## Advanced AI Techniques

## I. Bayesian Networks / 3. Structure Learning (1/2)

Wolfram Burgard, Luc de Raedt, Bernhard Nebel, Lars Schmidt-Thieme<br>Institute for Computer Science<br>University of Freiburg<br>http://www.informatik.uni-freiburg.de/

## 1. Checking Probalistic Independencies

## 2. Markov Equivalence and DAG patterns

## 3. PC Algorithm

- Assume, we know the whole structure of a bn except a single edge.
- This edge represents a single independence statement.
- Check it and include edge based on outcome of that test.

Advanced AI Techniques / 1. Checking Probalistic Independencies
Exact Check / Example (1/3)

If $X$ and $Y$ are independent, then

$$
p(X, Y)=p(X) \cdot p(Y)
$$

observed

| $Y=$ | 0 | 1 |
| ---: | :--- | :--- |
| $X=0$ | 3 | 6 |
| 1 | 1 | 2 |

observed relative frequencies $p(X, Y)$ :

| $Y=$ | 0 | 1 |
| ---: | :--- | :--- |
| $X=0$ | 0.25 | 0.5 |
| 1 | 0.083 | 0.167 |

expected relative frequencies $p(X) p(Y)$ :

| $Y=$ | 0 | 1 |
| ---: | :--- | :--- |
| $X=0$ | 0.25 | 0.5 |
| 1 | 0.083 | 0.167 |

If $X$ and $Y$ are independent, then

$$
p(X, Y)=p(X) \cdot p(Y)
$$

## observed

| $Y=$ | 0 | 1 |
| ---: | :---: | :---: |
| $X=0$ | 3000 | 6000 |
| 1 | 1000 | 2000 |

observed relative frequencies $p(X, Y)$ :

| $Y=$ | 0 | 1 |
| ---: | :--- | :--- |
| $X=0$ | 0.25 | 0.5 |
| 1 | 0.083 | 0.167 |

expected relative frequencies $p(X) p(Y)$ :

| $Y=$ | 0 | 1 |
| ---: | :--- | :--- |
| $X=0$ | 0.25 | 0.5 |
| 1 | 0.083 | 0.167 |

Wolfram Burgard, Luc de Raedt, Bernhard Nebel, Lars Schmidt-Thieme, Institute for Computer Science, University of Freiburg, Germany, Course on Advanced AI Techniques, winter term 2004

Advanced AI Techniques / 1. Checking Probalistic Independencies

## Exact Check / Example (3/3)

If $X$ and $Y$ are independent, then

$$
p(X, Y)=p(X) \cdot p(Y)
$$

observed

| $Y=\\|$ | 0 | 1 |
| ---: | :---: | :---: |
| $X=0$ | 2999 | 6001 |
| 1 | 1000 | 2000 |

observed relative frequencies $p(X, Y)$ :

| $Y=$ | 0 | 1 |
| ---: | :--- | :--- |
| $X=0$ | 0.2499167 | 0.5000833 |
| 1 | 0.0833333 | 0.1666667 |

expected relative frequencies $p(X) p(Y)$ :

| $Y=$ | 0 | 1 |
| ---: | :--- | :--- |
| $X=0$ | 0.2499375 | 0.5000625 |
| 1 | 0.0833125 | 0.1666875 |

## Definition 1. Gamma function

$$
\Gamma(a):=\int_{0}^{\infty} t^{a-1} e^{-t} d t
$$

converging for $a>0$.

## Lemma 1 ( $\Gamma$ is generalization of factorial).

(i) $\Gamma(n)=(n-1)$ ! for $n \in \mathbb{N}$.
(ii) $\frac{\Gamma(a+1)}{\Gamma(a)}=a$.


