

Using imsets for learning Bayesian networks

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Conditional Independence

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- Seeing the **length of hair** of a person will tell us more about his/her **gender** and conversely. It means, the value of G is dependent on the value of H .
- Knowing more about the **gender** will focus our belief on his/her **stature** - S is dependent on G and (through G) also on H .
- Nevertheless, if we know the **gender** of a person then **length of hair** of that person gives us no extra clue on his/her **stature** - H is independent of S given G .

Conditional Independence Statements

Definition (CI statement)

Let A, B, C be pairwise disjoint subsets of a set of variables N . Then the statement “ A is conditionally independent of B given C ” is a **CI statement** (over N), written as $I(A, B, C)$.

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Example (CI statement)

In Example 1 we have indicated only one CI statement, $I(H, S, G)$. On the other hand, we have indicated two dependence statements, namely $\neg I(G, H) = \neg I(G, H, \emptyset)$ and $\neg I(S, G)$.

Conditional Independence (CI) model

Definition (CI in PDs)

Let P be a discrete probability distribution over N . Given any $A \subseteq N$, let

- \mathbf{x}_A denote a configuration of values of variables $\mathbf{X}_A = \{X_i\}_{i \in A}$ and
- for $B \subseteq N \setminus A$ let $P(\mathbf{x}_A \mid \mathbf{x}_B)$ denote the conditional probability of $\mathbf{X}_A = \mathbf{x}_A$ given $\mathbf{X}_B = \mathbf{x}_B$.

The CI statement $I(A, B, C)$ is induced by probability distribution P over N if for all $\mathbf{x}_A, \mathbf{x}_B, \mathbf{x}_C$ such that $P(\mathbf{x}_C) > 0$

$$P(\mathbf{x}_A, \mathbf{x}_B \mid \mathbf{x}_C) = P(\mathbf{x}_A \mid \mathbf{x}_C) \cdot P(\mathbf{x}_B \mid \mathbf{x}_C) .$$

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$$P(h, s \mid g) = P(h \mid g) \cdot P(s \mid g) \text{ or, equivalently } P(h \mid g, s) = P(h \mid g)$$

What CI-statements are represented by a DAG?

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Two nodes a and b in a DAG G are **d-separated** by a set C if for all paths between a and b there is a node c ($c \neq a$ and $c \neq b$) such that either:

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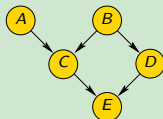
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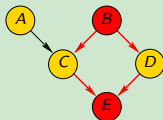
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$$I(A, D, B)$$

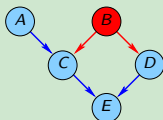
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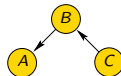
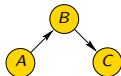
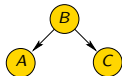
Example



$$\neg I(A, D, \{B, E\})$$

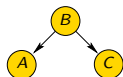
Equivalence classes of Bayesian networks

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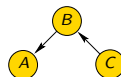
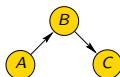


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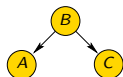


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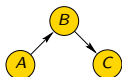


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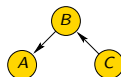
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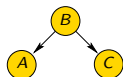


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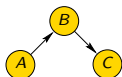


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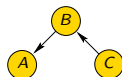
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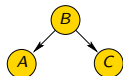
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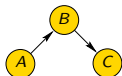
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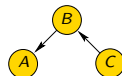
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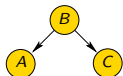


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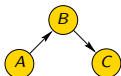
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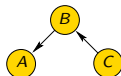
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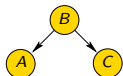
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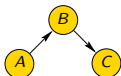
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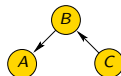
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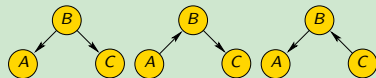
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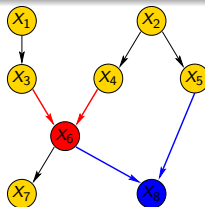
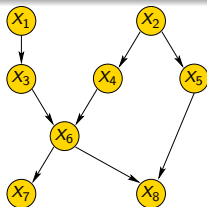
Definition (Immortality)

An **immortality** in a DAG G is an induced subgraph of G for a set $\{A, B, C\}$, where A, B, C are distinct nodes of G such that there are edges $A \rightarrow C$ and $B \rightarrow C$ and there is no edge between A and B in G .

