# Some characterization of clique trees and their application to statistical inference

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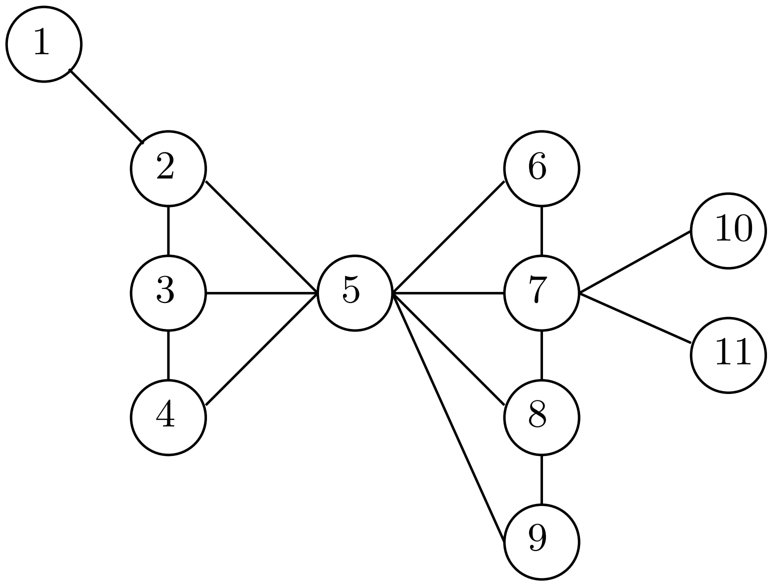
(Joint works with Hisayuki Hara and Satoshi Aoki)

# Contents

# Chordal graphs

- A graph is "chordal" if every circle of length $\geq 4$ has a chord

Example of a chordal graph



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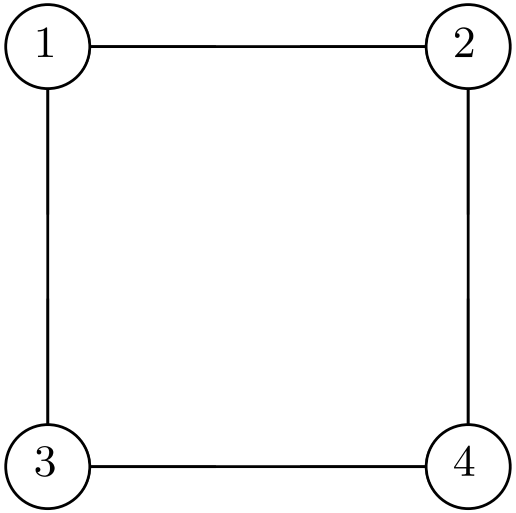
Example of non-chordal graph

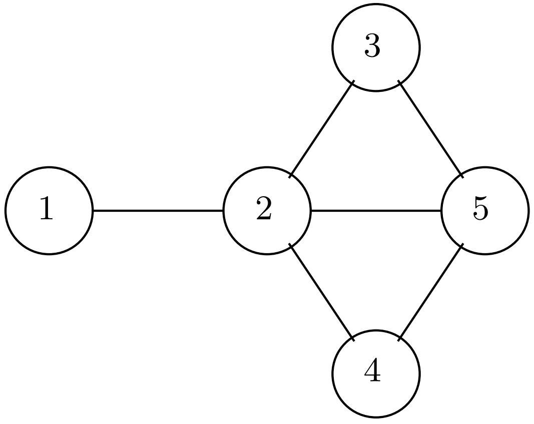


# Terminologies

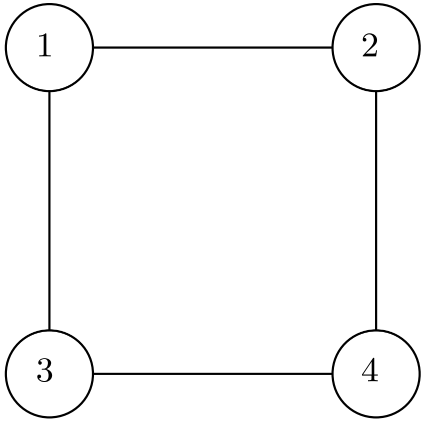
- clique ($\leftrightarrow$ face)
  the set of vertices which induces a complete subgraph
- maximal clique($\leftrightarrow$ facet)

# Minimal vertex separator

- Minimal vertex separator
  The minimal set of vertices which separates some pair of non-adjacent vertices
- A graph is chordal
  $\Leftrightarrow$ any minimal vertex separators induce cliques




