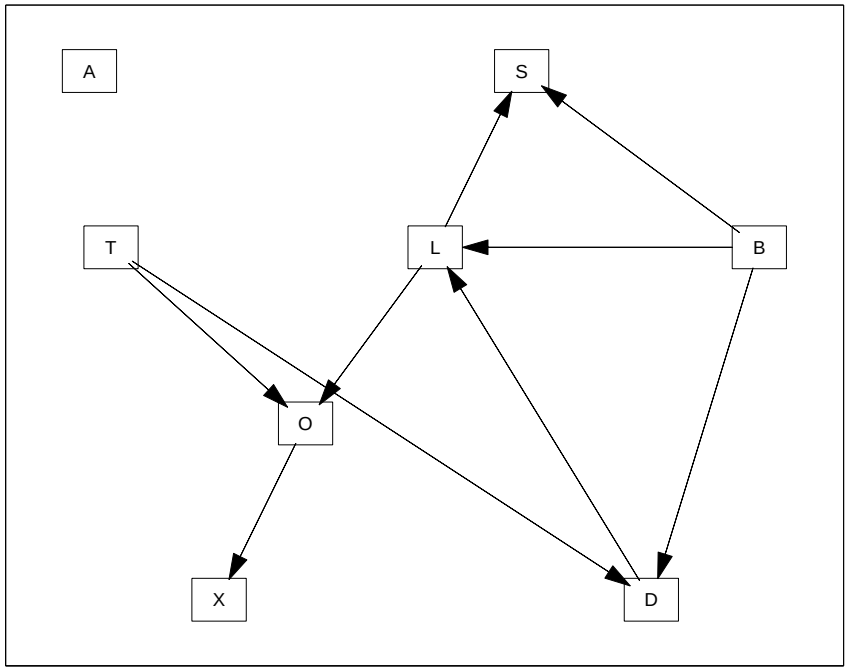
- exploration can begin from any given DAG

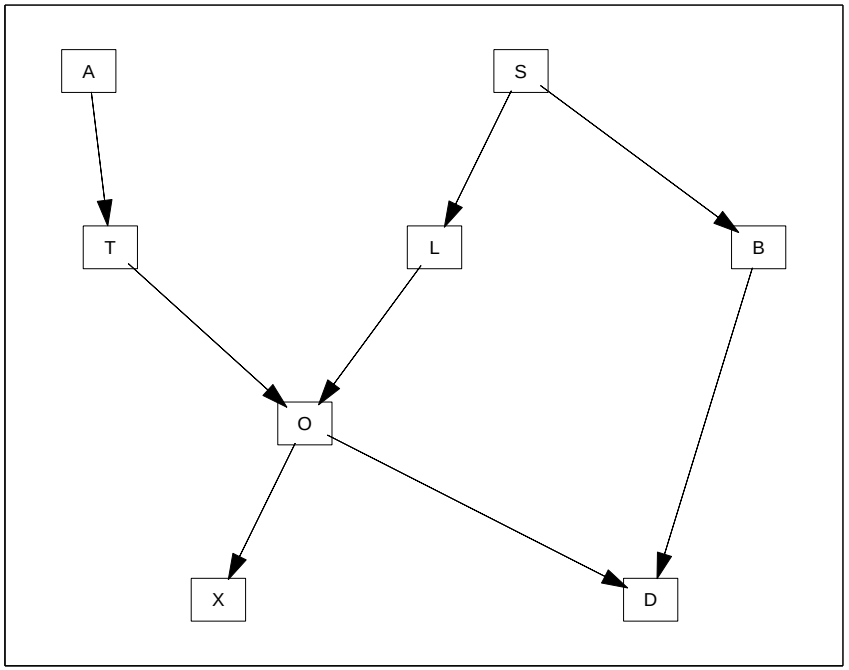
Example



- global score decomposition of this graph ?
- neighborhood ?
- local score computed to evaluate each neighbor ?

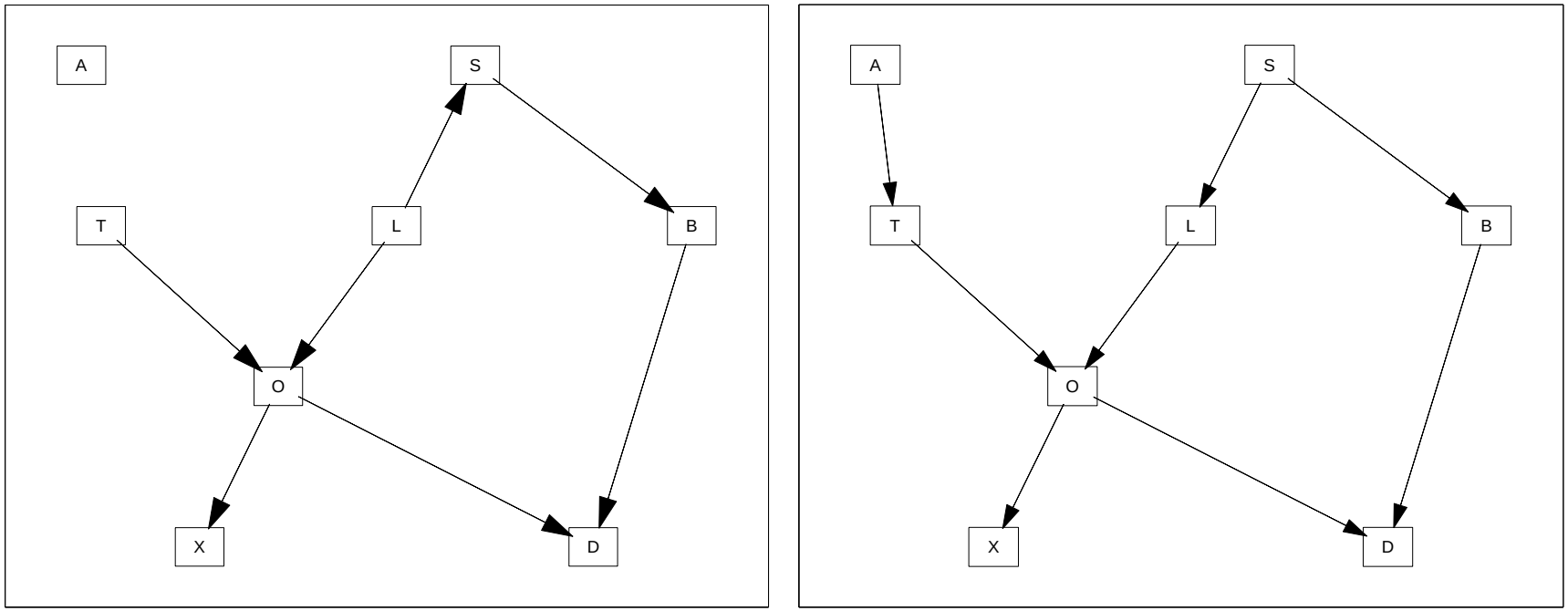
Example : obtained DAG vs. target one





start = empty graph. GS result = local optimum :-(

Example : obtained DAG vs. target one



start = MWST result. GS result is better