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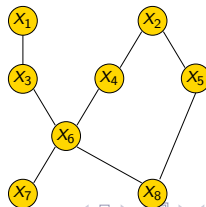
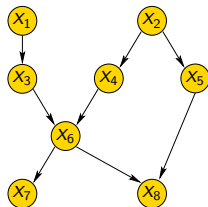
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Theorem

Bayesian networks belong to the same equivalence class iff they have the same underlying graph and the same set of immoralities.

Essential graphs

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The **essential graph** G^* of an equivalence class \mathcal{G} of DAGs over N is a hybrid graph over N defined as follows:

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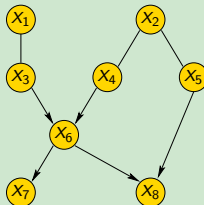
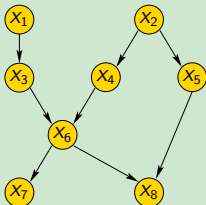
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Function $m : \mathcal{P}(N) \mapsto \mathbb{N}$ is sometimes called multiset. Thus, **imset** is an abbreviation from **I**nteger valued **M**ulti**S**ET. Studený (2001)

What is an imset? (an example)

Let $N = \{a, b, c\}$. An imset u over N is

\emptyset	$\{a\}$	$\{b\}$	$\{c\}$	$\{a, b\}$	$\{b, c\}$	$\{a, c\}$	$\{a, b, c\}$
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Using the convention we will write

$$u = \delta_{\{b\}} - \delta_{\{a,b\}} - \delta_{\{b,c\}} + \delta_{\{a,b,c\}}$$

Elementary imset

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Let $K \subseteq N$, $a, b \in N \setminus K$, and $a \neq b$.

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The **standard imset** for a DAG G is given by the formula

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Standard imset is another uniquely determined representative of an equivalence class of Bayesian networks.

\mathcal{M}_G will denote the set of CI-statements generated by a DAG G .

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Definition

Given two DAGs K, L over N , we say that they are **inclusion neighbors** and write $\mathcal{M}_K \sqsubset \mathcal{M}_L$ if

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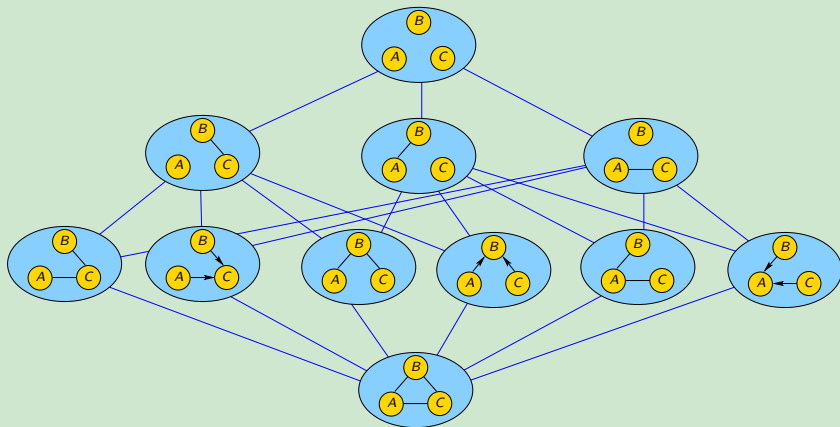
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We say that \mathcal{M}_L is an **upper neighbor** of \mathcal{M}_K or, dually, that \mathcal{M}_K is a **lower neighbor** of \mathcal{M}_L .

Search space for models of three variables

Example



Likelihood of data

- Let $D = \{\mathbf{x}^m, m = 1, \dots, M\}$ be the learning dataset, where \mathbf{x} is the vector of values of variable $\mathbf{X} = \{X_i\}_{i=1}^N$,

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The **likelihood** of D given G is the probability of data D being generated from the Bayesian network model with the structure given by directed acyclic graph G and representing joint probability distribution P is

$$P(D|G) = \prod_{m=1}^M P(\mathbf{X} = \mathbf{x}^m)$$

Lemma (Maximum loglikelihood)

The maximum log-likelihood for a given Bayesian network with graph G is

$$MLL(G|D) = \sum_{i=1}^N \sum_{k=1}^{r(i)} \sum_{j=1}^{q(i,G)} N(i,j,k) \log \frac{N(i,j,k)}{N(i,j)}$$

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Definition (Bayesian Information Criterion)

$$BIC(G|D) = MLL(G|D) - \frac{\log M}{2} d(G)$$

Greedy Equivalence Search (GES) algorithm

The GES algorithm starts with an empty graph and has two stages:

- 1 deleting CI-statements (which corresponds to edge additions and directing some edges)

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Theorem

In the limit of large datasets, if the CI-statements that hold in the dataset are exactly those of a Bayesian network then the algorithm terminates in the essential graph of this Bayesian network.