Wolfram Burgard, Luc de Raedt, Bernhard Nebel, Lars Schmidt-Thieme, Institute for Computer Science, University of Freiburg, Germany, Course on Advanced AI Techniques, winter term 2004

Advanced AI Techniques / 1. Checking Probalistic Independencies
Incomplete Gamma Function

## Definition 2. Incomplete Gamma function

$$
\gamma(a, x):=\int_{0}^{x} t^{a-1} e^{-t} d t
$$

defined for $a>0$ and $x \in[0, \infty]$.
Lemma 2.

$$
\gamma(a, \infty)=\Gamma(a)
$$


$\gamma$

$\gamma(5, x)$

## Definition 3. chi-square distribution ( $\chi^{2}$ ) has density

$$
p(x):=\frac{1}{2^{\frac{\mathrm{df}}{2}} \Gamma\left(\frac{\mathrm{df}}{2}\right)} x^{\frac{\mathrm{df}}{2}-1} e^{-\frac{x}{2}} ;
$$

defined on $] 0, \infty[$.
Its cumulative distribution function (cdf) is:

$$
p(X<x):=\frac{\gamma\left(\frac{\mathrm{df}}{2}, \frac{x}{2}\right)}{\Gamma\left(\frac{\mathrm{f}}{2}\right)} ;
$$


$\chi_{1}^{2}, \chi_{2}^{2}, \chi_{3}^{2}, \chi_{4}^{2}$

$\chi_{5}^{2}, \chi_{6}^{2}, \chi_{7}^{2}, \chi_{10}^{2}$

$\chi_{50}^{2}, \chi_{60}^{2}, \chi_{70}^{2}$

Wolfram Burgard, Luc de Raedt, Bernhard Nebel, Lars Schmidt-Thieme, Institute for Computer Science, University of Freiburg, Germany, Course on Advanced Al Techniques, winter term 2004
Advanced AI Techniques / 1. Checking Probalistic Independencies

## Lemma 3.

$$
E\left(\chi^{2}(x, \mathrm{df})\right)=\mathrm{df}
$$

A Java implementation of the incomplete gamma function (and thus of $\chi^{2}$ distribution) can be found, e.g., in COLT (http://dsd.lbl.gov/~hoschek/colt/), package cern.jet.stat, class Gamma.

Be careful, sometimes
$\tilde{\gamma}(a, x):=\frac{1}{\Gamma(a)} \int_{0}^{x} t^{a-1} e^{-t} d t=\frac{1}{\Gamma(a)} \gamma(a, x) \quad$ (e.g., R)
or
$\tilde{\gamma}(a, x):=\int_{x}^{\infty} t^{a-1} e^{-t} d t \quad=\Gamma(a)-\gamma(a, x)$
(e.g., Maple)
are referenced as incomplete gamma function.

Let $X, Y$ be random variables, $D \subseteq \operatorname{dom}(X) \times \operatorname{dom}(Y)$ and for two values $x \in \operatorname{dom}(X), y \in \operatorname{dom}(Y)$

$$
\begin{aligned}
c_{X=x} & :=\left|\left\{d \in D \mid d_{\mid X}=x\right\}\right| \\
c_{Y=y} & :=\left|\left\{d \in D \mid d_{\mid X}=x\right\}\right| \\
c_{X=x, Y=y} & :=\left|\left\{d \in D \mid d_{\mid X}=x, d_{\mid Y}=y\right\}\right|
\end{aligned}
$$

## their counts.

Advanced AI Techniques / 1. Checking Probalistic Independencies

$$
\chi^{2} \text { and } G^{2} \text { statistics / Just } 2 \text { Variables }
$$

If $X, Y$ are independent, then

$$
p(X, Y)=p(X) p(Y)
$$

and thus

$$
E\left(c_{X=x, Y=y} \mid c_{X=x}, c_{Y=y}\right)=\frac{c_{X=x} \cdot c_{Y=y}}{|D|}
$$

Then the statistics

$$
\chi^{2}:=\sum_{x \in \operatorname{dom}(X)} \sum_{y \in \operatorname{dom}(Y)} \frac{\left(c_{X=x, Y=y}-\frac{c_{X=x} \cdot c_{Y=y}}{|D|}\right)^{2}}{\frac{c_{X X x} \cdot c_{Y=y}}{|D|}}
$$

as well as

$$
G^{2}:=2 \sum_{x \in \operatorname{dom}(X)} \sum_{y \in \operatorname{dom}(Y)} c_{X=x, Y=y} \cdot \ln \left(\frac{c_{X=x, Y=y}}{\left(\frac{\left.c_{X=x^{\prime} \cdot C_{Y=y}}^{|D|}\right)}{|n|}\right)}\right.
$$

are asymptotically $\chi^{2}$-distributed with
$\mathrm{df}=(|\operatorname{dom}(X)|-1)(|\operatorname{dom}(Y)|-1)$ degrees of freedom.

