Advanced AI Techniques

I. Bayesian Networks / 4. Constrained-based Structure Learning (1/2)

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Advanced AI Techniques

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1. Checking Probabilistic Independencies

2. Markov Equivalence and DAG patterns

3. PC Algorithm

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Types of Methods for Structure Learning

There are three types of structure learning algorithms for Bayesian networks:

1. **constrained-based learning** (e.g., PC),
2. **searching with a target function** (e.g., K2),
3. **hybrid methods** (e.g., sparse candidate).

Computing the Skeleton

Lemma 1 (Edge Criterion). *Let $G := (V, E)$ be a DAG and $X, Y \in V$. Then it is equivalent:*

(i) X and Y cannot be separated by any $\mathcal{Z}$, i.e.,

$$\neg I_G(X, Y \mid \mathcal{Z}) \quad \forall \mathcal{Z} \subseteq V \setminus \{X, Y\}$$

(ii) There is an edge between X and Y, i.e.,

$$(X, Y) \in E \text{ or } (Y, X) \in E$$

Definition 1. Any $\mathcal{Z} \subseteq V \setminus \{X, Y\}$ with $I_G(X, Y \mid \mathcal{Z})$ is called a **separator of** X **and** Y.

$$\mathrm{Sep}(X, Y) := \{\mathcal{Z} \subseteq V \setminus \{X, Y\} \mid I_G(X, Y \mid \mathcal{Z})\}$$

Computing the Skeleton / Separators

```
separators-basic(set of variables V, independency relation I) :
Allocate S : P²(V) → P(V) ∪ {none}
for {X, Y} ⊆ V do
    S({X, Y}) := none
    for T ⊆ V \ {X, Y} do
        if I(X, Y | T)
            S({X, Y}) := T
            break
        fi
    od
od
return S
```

Figure 1: Compute a separator for each pair of variables.

Example / 1/3 – Computing the Skeleton

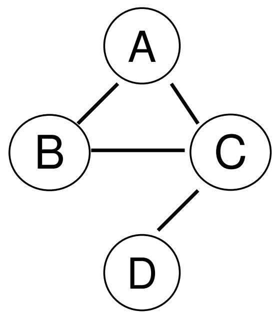
Let I be the following independency structure:

$$I(A, D \,|\, C), \quad I(A, D \,|\, \{C, B\}), \quad I(B, D)$$

Then we can compute the following separators:

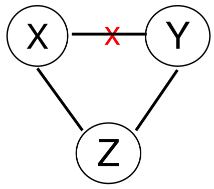
$$S(A, B) := \text{none}$$
$$S(A, C) := \text{none}$$
$$S(A, D) := \{C\}$$
$$S(B, C) := \text{none}$$
$$S(B, D) := \emptyset$$
$$S(C, D) := \text{none}$$

Thus, the skeleton of the Bayesian Network representing I looks like



Computing the V-structure

Lemma 2 (Uncoupled Head-to-head Meeting Criterion). *Let $G := (V, E)$ be a DAG, $X, Y, Z \in V$ with*



Then it is equivalent:

(i) $X \rightarrow Z \leftarrow Y$ is an uncoupled head-to-head meeting, i.e.,

$$(X, Z), (Y, Z) \in E, (X, Y), (Y, X) \notin E$$

(ii) Z is not contained in any separator of X and Y, i.e.,

$$Z \notin S \quad \forall S \in \text{Sep}(X, Y)$$

(iii) Z is not contained in at least one separator of X and Y, i.e.,

$$Z \notin S \quad \exists S \in \text{Sep}(X, Y)$$

Computing Skeleton and V-structure

vstructure(set of variables V, independency relation I) :
$S :=$ *separators*(V, I)
$G := (V, E)$ with $E := \{\{X, Y\} \mid S(\{X, Y\}) = \text{none}\}$
for $X, Y, Z \in V$ with $X - Z - Y, X \not- Y$ **do**
    if $Z \notin S(X, Y)$
        orient $X - Z - Y$ as $X \rightarrow Z \leftarrow Y$
    fi
od
return G

Figure 2: Compute skeleton and v-structure.

learn-structure-pc(set of variables V, independency relation I) :
$G :=$ *vstructure*(V, I)
saturate(G)
return G

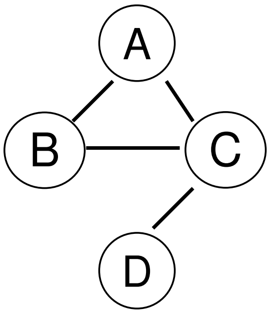
Figure 3: Learn structure of a Bayesian Network (SGS/PC algorithm, [SGS00]).