Comparison of Chickering's GES with our imset version

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- This allows a very easy recomputation of the criteria (two values of a data imset are added and two subtracted).
- From each equivalence class no more than one model is generated.

Experiments with the imset version of GES

We implemented the imset version of GES in R.

The code is freely available from: <http://www.utia.cz/vomlel/imset>

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Model	# variables	# selected nb.	# evaluated nb.
abcde - lower nb.	5	4	60
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asia - lower nb.	8	8	389
- upper nb.		0	8
abcedefghi - lower nb.	9	10	621
- upper nb.		0	10
boerlage92 - lower nb.	23	35	19607
- upper nb.		0	47
alarm - lower nb.	37	52	65787
- upper nb.		1	128

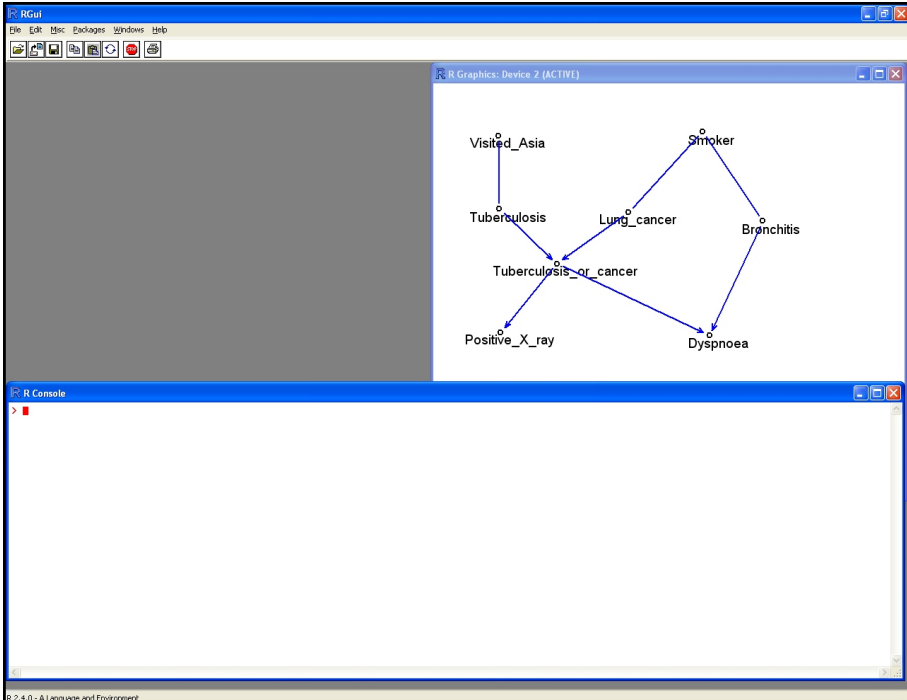
Experiments with the imset version of GES

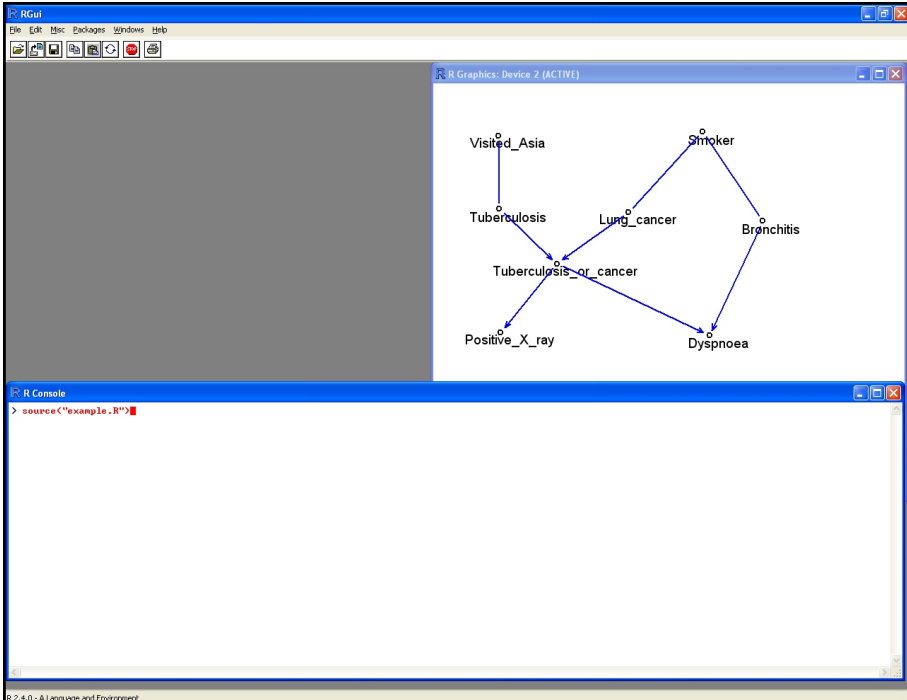
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For the alarm model there are more than $2^{\frac{37 \cdot 36}{2}} = 2^{666}$ essential graphs.