Generally, the statistics have the form

$$
\begin{aligned}
\chi^{2} & =\sum \frac{(\text { observed }- \text { expected })^{2}}{\text { expected }} \\
G^{2} & =\sum \text { observed } \ln \left(\frac{\text { observed }}{\text { expected }}\right)
\end{aligned}
$$

$\chi^{2}=0$ and $G^{2}=0$ for exact independent variables.

The larger $\chi^{2}$ and $G^{2}$, the more likely / stronger the depedency between $X$ and $Y$.

Advanced AI Techniques / 1. Checking Probalistic Independencies
Testing Independency / more formally

More formally, under the
null hypothesis of independency of $X$ and $Y$,
the probability for $\chi^{2}$ and $G^{2}$ to have the computed values (or even larger ones) is

$$
p_{\chi_{\mathrm{df}}^{2}}\left(X>\chi^{2}\right) \quad \text { and } \quad p_{\chi_{\mathrm{df}}^{2}}\left(X>G^{2}\right)
$$

Let $p_{0}$ be a given threshold called significance level and often choosen as 0.05 or 0.01 .

- If $p\left(X>\chi^{2}\right)<p_{0}$, we can reject the null hypothesis and thus accept its alternative hypothesis of dependency of $X$ and $Y$.
i.e., add the edge between $X$ and $Y$.
- If $p\left(X>\chi^{2}\right) \geq p_{0}$, we cannot reject the null hypothesis.

Here, we then will accept the null hypothesis, i.e., not add the edge between $X$ and $Y$.
observed

| $Y=$ | 0 | 1 |
| ---: | :--- | :--- |
| $X=0$ | 3 | 6 |
| 1 | 1 | 2 |

margins

| $Y=$ | 0 | 1 | $\sum$ |
| ---: | :--- | :--- | :--- |
| $X=0$ | 3 | 6 | 9 |
| 1 | 1 | 2 | 3 |
| $\sum$ | 4 | 8 | 12 |

expected

| $Y=$ | 0 | 1 | $\sum$ |
| ---: | :--- | :--- | :--- |
| $X=0$ | 3 | 6 | 9 |
| 1 | 1 | 2 | 3 |
| $\sum$ | 4 | 8 | 12 |

$$
\chi^{2}=G^{2}=0 \quad \text { and } \quad p(X>0)=1
$$

Hence, for any significance level $X$ and $Y$ are considered independent.


Wolfram Burgard, Luc de Raedt, Bernhard Nebel, Lars Schmidt-Thieme, Institute for Computer Science, University of Freiburg, Germany, Course on Advanced Al Techniques, winter term 2004

Advanced AI Techniques / 1. Checking Probalistic Independencies
Example 2 (1/2)
observed

| $Y=$ | 0 | 1 |
| ---: | :--- | :--- |
| $X=0$ | 6 | 1 |
| 1 | 2 | 4 |

margins

| $Y=$ | 0 | 1 | $\sum$ |
| ---: | :--- | :--- | :--- |
| $X=0$ | 6 | 1 | 7 |
| 1 | 2 | 4 | 6 |
| $\sum$ | 8 | 5 | 13 |

## expected

| $Y=$ | 0 | 1 | $\sum$ |
| ---: | :---: | :---: | :---: |
| $X=0$ | 4.31 | 2.69 | 7 |
| 1 | 3.69 | 2.31 | 6 |
| $\sum$ | 8 | 5 | 13 |

$$
\begin{aligned}
\chi^{2} & =\frac{(6-4.31)^{2}}{4.31}+\frac{(1-2.69)^{2}}{2.69}+\frac{(2-3.69)^{2}}{3.69}+\frac{(4-2.31)^{2}}{2.31} \\
& =3.75
\end{aligned}
$$

$$
\rightsquigarrow p_{\chi_{1}^{2}}(X>3.75)=0.053
$$

i.e., with a significance level of $p_{0}=0.05$
we would not be able to reject the null hypothesis of independency of $X$ and $Y$.


If we use $G^{2}$ instead of $\chi^{2}$,

$$
G^{2}=3.94, \quad p_{\chi_{1}^{2}}(X>3.94)=0.047
$$

with a significance level of $p_{0}=0.05$
we would have to reject the null hypothesis of independency of $X$ and $Y$.