Example / 2/3 – Computing the V-Structure

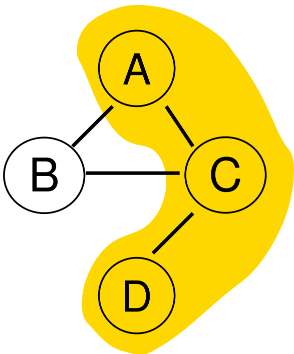
Separators:

$$S(A,B) := \text{none}$$
$$S(A,C) := \text{none}$$
$$S(A,D) := \{C\}$$
$$S(B,C) := \text{none}$$
$$S(B,D) := \emptyset$$
$$S(C,D) := \text{none}$$

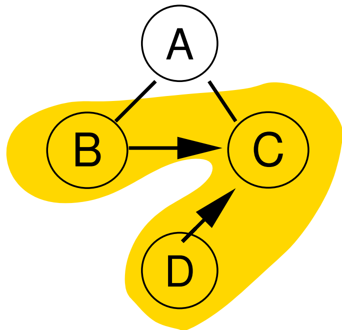
Skeleton:



Checking A–C–D:

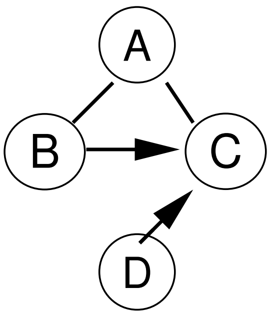


Checking B–C–D:

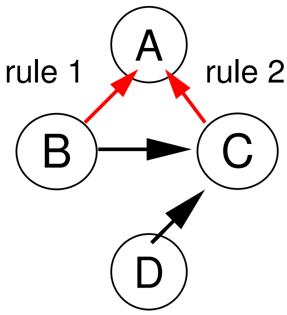


Example / 3/3 – Saturating

Skeleton and v-structure:



Saturating:



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Number of Independency Tests

Let there be n variables.
For each of the $\binom{n}{2}$ pairs of variables, there are 2^{n-2} candidates for possible separators.

$$\text{number of } I\text{-tests} = \binom{n}{2} 2^{n-2}$$

Example: $n = 4$:

$$\binom{n}{2} 2^{n-2} = \binom{4}{2} 2^2 = 6 \cdot 4 = 24$$

If we start with small separators and stop once a separator has been found, we still have to check

$$4 \cdot (1 + 2 + 1) + 1 \cdot (1 + 2) + 1 \cdot 1 = 20$$

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Number of Independency Tests

Can we reduce the number of tests for a given pair of variable by reusing results for other pairs of variables?

Lemma 3. *Let $G := (V, E)$ be a DAG and $X, Y \in V$ separated. Then*

$$I(X, Y \mid \text{pa}(X)) \quad \textit{or} \quad I(X, Y \mid \text{pa}(Y))$$

As we do not know directions of edges at the the skeleton recovery step, we use the weaker result:

$$I(X, Y \mid \text{fan}(X)) \quad \text{or} \quad I(X, Y \mid \text{fan}(Y))$$

Computing the Skeleton / Separators

separators-remove-edges(separator map S, skeleton graph G, independency relation I)
$i := 0$
while $\exists X \in V : |\operatorname{fan}_G(X)| > i$ **do**
    for $\{X,Y\} \in E$ with $\operatorname{fan}_G(X)| > i$ or $\operatorname{fan}_G(Y)| > i$ **do**
        for $T \in \mathcal{P}^i(\operatorname{fan}_G(X) \setminus \{Y\}) \cup \mathcal{P}^i(\operatorname{fan}_G(Y) \setminus \{X\})$ **do**
            if $I(X, Y \mid T)$
                $S(\{X,Y\}) := T$
                $E := E \setminus \{\{X,Y\}\}$
                break
            fi
        od
    od
    $i := i + 1$
od
return S

separators-interlaced(set of variables V, independency relation I) :
Allocate $S : \mathcal{P}^2(V) \rightarrow \mathcal{P}(V) \cup \{\text{none}\}$
$S(\{X,Y\}) := \text{none} \quad \forall \{X,Y\} \subseteq V$
$G := (V, E)$ with $E := \mathcal{P}^2(V)$
separators-remove-edges(S, G, I)
return S

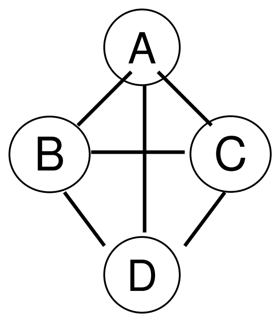
Figure 4: Compute a separator for each pair of variables.