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R Graphics: Device 2 (ACTIVE)

Visited_o_Asia Smoker

Tuberculo_osis Lung_o_cancer Bronchitis

Tuberculosis_o_or_cancer

Positive_o_X_ray Dyspnoea

R Console

```
> source("example.R")
[1] learning the node1 from data
[1] "first going down ..."
1: ■
```

R 2.4.0 - A Language and Environment

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R Graphics: Device 2 (ACTIVE)

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1:
[1] -u< Dyspnoea , Bronchitis ! >
1: ■
```

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R Graphics: Device 2 (ACTIVE)

```
graph TD
    Visited_Asia((Visited_Asia))
    Smoker((Smoker))
    Tuberculosis((Tuberculosis))
    Lung_cancer((Lung_cancer))
    Bronchitis((Bronchitis))
    Tuberculosis_or_cancer((Tuberculosis_or_cancer))
    Positive_X_ray((Positive_X_ray))
    Dyspnoea((Dyspnoea))
    Bronchitis --> Dyspnoea
```

R Console

```
> source("example.R")
[1] learning the model from data
[1] "first going down ..."
1:
1: -u< Dyspnoea , Bronchitis ! >
1:
[1] BIC criteria value: -272961.807754096
1: ■
```

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R Graphics: Device 2 (ACTIVE)

```
graph TD; Visited_Asia --> Tuberculosis; Visited_Asia --> Lung_cancer; Visited_Asia --> Positive_X_ray; Smoker --> Lung_cancer; Smoker --> Bronchitis; Tuberculosis --> Tuberculosis_or_cancer; Lung_cancer --> Tuberculosis_or_cancer; Lung_cancer --> Positive_X_ray; Bronchitis --> Dyspnoea; Tuberculosis_or_cancer --> Positive_X_ray; Positive_X_ray --> Dyspnoea;
```

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```

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R Graphics: Device 2 (ACTIVE)

```
graph TD; Visited_Asia((Visited_Asia)); Smoker((Smoker)); Tuberculosis((Tuberculosis)); Lung_cancer((Lung_cancer)); Bronchitis((Bronchitis)); Tuberculosis_or_cancer((Tuberculosis_or_cancer)); Positive_X_ray((Positive_X_ray)); Dyspnoea((Dyspnoea)); Tuberculosis --> Tuberculosis_or_cancer; Lung_cancer --> Tuberculosis_or_cancer; Lung_cancer --> Bronchitis; Bronchitis --> Dyspnoea;
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[1] learning the model from data
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[1] -u< Tuberculosis_or_cancer , Lung_cancer ! >
1:
[1] BIC criteria value: -254182.414471906
1: ■
```

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```
graph TD
    Visited_Asia((Visited_Asia))
    Smoker((Smoker))
    Tuberculosis((Tuberculosis))
    Lung_cancer((Lung_cancer))
    Bronchitis((Bronchitis))
    Tuberculosis_or_cancer((Tuberculosis_or_cancer))
    Positive_X_ray((Positive_X_ray))
    Dyspnoea((Dyspnoea))

    Tuberculosis --> Lung_cancer
    Lung_cancer --> Tuberculosis_or_cancer
    Lung_cancer --> Bronchitis
    Bronchitis --> Dyspnoea
```