$\mathcal{S} = \{\{2\}, \{2, 5\}\}$

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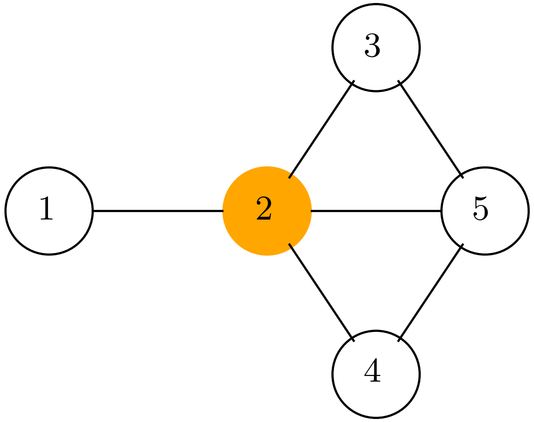


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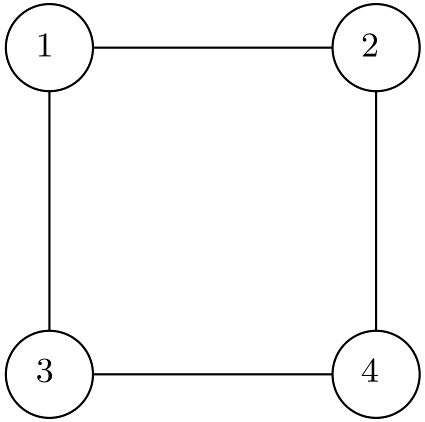


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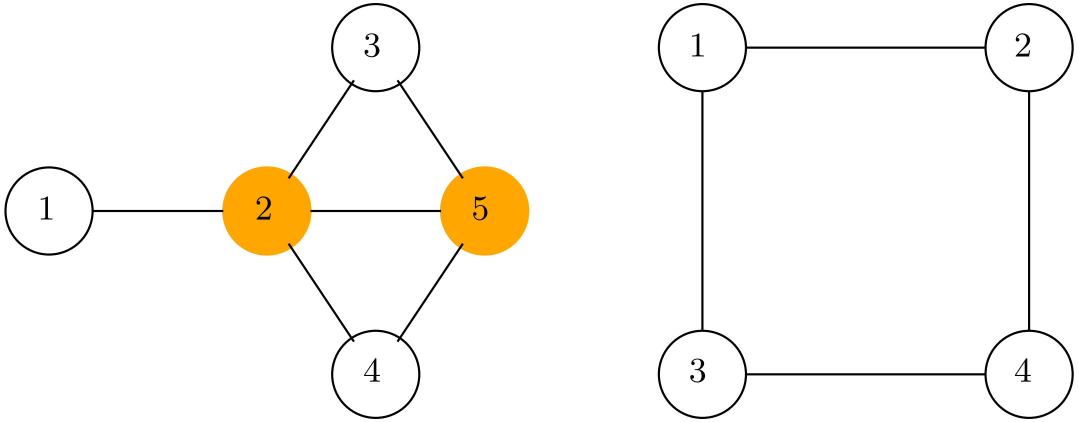


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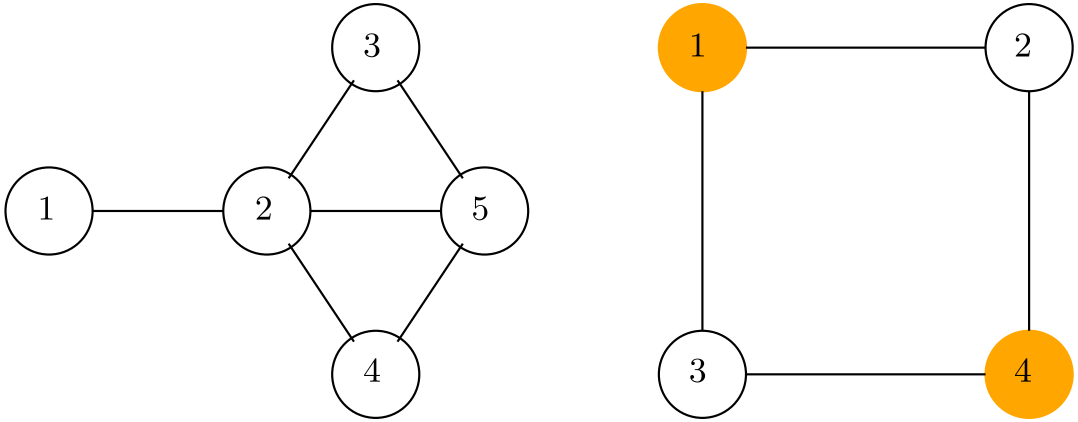