Example / Computing the Separators (1/3)

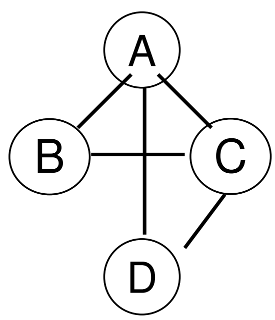
$$I(A, D \mid C), \quad I(A, D \mid \{C, B\}), \quad I(B, D)$$

$i = 0$:
A, B, $T = \emptyset$: —
C, $T = \emptyset$: —
D, $T = \emptyset$: —
B, C, $T = \emptyset$: —
D, $T = \emptyset$: $D(\{B, D\}) = \emptyset$
C, D, $T = \emptyset$: —

initial graph:



after update for B, D:



Example / Computing the Separators (2/3)

$$I(A, D \mid C), \quad I(A, D \mid \{C, B\}), \quad I(B, D)$$

$i = 1:$

$A,\ B,\ T = \{C\}, \{D\}$: —

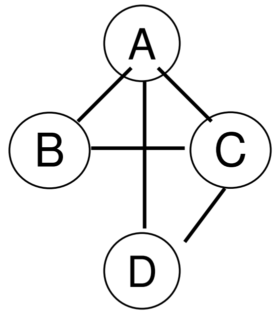
$C,\ T = \{B\}, \{D\}$: —

$D,\ T = \{B\}, \{C\}$: $S(\{A, D\}) = \{C\}$

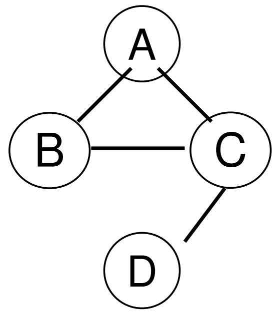
$B,\ C,\ T = \{A\}, \{D\}$: —

$C,\ D,\ T = \{A\}, \{B\}$: —

after update for B, D:



after update for A, D:



Example / Computing the Separators (3/3)

$$I(A, D \mid C), \quad I(A, D \mid \{C, B\}), \quad I(B, D)$$

$i = 2:$

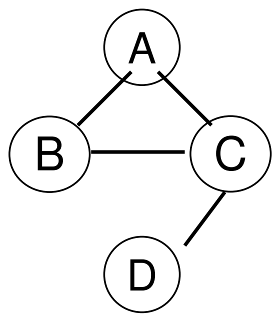
$A,\ C,\ T = \{B, D\}$: —

$B,\ C,\ T = \{A, D\}$: —

$C,\ D,\ T = \{A, B\}$: —

total: 19 I-tests.

after update for A, D:



Algorithms – SGS vs. PC

SGS/PC with `separators-basic` is called **SGS algorithm** ([SGS00], 1990).

SGS/PC with `separators-interlaced` is called **PC algorithm** ([SGS00], 1991).

Implementations are available:

- in Tetrad
  `http://www.phil.cmu.edu/projects/tetrad/`
  (class files & javadocs, no sources)

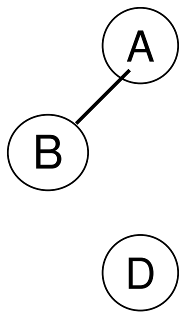
- in Hugin (commercial).

Another Example

Let I be the following independency structure:

$$I(A, D \,|\, B), \quad I(B, D)$$

PC computes the following DAG pattern:



But this is not even a representation of I, as it implies

$$I_G(A, D \,|\, \emptyset)$$

Representation and Faithfulness Tests

PC computes the DAG pattern of an independency relation

if there exists one at all !

Remember: not any independency relation has a faithful DAG representation.

But how do we know if an independency relation has a faithful DAG representation?

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Representation and Faithfulness Tests

There is no easy way to decide if a given independency relation has a faithful DAG representation.

So just check ex-post if the DAG pattern we have found is a faithful representation.

Check:

1. compute all $I_G(X, Y \mid \mathcal{Z})$ and check if $I(X, Y \mid \mathcal{Z})$ (representation),

2. check for each $I(X, Y \mid \mathcal{Z})$ if $I_G(X, Y \mid \mathcal{Z})$ (faithfulness).

As there is no easy way to enumerate $I_G(X, Y \mid \mathcal{Z})$ for a DAG pattern G directly, we draw a representative H and then enumerate $I_H(X, Y \mid \mathcal{Z})$ (remember that $I_H = I_G$).