R Console

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[1] learning the model from data
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[1] -u< Dyspnoea , Bronchitis ! >
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[1] BIC criteria value: -272961.807754096
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1:
[1] BIC criteria value: -254182.414471906
1:
[1] -u< Tuberculosis_or_cancer , Positive_X_ray ! >
1: ■
```

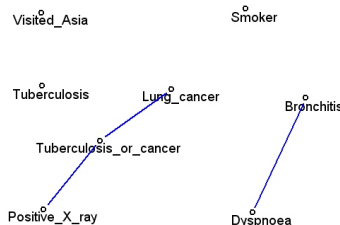
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```
graph TD
    Visited_Asia --> Lung_cancer
    Smoker --> Lung_cancer
    Tuberculosis --> Tuberculosis_or_cancer
    Lung_cancer --> Tuberculosis_or_cancer
    Tuberculosis_or_cancer --> Positive_X_ray
    Bronchitis --> Dyspnoea
    Lung_cancer --> Bronchitis
```

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[1] learning the model from data
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1:
[1] -u< Tuberculosis_or_cancer , Lung_cancer ! >
1:
[1] BIC criteria value: -254182.414471906
1:
[1] -u< Tuberculosis_or_cancer , Positive_X_ray ! >
1:
[1] BIC criteria value: -251673.946500418
1: ■
```

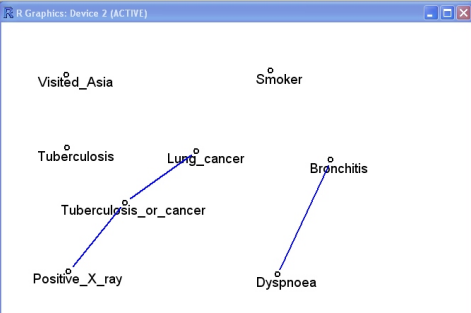
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```
graph TD
    Visited_Asia((Visited_Asia)) --- Lung_cancer((Lung_cancer))
    Smoker((Smoker)) --- Lung_cancer
    Tuberculosis((Tuberculosis)) --- Tuberculosis_or_cancer((Tuberculosis_or_cancer))
    Lung_cancer --- Tuberculosis_or_cancer
    Tuberculosis_or_cancer --- Positive_X_ray((Positive_X_ray))
    Bronchitis((Bronchitis)) --- Dyspnoea((Dyspnoea))
    Tuberculosis_or_cancer --- Lung_cancer
```

R Console

```
> source("example.R")
[1] learning the model from data
[1] "first going down ..."
1:
[1] -u< Dyspnoea , Bronchitis ! >
1:
[1] BIC criteria value: -272961.807754096
1:
[1] -u< Tuberculosis_or_cancer , Lung_cancer ! >
1:
[1] BIC criteria value: -254182.414471906
1:
[1] -u< Tuberculosis_or_cancer , Positive_X_ray ! >
1:
[1] BIC criteria value: -251673.946500448
1:
[1] -u< Tuberculosis_or_cancer , Tuberculosis ! Lung_cancer >
1: ■
```

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```

graph TD
    Visited_Asia --> Tuberculosis
    Visited_Asia --> Lung_cancer
    Visited_Asia --> Positive_X_ray
    Smoker --> Lung_cancer
    Tuberculosis --> Tuberculosis_or_cancer
    Lung_cancer --> Tuberculosis_or_cancer
    Bronchitis --> Dyspnoea
    Tuberculosis_or_cancer --> Positive_X_ray
  
```

R Console

```

> source("example.R")
[1] learning the model from data
[1] "first going down ..."
1:
[1] -u< Dyspnoea , Bronchitis ! >
1:
[1] BIC criteria value: -272961.807754096
1:
[1] -u< Tuberculosis_or_cancer , Lung_cancer ! >
1:
[1] BIC criteria value: -254182.414471906
1:
[1] -u< Tuberculosis_or_cancer , Positive_X_ray ! >
1:
[1] BIC criteria value: -251673.946500448
1:
[1] -u< Tuberculosis_or_cancer , Tuberculosis ! Lung_cancer >
1:
[1] BIC criteria value: -233597.143438138
1: █
  
```

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R Graphics: Device 2 (ACTIVE)

```

graph TD
    Visited_Asia --> Tuberculosis
    Visited_Asia --> Lung_cancer
    Smoker --> Bronchitis
    Tuberculosis --> Tuberculosis_or_cancer
    Lung_cancer --> Tuberculosis_or_cancer
    Lung_cancer --> Positive_X_ray
    Bronchitis --> Dyspnoea
    Tuberculosis_or_cancer --> Positive_X_ray
  
```

R Console