Here, we then accept the alternative, depedency of $X$ and $Y$.


Advanced AI Techniques / 1. Checking Probalistic Independencies
count variables / general case

Let $\mathcal{V}$ be a set of random variables.

We write $v \in \mathcal{V}$ as abbreviation for $v \in \prod \operatorname{dom}(\mathcal{V})$.
For a dataset $D \subseteq \prod \operatorname{dom}(\mathcal{V})$ and

- each subset $\mathcal{X} \subseteq \mathcal{V}$ of variables and
- each configuration $x \in \mathcal{X}$ of these variables
let

$$
c_{\mathcal{X}=x}:=\left|\left\{d \in D \mid d_{\mid \mathcal{X}}=x\right\}\right|
$$

be a (random) variable containing the frequencies of occurences of $\mathcal{X}=x$ in the data.

Advanced AI Techniques / 1. Checking Probalistic Independencies $G^{2}$ statistics / general case

Let $\mathcal{X}, \mathcal{Y}, \mathcal{Z} \subseteq \mathcal{V}$ be three disjoint subsets of variables. If

$$
I(\mathcal{X}, \mathcal{Y} \mid \mathcal{Z})
$$

then

$$
p(\mathcal{X}, \mathcal{Y}, \mathcal{Z})=\frac{p(\mathcal{X}, \mathcal{Z}) p(\mathcal{Y}, \mathcal{Z})}{p(\mathcal{Z})}
$$

and thus for each configuration $x \in \mathcal{X}, y \in \mathcal{Y}$, and $z \in \mathcal{Z}$

$$
E\left(c_{\mathcal{X}=x, \mathcal{Y}=y, \mathcal{Z}=z} \mid c_{\mathcal{X}=x, \mathcal{Z}=z}, c_{\mathcal{Y}=y, \mathcal{Z}=z}\right)=\frac{c_{\mathcal{X}=x, \mathcal{Z}=z} c_{\mathcal{Y}=y, \mathcal{Z}=z}}{c_{\mathcal{Z}=z}}
$$

The statistics

$$
G^{2}:=2 \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} \sum_{z \in \mathcal{Z}} c_{\mathcal{X}=x, \mathcal{Y}=y, \mathcal{Z}=z} \cdot \ln \left(\frac{c_{\mathcal{X}=x, \mathcal{Y}=y, \mathcal{Z}=z} \cdot c_{\mathcal{Z}=z}}{c_{\mathcal{X}=x, \mathcal{Z}=z} \cdot c_{\mathcal{Y}=y, \mathcal{Z}=z}}\right)
$$

is asymptotically $\chi^{2}$-distributed with

$$
\mathrm{df}=\prod_{X \in \mathcal{X}}(|\operatorname{dom} X|-1) \prod_{Y \in \mathcal{Y}}(|\operatorname{dom} Y|-1) \prod_{Z \in \mathcal{Z}}|\operatorname{dom} Z|
$$

degrees of freedom.

Advanced AI Techniques / 1. Checking Probalistic Independencies

Recommendations [SGS00, p. 95]:

- As heuristics, reduce degrees of freedom by 1 for each structural zero:
df ${ }^{\text {reduced }}:=\mathrm{df}-\left|\left\{(x, y, z) \in \mathcal{X} \times \mathcal{Y} \times \mathcal{Z} \mid c_{\mathcal{X}=x, \mathcal{Y}=y, \mathcal{Z}=z}=0\right\}\right|$
- Use $G^{2}$ instead of $\chi^{2}$.
- If $|D|<10 \mathrm{df}$, assume conditional dependency.


## Problems:

- null hypothesis is accepted if it is not rejected.
(especially problematic for small samples)
- repeated testing.


## 1. Checking Probalistic Independencies

## 2. Markov Equivalence and DAG patterns

## 3. PC Algorithm

Definition 4. Let $G, H$ be two graphs on a set $V$ (undirected or DAGs).
$G$ and $H$ are called markov-equivalent, if they have the same independency model, i.e.

$$
I_{G}(X, Y \mid Z) \Leftrightarrow I_{H}(X, Y \mid Z), \quad \forall X, Y, Z \subseteq V
$$

The notion of markov-equivalence for undirected graphs is uninteresting, as every undirected graph is markovequivalent only to itself (corollary of uniqueness of minimal representation!).