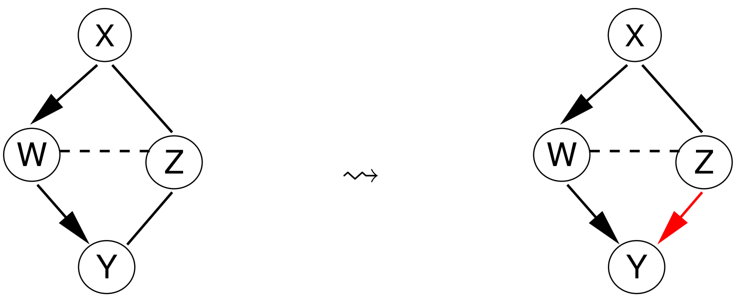
Draw a Representative of a DAG pattern

```
draw-representative(DAG pattern G) :
saturate(G)
while G has unoriented edges do
        draw an edge from G an orient it arbitrarily
        saturate(G)
od
return G
```

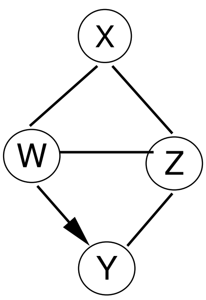
Figure 5: Draw a representative of a DAG pattern.

Draw a Representative of a DAG pattern

Here, rule 4 is necessary in `saturate`.

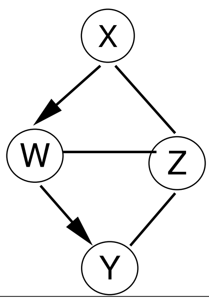


Start with DAG pattern



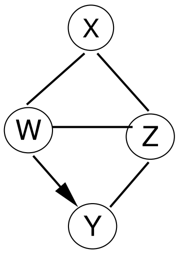
that is already saturated

and choose as next edge X–W and orient it as $X \to W$. Then rule 4 has to be applied to saturate the resulting DAG pattern

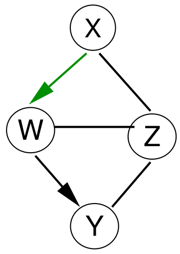


Draw a Representative of a DAG pattern / Example

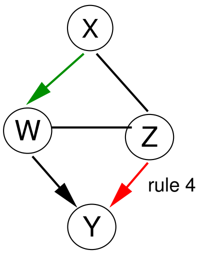
step 1a: saturate.



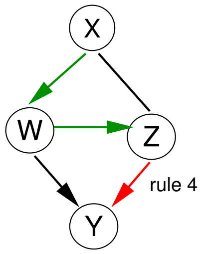
step 1b: orient any unoriented edge:



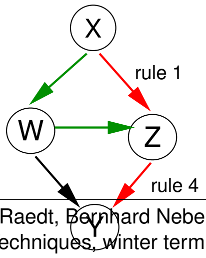
step 2a: saturate.



step 2b: orient any unoriented edge:



step 3a: saturate.



done.

Representation and Faithfulness Tests

If $I = I_p$ the probabilistic independency relation of a JPD p, then for (1) it suffices to check the Markov property, i.e.,

$$\text{for all } X \text{ check if } I_p(X, \mathrm{nondesc}(X) \setminus \mathrm{pa}(X) \,|\, \mathrm{pa}(X))$$

It even suffices to check for any topological ordering $\sigma = (X_1, \ldots, X_n)$ if

$$I_p(\sigma(i), \sigma(\{1, \ldots, i-1\}) \setminus \mathrm{pa}(\sigma(i)) \,|\, \mathrm{pa}(\sigma(i)))$$

A Third Method to Compute Separators

`separators-interlaced` computes separators top-down by

- starting with a complete graph and then
- successively thining the graph.

Therefore, we have to start checking with lots of candidates for possible separators.

A Third Method to Compute Separators

separators-add-edges(separator map S, skeleton graph G, independency relation I) :
$S(\{X,Y\}) := \text{argmin}_{T\subseteq \text{fan}_G(X), T\subseteq \text{fan}_G(Y)}\, g(X,Y,T) \quad \forall \{X,Y\}\in \mathcal{P}^2(V)$
$\{X_0,Y_0\} := \text{argmax}_{\{X,Y\}\in\mathcal{P}^2(V)}\, g(X,Y,S(\{X,Y\}))$
while $\neg I(X_0,Y_0 \,|\, S(\{X_0,Y_0\}))$ **do**
    $E := E \cup \{\{X_0,Y_0\}\}$
    $S(\{X_0,Y_0\}) :=$ none
    $S(\{X,Y\}) := \text{argmin}_{T\subseteq \text{fan}_G(X), T\subseteq \text{fan}_G(Y)}\, g(X,Y,T) \quad \forall \{X,Y\}\in \mathcal{P}^2(V)\setminus E, X\in\{X_0,Y_0\}$
    $\{X_0,Y_0\} := \text{argmax}_{\{X,Y\}\in\mathcal{P}^2(V)\setminus E}\, g(X,Y,S(\{X,Y\}))$
od
return S