```

> source("example.R")
[1] learning the model from data
[1] "first going down ..."
1:
[1] -u< Dyspnoea , Bronchitis ! >
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[1] BIC criteria value: -272961.807754096
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1:
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1:
[1] BIC criteria value: -251673.946500448
1:
[1] -u< Tuberculosis_or_cancer , Tuberculosis ! Lung_cancer >
1:
[1] BIC criteria value: -233597.143438138
1:
[1] -u< Smoker , Bronchitis ! >
1:

```

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R Graphics: Device 2 (ACTIVE)

```
graph TD; Visited_Asia --> Tuberculosis; Visited_Asia --> Lung_cancer; Visited_Asia --> Tuberculosis_or_cancer; Visited_Asia --> Positive_X_ray; Smoker --> Bronchitis; Bronchitis --> Dyspnoea; Tuberculosis --> Tuberculosis_or_cancer; Lung_cancer --> Tuberculosis_or_cancer;
```

R Console

```
> source("example.R")
[1] learning the model from data
[1] "first going down ..."
1:
[1] -u< Dyspnoea , Bronchitis ! >
1:
[1] BIC criteria value: -272961.807754096
1:
[1] -u< Tuberculosis_or_cancer , Lung_cancer ! >
1:
[1] BIC criteria value: -254182.414471906
1:
[1] -u< Tuberculosis_or_cancer , Positive_X_ray ! >
1:
[1] BIC criteria value: -251673.946500448
1:
[1] -u< Tuberculosis_or_cancer , Tuberculosis ! Lung_cancer >
1:
[1] BIC criteria value: -233597.143438138
1:
[1] -u< Smoker , Bronchitis ! >
1:
[1] BIC criteria value: -228979.728973490
1: ■
```

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R Graphics: Device 2 (ACTIVE)

```
graph TD; Visited_Asia --> Tuberculosis; Visited_Asia --> Lung_cancer; Smoker --> Bronchitis; Bronchitis --> Dyspnoea; Tuberculosis --> Tuberculosis_or_cancer; Lung_cancer --> Tuberculosis_or_cancer; Tuberculosis_or_cancer --> Positive_X_ray;
```

R Console

```
> source("example.R")
[1] learning the model from data
[1] "first going down ..."
1:
[1] -u< Dyspnoea , Bronchitis ! >
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[1] BIC criteria value: -272961.807754096
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1:
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1:
[1] -u< Tuberculosis_or_cancer , Positive_X_ray ! >
1:
[1] BIC criteria value: -251673.946500448
1:
[1] -u< Tuberculosis_or_cancer , Tuberculosis ! Lung_cancer >
1:
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1:
[1] -u< Smoker , Bronchitis ! >
1:
[1] BIC criteria value: -228979.728973490
1:
[1] -u< Tuberculosis_or_cancer , Dyspnoea ! Bronchitis >
1: ■
```

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R Graphics: Device 2 (ACTIVE)

```

graph TD
    Visited_Asia --> Tuberculosis
    Smoker --> Bronchitis
    Tuberculosis --> Tuberculosis_or_cancer
    Lung_cancer --> Tuberculosis_or_cancer
    Bronchitis --> Dyspnoea
    Tuberculosis_or_cancer --> Positive_X_ray
    Tuberculosis_or_cancer --> Dyspnoea
  
```

R Console