Why is markov-equivalence important?

1. in structure learning, the set of all graphs over $V$ is our search space.
$\rightsquigarrow$ if we can restrict searching to equivalence classes, the search space becomes smaller.
2. if we interpret the edges of our graph as causal relationships between variables, it is of interest,

- which edges are necessary
(i.e., occur in all instances of the equivalence class), and
- which edges are only possible
(i.e., occur in some instances of the equivalence class, but not in some others; i.e., there are alternative explanations).

Definition 5. Let $G$ be a directed graph. We call a chain

$$
p_{1}-p_{2}-p_{3}
$$

uncoupled if there is no edge between $p_{1}$ and $p_{3}$.

Lemma 4 (markov-equivalence criterion, [PGV90]). Let $G$ and $H$ be two DAGs on the vertices $V$.
$G$ and $H$ are markov-equivalent if and only if
(i) $G$ and $H$ have the same links $(u(G)=u(H))$ and
(ii) $G$ and $H$ have the same uncoupled head-to-head meetings.

The set of uncoupled head-to-head meetings is also denoted as V-structure of $G$.

Markov-equivalence / examples


Figure 1: Example for markov-equivalent DAGs.


Figure 2: Which minimal DAG-representations of $I$ are equivalent? [CGH97, p. 240]

Advanced AI Techniques / 2. Markov Equivalence and DAG patterns

## Directed graph patterns

ALBERT-LUDWIGSUNIVERSITÄT FREIBURG

Definition 6. Let $V$ be a set and $E \subseteq V^{2} \cup \mathcal{P}^{2}(V)$ a set of ordered and unordered pairs of elements of $V$ with $(v, w),(w, v) \notin E$ for $v, w \in V$ with $\{v, w\} \in E$.
Then $G:=(V, E)$ is called a directed graph pattern. The elements of $V$ are called vertices, the elemtents of $E$ edges: unordered pairs are called undirected edges, ordered pairs directed edges.

We say, a directed graph pattern $H$ is a pattern of the directed graph $G$, if there is an orientation of the unoriented edges of $H$ that yields $G$, i.e.

$$
\begin{aligned}
&(v, w) \in E_{G} \Rightarrow\left\{\begin{array}{l}
(v, w) \in E_{H} \text { or } \\
\{v, w\} \in E_{H}
\end{array}\right. \\
&(v, w) \in E_{G} \Leftarrow(v, w) \in E_{H}
\end{aligned}
$$

$$
\left.\begin{array}{l}
(v, w) \in E_{G} \text { or } \\
(w, v) \in E_{G}
\end{array}\right\} \Leftarrow\{v, w\} \in E_{H}
$$



Figure 3: Directed graph pattern.

Definition 7. A directed graph pattern $H$ is called an acyclic directed graph pattern (DAG pattern), if

- it is the directed graph pattern of a DAG $G$ or equivalently
- $G$ does not contain a completely directed cycle, i.e. there is no sequence $v_{1}, \ldots, v_{n} \in V$ with $\left(v_{i}, v_{i+1}\right) \in E$ for $i=1, \ldots, n-1$ (i.e. the directed graph got by dropping undirected edges is a DAG).


Figure 4: DAG pattern.


Figure 5: Directed graph pattern that is not a DAG pattern.

Advanced AI Techniques / 2. Markov Equivalence and DAG patterns
DAG patterns represent markov equivalence classest Ersitīt freiburg

Lemma 5. Each markov equivalence class corresponds uniquely to a DAG pattern $G$ :

The markov equivalence class consists of all DAGs that $G$ is a pattern of, i.e., that give $G$ by dropping the directions of some edges that are not part of an uncoupled head-to-head meeting,
(ii) The DAG pattern contains a directed edge $(v, w)$, if all representatives of the markov equivalence class contain this directed edge, otherwise (i.e. if some representatives have $(v, w)$, some others $(w, v)$ ) the DAG pattern contains the undirected edge $\{v, w\}$.

The directed edges of the DAG pattern are also called irreversible or compelled, the undirected edges are also called reversible.

## Advanced AI Techniques / 2. Markov Equivalence and DAG patterns

DAG patterns represent markov equivalence classes / exampleit freiburg


Figure 6: DAG pattern and its markov equivalence class representatives.