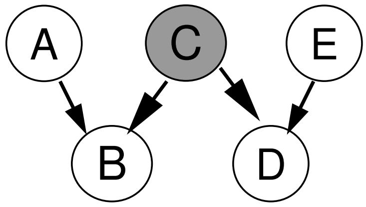
separators-bottumup(set of variables V, independency relation I) :
Allocate $S : \mathcal{P}^2(V) \to \mathcal{P}(V) \cup \{\text{none}\}$
$G := (V,E)$ with $E := \emptyset$
separators-add-edges(S,G,I)
separators-remove-edges(S,G,I)
return S

Figure 6: Compute a separator for each pair of variables [TASB03].

Embedded Faithfulness

Let I be the following independency structure:

$$I(A, D), \quad I(A, E), \quad I(A, E \mid B), \quad I(A, E \mid D), \quad I(B, E)$$



Assume C to be hidden.

d-separations between variables A,B,D, and E:

$$I(A, D), \quad I(A, E), \quad I(A, E \mid B), \quad I(A, E \mid D), \quad I(B, E)$$

Embedded Faithfulness

Definition 2. Let I be an independency relation on the variables V and G be a DAG with vertices $W \supseteq V$.

I **is embedded in** G, if all independency statements entailed by G between variables from V hold in I:

$$I_G(\mathcal{X}, \mathcal{Y} \mid \mathcal{Z}) \Rightarrow I(\mathcal{X}, \mathcal{Y} \mid \mathcal{Z}) \quad \forall \mathcal{X}, \mathcal{Y}, \mathcal{Z} \subseteq V$$

I **is embedded faithfully in** G, if the independency statements entailed by G are exactly I:

$$I_G(\mathcal{X}, \mathcal{Y} \mid \mathcal{Z}) \Leftrightarrow I(\mathcal{X}, \mathcal{Y} \mid \mathcal{Z}) \quad \forall \mathcal{X}, \mathcal{Y}, \mathcal{Z} \subseteq V$$

Many independency relations w./o. faithful DAG representation can be embedded faithfully.

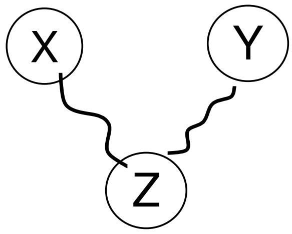
But not every independency relation can be embedded faithfully.

Embedded Faithfulness / Example

Let I be the independency relation [Nea03, ex. 2.13, p. 103]

$$I(X, Y), \quad I(X, Y \mid Z)$$

Assume, I can be embedded faithfully in a DAG G.



- As $\neg I(X, Z)$, there must be chain $X \sim Z$ w./o. head-to-head meetings.
- As $\neg I(Z, Y)$, there must be chain $Y \sim Z$ w./o. head-to-head meetings.

Now, concatenate both chains $X \sim Z \sim Y$:

- eihter $X \sim\!\rightarrow Z \leftarrow\!\sim Y$, and then the chain is not blocked by Z, i.e., not $I(X, Y \mid Z)$,
- or not $X \sim\!\rightarrow Z \leftarrow\!\sim Y$, and then the chain is not blocked by $\emptyset$, i.e., not $I(X, Y)$.

There are variants of the PC algorithm for finding faithful embeddings of a given independency relation:

- Causal Inference (CI) and
- Fast Causal Inference Algorithms (FCI; [SGS00])

See also [Nea03, ch. 10.2].

References

[Nea03] Richard E. Neapolitan. *Learning Bayesian Networks*. Prentice Hall, 2003.

[SGS00] Peter Spirtes, Clark Glymour, and Richard Scheines. *Causation, Prediction, and Search*. MIT Press, 2 edition, 2000.

[TASB03] I. Tsamardinos, C. F. Aliferis, A. Statnikov, and L. E. Brown. Scaling-up bayesian network learning to thousands of variables using local learning technique. Technical report, DSL TR-03-02, March 12, 2003, Vanderbilt University, Nashville, TN, USA, 2003.