```

> source("example.R")
[1] learning the model from data
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1:
[1] -u< Dyspnoea , Bronchitis ! >
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[1] -u< Smoker , Bronchitis ! >
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[1] BIC criteria value: -228979.728973490
1:
[1] -u< Tuberculosis_or_cancer , Dyspnoea ! Bronchitis >
1:
[1] BIC criteria value: -226168.238717828
1:

```

R 2.4.0 - A Language and Environment

RGui

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R Graphics: Device 2 (ACTIVE)

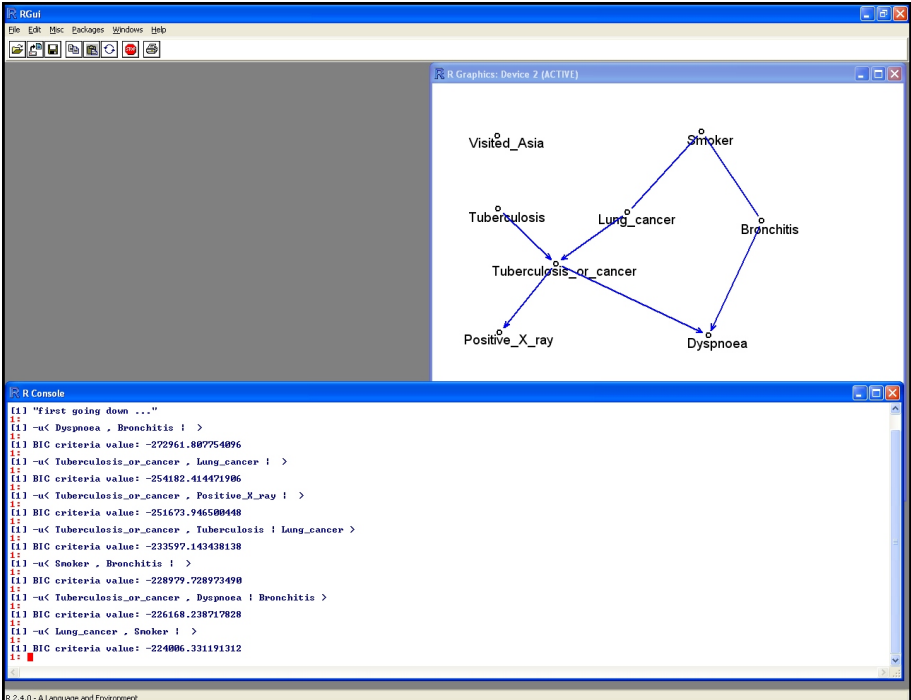
```
graph TD; Visited_Asia --> Tuberculosis; Visited_Asia --> Lung_cancer; Visited_Asia --> Tuberculosis_or_cancer; Visited_Asia --> Positive_X_ray; Visited_Asia --> Dyspnoea; Smoker --> Bronchitis; Bronchitis --> Tuberculosis_or_cancer; Bronchitis --> Dyspnoea; Tuberculosis --> Tuberculosis_or_cancer; Lung_cancer --> Tuberculosis_or_cancer; Tuberculosis_or_cancer --> Positive_X_ray; Tuberculosis_or_cancer --> Dyspnoea;
```

R Console

```
> source("example.R")
[1] learning the model from data
[1] "first going down ..."
1:
[1] -u< Dyspnoea , Bronchitis ! >
1:
[1] BIC criteria value: -272961.807754096
1:
[1] -u< Tuberculosis_or_cancer , Lung_cancer ! >
1:
[1] BIC criteria value: -254182.414471906
1:
[1] -u< Tuberculosis_or_cancer , Positive_X_ray ! >
1:
[1] BIC criteria value: -251673.946500448
1:
[1] -u< Tuberculosis_or_cancer , Tuberculosis ! Lung_cancer >
1:
[1] BIC criteria value: -233597.143438138
1:
[1] -u< Smoker , Bronchitis ! >
1:
[1] BIC criteria value: -228979.728973490
1:
[1] -u< Tuberculosis_or_cancer , Dyspnoea ! Bronchitis >
1:
[1] BIC criteria value: -226168.238717828
1:
[1] -u< Lung_cancer , Smoker ! >
1:
```

R 2.4.0 - A Language and Environment

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R Graphics: Device 2 (ACTIVE)

```

graph TD
    Visited_Asia((Visited_Asia)) --> Tuberculosis((Tuberculosis))
    Smoker((Smoker)) --> Lung_cancer((Lung_cancer))
    Smoker((Smoker)) --> Bronchitis((Bronchitis))
    Tuberculosis((Tuberculosis)) --> Tuberculosis_or_cancer((Tuberculosis_or_cancer))
    Lung_cancer((Lung_cancer)) --> Tuberculosis_or_cancer((Tuberculosis_or_cancer))
    Bronchitis((Bronchitis)) --> Dyspnoea((Dyspnoea))
    Tuberculosis_or_cancer((Tuberculosis_or_cancer)) --> Positive_X_ray((Positive_X_ray))
    Tuberculosis_or_cancer((Tuberculosis_or_cancer)) --> Dyspnoea((Dyspnoea))
    