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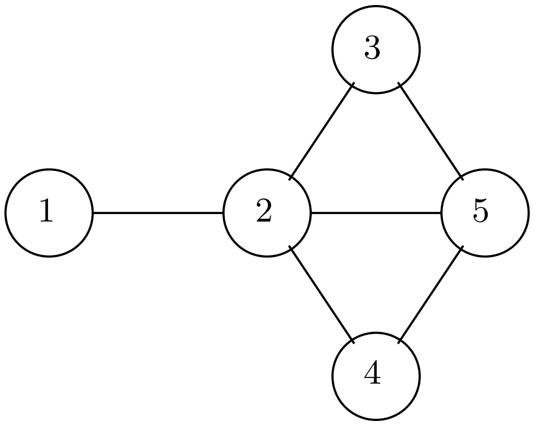


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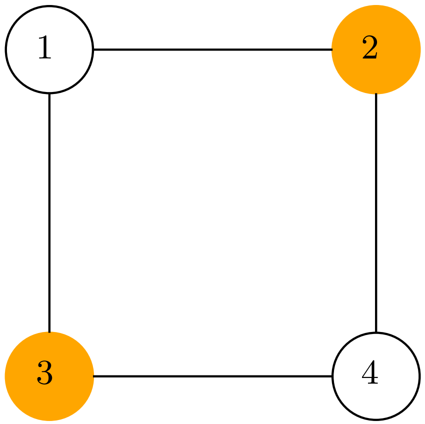


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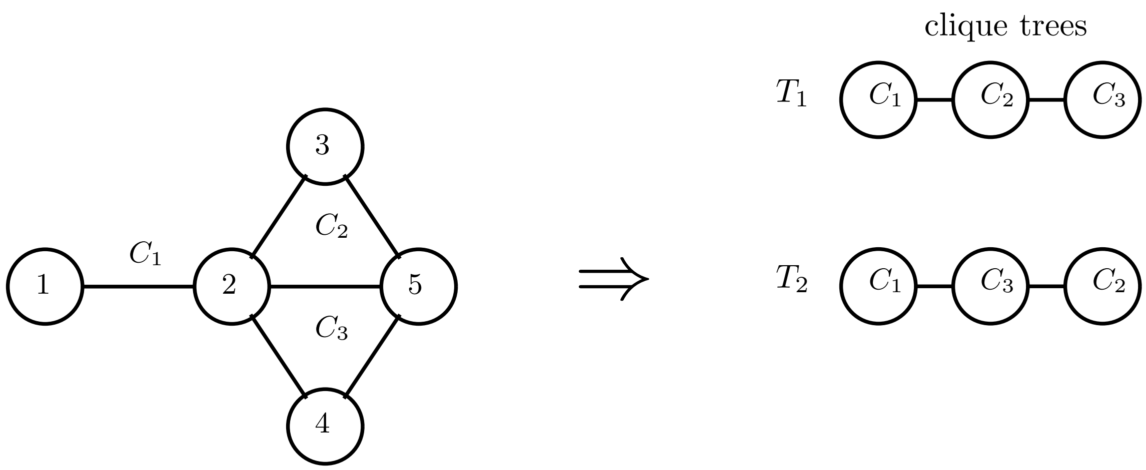
# Clique tree

- A clique tree $T = (\mathcal{C}, \mathcal{E})$
  $\forall C, \forall C' \in \mathcal{C}$ and any $C'' \in \mathcal{C}$ on the unique path in $T$ between $C$ and $C'$