Wolfram Burgard, Luc de Raedt, Bernhard Nebel, Lars Schmidt-Thieme, Institute for Computer Science, University of Freiburg, Germany,
Advanced AI Techniques / 2. Markov Equivalence and DAG patterns
DAG patterns represent markov equivalence classes' Ersitait freiburg
But beware, not every DAG pattern represents a Markov-equivalence class!

## Example:


is not a DAG pattern of a Markov-equivalence class, but

is.

DAG patterns represent markov equivalence classest Ersitait freiburg
But just skeleton plus uncoupled head-to-head meetings do not make a DAG pattern that represents a markov-equivalence class either.
Example:

is not a DAG pattern that represents a Markov-equivalence class, as any of its represenatives also has $Z \rightarrow W$. But

is.
Wolfram Burgard, Luc de Raedt, Bernhard Nebel, Lars Schmidt-Thieme, Institute for Computer Science, University of Freiburg, Germany, Course on Advanced AI Techniques, winter term 2004
Advanced AI Techniques / 2. Markov Equivalence and DAG patterns

So, to compute the DAG pattern that represents the equivalence class of a given DAG,

1. start with the skeleton plus all head-to-head-meetings,
2. add entailed edges successively (saturating).
rule 1:

rule 2 :

rule 3 :

rule 4:

$\leadsto$


Dashed link can be $W \rightarrow Z, W \leftarrow Z$, or $W-Z$ (so rule 4 is actually a compact notation for 3 rules).
Wolfram Burgard, Luc de Raedt, Bernhard Nebel, Lars Schmidt-Thieme, Institute for Computer Science, University of Freiburg, Germany, Course on Advanced Al Techniques, winter term 2004
Advanced AI Techniques / 2. Markov Equivalence and DAG patterns

```
l saturate(graph pattern G}=(V,E))\mathrm{ :
2 apply rules 1-4 to }G\mathrm{ until no more rule matches
3 return }
dag-pattern(graph G = (V,E)) :
H:=(V,F) with F:={{x,y}|(x,y)\inE}
3 for }X->Z\leftarrowY\mathrm{ uncoupled head-to-head-meeting in G 㶾
4 orient }X->Z\leftarrowY\mathrm{ in }
5 Od
6 saturate( }H\mathrm{ )
7 return H
```

Figure 7: Algorithm for computing the DAG pattern of the Markov-equivalence class of a given DAG.

Lemma 6. For a given graph $G$, algorithm 7 computes correctly the DAG pattern that represents its Markov-equivalence class.
Furthermore, here, even the rule set $1-3$ will do and is non-redundant.

## See [Mee95] for a proof.

What follows, is an alternative algorithm for computing DAG patterns that represent the Markov-equivalence class of a given DAG.

Advanced AI Techniques / 2. Markov Equivalence and DAG patterns
Toplogical edge ordering

Definition 8. Let $G:=(V, E)$ be a directed graph.
A bijective map

$$
\tau:\{1, \ldots,|E|\} \rightarrow E
$$

is called an ordering of the edges of $G$.

## An edge ordering $\tau$ is called topological edge ordering if

(i) numbers increase on all paths, i.e.

$$
\tau^{-1}(x, y)<\tau^{-1}(y, z)
$$

for paths $x \rightarrow y \rightarrow z$ and
(ii) shortcuts have larger numbers, i.e. for $x, y, z$ with
it is


$$
\tau^{-1}(x, y)<\tau^{-1}(y, z) \stackrel{!}{<} \tau^{-1}(x, z)
$$



Figure 8: Example for a topological edge ordering.

```
l topological-edge-ordering}(G=(V,E))
\sigma:= topological-ordering(G)
E':=E
for}i=1,\ldots,|E|\underline{\mathbf{do}
    Let }(v,w)\in\mp@subsup{E}{}{\prime}\mathrm{ with }\mp@subsup{\sigma}{}{-1}(w)\mathrm{ minimal and then with }\mp@subsup{\sigma}{}{-1}(v)\mathrm{ maximal
    \tau(i):= (v,w)
    E ^ { \prime } : = E ^ { \prime } \ \{ ( v , w ) \}
od
return}
```

Figure 9: Algorithm for computing a topological edge ordering of a DAG.