```

R Console

```

[1] -u< Dyspnoea , Bronchitis ! >
[1] BIC criteria value: -272961.807754096
[1] -u< Tuberculosis_or_cancer , Lung_cancer ! >
[1] BIC criteria value: -254182.414471906
[1] -u< Tuberculosis_or_cancer , Positive_X_ray ! >
[1] BIC criteria value: -251673.946500448
[1] -u< Tuberculosis_or_cancer , Tuberculosis ! Lung_cancer >
[1] BIC criteria value: -233597.143438138
[1] -u< Smoker , Bronchitis ! >
[1] BIC criteria value: -228979.728973490
[1] -u< Tuberculosis_or_cancer , Dyspnoea ! Bronchitis >
[1] BIC criteria value: -226168.238717828
[1] -u< Lung_cancer , Smoker ! >
[1] BIC criteria value: -224006.331191312
[1] -u< Tuberculosis , Visited_Asia ! >

```

R 2.4.0 - A Language and Environment

RGui

File Edit Misc Packages Windows Help

R Graphics: Device 2 (ACTIVE)

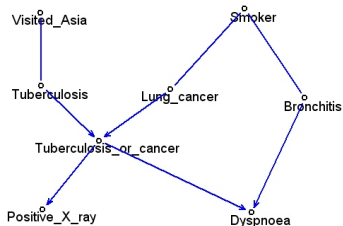
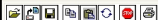
```
graph TD; Visited_Asia((Visited_Asia)) --> Tuberculosis((Tuberculosis)); Smoker((Smoker)) --> Lung_cancer((Lung_cancer)); Smoker((Smoker)) --> Bronchitis((Bronchitis)); Tuberculosis((Tuberculosis)) --> Tuberculosis_or_cancer((Tuberculosis_or_cancer)); Lung_cancer((Lung_cancer)) --> Tuberculosis_or_cancer((Tuberculosis_or_cancer)); Lung_cancer((Lung_cancer)) --> Dyspnoea((Dyspnoea)); Bronchitis((Bronchitis)) --> Dyspnoea((Dyspnoea)); Tuberculosis_or_cancer((Tuberculosis_or_cancer)) --> Positive_X_ray((Positive_X_ray)); Tuberculosis_or_cancer((Tuberculosis_or_cancer)) --> Dyspnoea((Dyspnoea));
```

R Console

```
[1] BIC criteria value: -272961.807754096
1: -u< Tuberculosis_or_cancer , Lung_cancer ! >
1: BIC criteria value: -254182.414471906
1: -u< Tuberculosis_or_cancer , Positive_X_ray ! >
1: BIC criteria value: -251673.946500448
1: -u< Tuberculosis_or_cancer , Tuberculosis ! Lung_cancer >
1: BIC criteria value: -233597.143438138
1: -u< Smoker , Bronchitis ! >
1: BIC criteria value: -228979.728973490
1: -u< Tuberculosis_or_cancer , Dyspnoea ! Bronchitis >
1: BIC criteria value: -226168.238717828
1: -u< Lung_cancer , Smoker ! >
1: BIC criteria value: -224006.331191312
1: -u< Tuberculosis , Visited_Asia ! >
1: BIC criteria value: -223982.552597421
1: █
```

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```

1:
[1] BIC criteria value: -223982.552597421
1:
[1] BIC criteria value: -223982.552597421
[1] "second going up ..."
[1] BIC criteria value: -223982.552597421
[1] A best essential graph for the given data is plotted now.
[1] Algorithm went through:
[1] Lower neighbours: 8
[1] - evaluations (incl. cache): 389
[1] - Chickering eval. (incl. cache): 546
[1] Upper neighbours: 0
[1] - evaluations (incl. cache): 8
[1] - Chickering eval. (incl. cache): 8
[1] BIC criteria value: -223982.552597421
[1] MLL criteria value: -223878.936268237
[1] "structural inset:"
[1] < > = 1
[1] < Tuberculosis_or_cancer > = 1
[1] < Tuberculosis_or_cancer Positive_X_ray > = -1
[1] < Tuberculosis_or_cancer Bronchitis > = 1
[1] < Tuberculosis_or_cancer Dyspnoea Bronchitis > = -1
[1] < Smoker > = 1
[1] < Smoker Bronchitis > = -1
[1] < Tuberculosis_or_cancer Tuberculosis Lung_cancer > = -1
[1] < Tuberculosis_or_cancer Tuberculosis Lung_cancer Smoker Visited_Asia Dyspnoea Bronchitis Positive_X_ray > = 1
[1] < Lung_cancer Smoker > = -1
[1] < Tuberculosis Visited_Asia > = -1
[1] < Tuberculosis Lung_cancer > = 1
[1] >

```