$$C \cap C' \subseteq C'' \rightarrow \text{ junction property}$$



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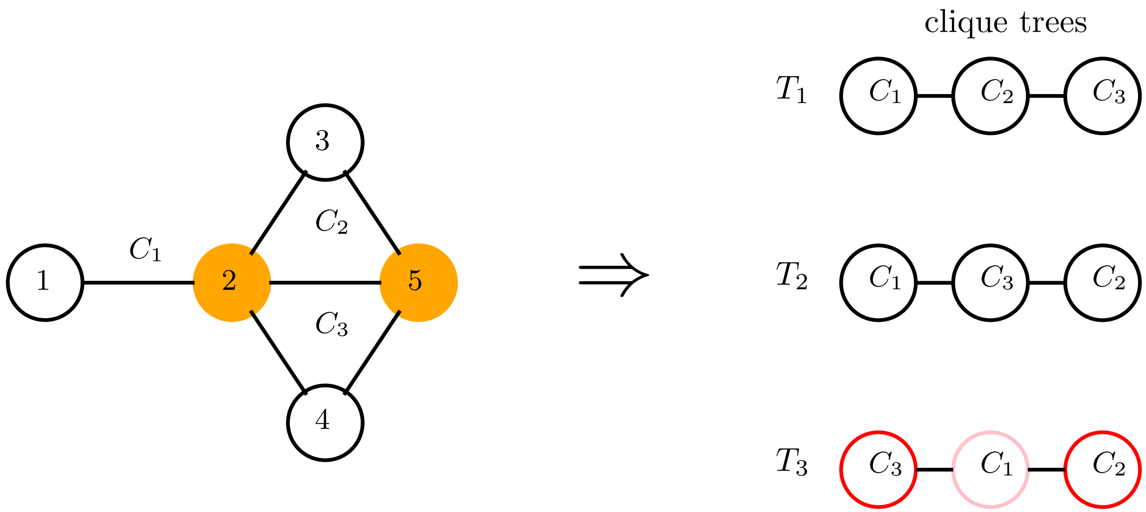

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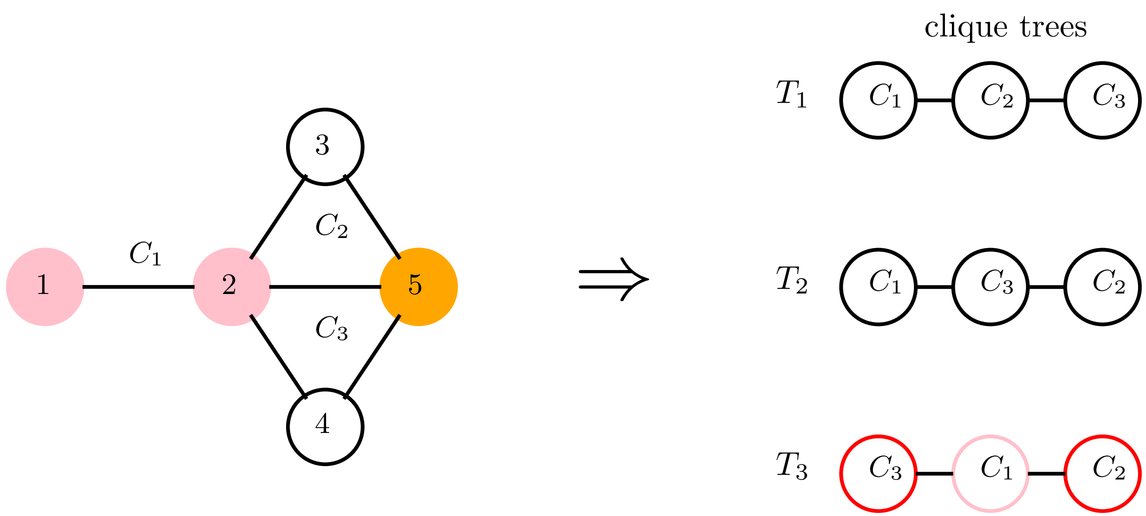

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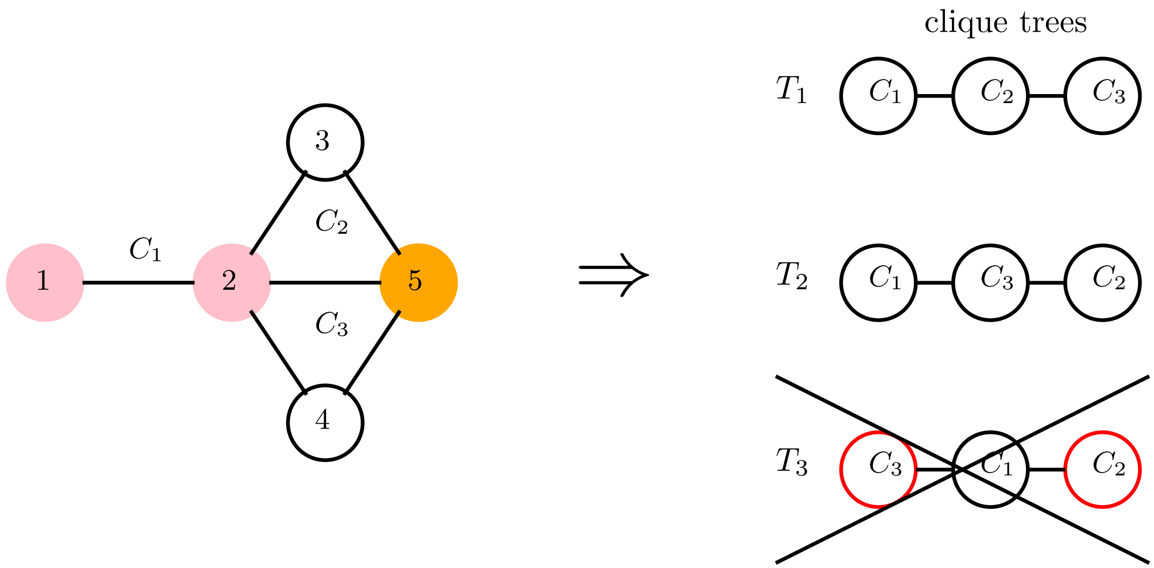