Wolfram Burgard, Luc de Raedt, Bernhard Nebel, Lars Schmidt-Thieme, Institute for Computer Science, University of Freiburg, Germany,
Advanced AI Techniques / 2. Markov Equivalence and DAG patterns

```
dag-pattern \((G=(V, E))\) :
\(\tau:=\) topological-edge-ordering \((G)\)
\(E_{\text {irr }}:=\emptyset\)
\(E_{\text {rev }}:=\emptyset\)
\(E_{\text {rest }}:=E\)
while \(E_{\text {rest }} \neq \emptyset \underline{\text { do }}\)
    Let \((y, z) \in E_{\text {rest }}\) with \(\tau^{-1}(y, z)\) minimal
            [label pa \((z):]\)
            if \(\exists(x, y) \in E_{\text {irr }}\) with \((x, z) \notin E\)
            \(E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid x^{\prime} \in \operatorname{pa}(z)\right\}\)
            else
                \(E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, y\right) \in E_{\text {irr }}\right\}\)
                if \(\exists(x, z) \in E\) with \(x \notin\{y\} \cup \mathrm{pa}(y)\)
                    \(E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, z\right) \in E_{\text {rest }}\right\}\)
            else
                        \(E_{\text {rev }}:=E_{\text {rev }} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, z\right) \in E_{\text {rest }}\right\}\)
                fi
            fi
            \(E_{\text {rest }}:=E \backslash E_{\text {irr }} \backslash E_{\text {rev }}\)
od
\(\underline{\text { return }} \bar{G}:=\left(V, E_{\text {irr }} \cup\left\{\{v, w\} \mid(v, w) \in E_{\text {rev }}\right\}\right)\)
```

Figure 10: Algorithm for computing the DAG pattern representing the markov equivalence class of

Lemma 7 ([Chi95]). Let $G$ be a DAG and $x, y, z$ three vertices of $G$ that are pairwise adjacent. If any two of the connecting edges are reversible, then the third one is also.

Advanced AI Techniques / 2. Markov Equivalence and DAG patterns

```
dag-pattern \((G=(V, E))\) :
\(\tau:=\) topological-edge-ordering \((G)\)
\(E_{\text {irr }}:=\emptyset\)
\(E_{\text {rev }}:=\emptyset\)
\(E_{\text {rest }}:=E\)
\(\underline{\text { while }} E_{\text {rest }} \neq \emptyset \underline{\text { do }}\)
Let \((y, z) \in E_{\text {rest }}\) with \(\tau^{-1}(y, z)\) minimal
    [label pa(z):]
        if \(\exists(x, y) \in E_{\text {irr }}\) with \((x, z) \notin E\)
            \(E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid x^{\prime} \in \operatorname{pa}(z)\right\}\)
        else
            \(E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, y\right) \in E_{\text {irr }}\right\}\)
            if \(\exists(x, z) \in E\) with \(x \notin\{y\} \cup \mathrm{pa}(y)\)
                \(E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, z\right) \in E_{\text {rest }}\right\}\)
            else
                \(E_{\text {rev }}:=E_{\text {rev }} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, z\right) \in E_{\text {rest }}\right\}\)
            \(\underline{f}\)
            fi
            \(E_{\text {rest }}:=E \backslash E_{\text {irr }} \backslash E_{\text {rev }}\)
        od
        \(\underline{\text { return }} \bar{G}:=\left(V, E_{\text {irr }} \cup\left\{\{v, w\} \mid(v, w) \in E_{\text {rev }}\right\}\right)\)
```

a) $x^{\prime}=y$ :

b) $x^{\prime} \neq y$ : case 1) $x^{\prime}$ and $y$ not adjacent:

case 2) $x^{\prime}$ and $y$ adjacent:

dag-pattern $(G=(V, E))$ :
$\tau:=$ topological-edge-ordering $(G)$
$E_{\text {irr }}:=\emptyset$
$E_{\text {rev }}:=\emptyset$
$E_{\text {rest }}:=E$
while $E_{\text {rest }} \neq \emptyset \underline{\text { do }}$
Let $(y, z) \in E_{\text {rest }}$ with $\tau^{-1}(y, z)$ minimal
[label $\mathrm{pa}(z):]$
if $\exists(x, y) \in E_{\text {irr }}$ with $(x, z) \notin E$ $E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid x^{\prime} \in \operatorname{pa}(z)\right\}$
else
$E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, y\right) \in E_{\text {irr }}\right\}$
if $\exists(x, z) \in E$ with $x \notin\{y\} \cup \mathrm{pa}(y)$

$$
E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, z\right) \in E_{\text {rest }}\right\}
$$

else

$$
E_{\mathrm{rev}}:=E_{\mathrm{rev}} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, z\right) \in E_{\mathrm{rest}}\right\}
$$

fi

## fi

case 1) $(y, z)$ is irreversible:

case 2) $(y, z)$ is reversible:

$E_{\text {rest }}:=E \backslash E_{\text {irr }} \backslash E_{\text {rev }}$
od
$\underline{\text { return }} \bar{G}:=\left(V, E_{\text {irr }} \cup\left\{\{v, w\} \mid(v, w) \in E_{\text {rev }}\right\}\right)$

Wolfram Burgard, Luc de Raedt, Bernhard Nebel, Lars Schmidt-Thieme, Institute for Computer Science, University of Freiburg, Germany, Course on Advanced AI Techniques, winter term 2004
Advanced AI Techniques / 2. Markov Equivalence and DAG patterns

```
dag-pattern \((G=(V, E))\) :
\(\tau:=\) topological-edge-ordering \((G)\)
    \(E_{\text {irr }}:=\emptyset\)
    \(E_{\text {rev }}:=\emptyset\)
    \(E_{\text {rest }}:=E\)
    while \(E_{\text {rest }} \neq \emptyset \underline{\text { do }}\)
            Let \((y, z) \in E_{\text {rest }}\) with \(\tau^{-1}(y, z)\) minimal
            [label \(\mathrm{pa}(z):]\)
            if \(\exists(x, y) \in E_{\text {irr }}\) with \((x, z) \notin E\)
            \(E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid x^{\prime} \in \operatorname{pa}(z)\right\}\)
            else
                \(E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, y\right) \in E_{\text {irr }}\right\}\)
                if \(\exists(x, z) \in E\) with \(x \notin\{y\} \cup \mathrm{pa}(y)\)
                \(E_{\text {irr }}:=E_{\text {irr }} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, z\right) \in E_{\text {rest }}\right\}\)
            else
                \(E_{\text {rev }}:=E_{\text {rev }} \cup\left\{\left(x^{\prime}, z\right) \mid\left(x^{\prime}, z\right) \in E_{\text {rest }}\right\}\)
                fi
            fi
            \(E_{\text {rest }}:=E \backslash E_{\text {irr }} \backslash E_{\text {rev }}\)
    od
    \(\underline{\text { return }} \bar{G}:=\left(V, E_{\text {irr }} \cup\left\{\{v, w\} \mid(v, w) \in E_{\text {rev }}\right\}\right)\)
```

a) $x^{\prime}=x$ :

b) $x^{\prime} \neq x$ : case 1) $\left(x^{\prime}, y\right)$ irreversible

case 2) $\left(x^{\prime}, y\right)$ is reversible:


## 1. Checking Probalistic Independencies

## 2. Markov Equivalence and DAG patterns

## 3. PC Algorithm

[CGH97] Enrique Castillo, José Manuel Gutiérrez, and Ali S. Hadi. Expert Systems and Probabilistic Network Models. Springer, New York, 1997.
[Chi95] D. Chickering. A transformational characterization of equivalent bayesian network structures. In Philippe Besnard and Steve Hanks, editors, Proceedings of the Eleventh Conference on Uncertainty in Artificial Intelligence, pages 87-98. Morgan Kaufmann, 1995.
[Mee95] C. Meek. Causal inference and causal explanation with background knowledge. In Proceedings of Eleventh Conference on Uncertainty in Artificial Intelligence, Montreal, QU, pages 403-418. Morgan Kaufmann, August 1995.
[PGV90] J. Pearl, D. Geiger, and T. S. Verma. The logic of influence diagrams. In R. M. Oliver and J. Q. Smith, editors, Influence Diagrams, Belief Networks and Decision Analysis. Wiley, Sussex, 1990. (a shorter version originally appeared in Kybernetica, Vol. 25, No. 2, 1989).
[SGS00] Peter Spirtes, Clark Glymour, and Richard Scheines. Causation, Prediction, and Search. MIT Press, 2 edition, 2000.