$T_3$ is not a clique tree

## Properties of clique trees

- A graph is chordal $\Leftrightarrow$ there exists a clique tree
- For $C$ and $C'$ s.t. $(C, C') \in \mathcal{E}$, $C \cap C' \in \mathcal{S}$
  $\longrightarrow$ every edge corresponds to m.v.s.
- $\mathcal{T}$ : the set of clique trees for a graph $G$
- In general clique trees are not uniquely defined (e.g. Hara and Takemura(2006))

# Properties of clique trees

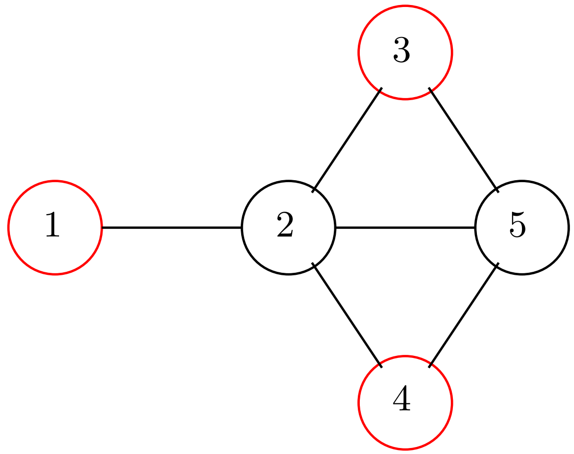
- Clique trees appear in many practical problem
  - Local computation of the marginal distribution in Baysian network (Junction tree algorithm)
  - Efficient computation of the MLE in the statistical model determined by “not” chordal graph
  - Calculation of a Markov basis for a decomposable model (Dobra(2004))

# Simplicial vertex and p.e.o.

- Simplicial vertex

  $v \in V$ s.t. $N_G(v)$ induces a clique

  (where $N_G(v)$ denotes the open adjacency set of $v$)



# Properties of simplicial vertex

For a maximal clique $C \in \mathcal{C}$, we denote by

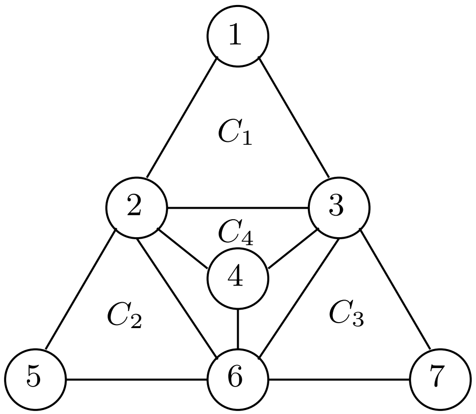
- $\mathrm{Simp}(C)$ : the set of simplicial vertices in $C$
- $\mathrm{Sep}(C)$ : the set of non-simplicial vertices in $C$
- $C = \mathrm{Simp}(C) \cup \mathrm{Sep}(C)$ $\longrightarrow$ disjoint union.
- a simplicial clique : $C \in \mathcal{C}$ s.t. $\mathrm{Simp}(C) \neq \emptyset$

# Boundary cliques and endpoints in clique trees

**Definition 1** (Boundary clique(Shibata(1988)))**.**
*A simplicial clique $C$ is a boundary clique if*

$$\exists C' \in \mathcal{C} \quad s.t. \quad \mathrm{Sep}(C) = C \cap C'.$$

*Then we call $C'$ dominant clique for $C$.*



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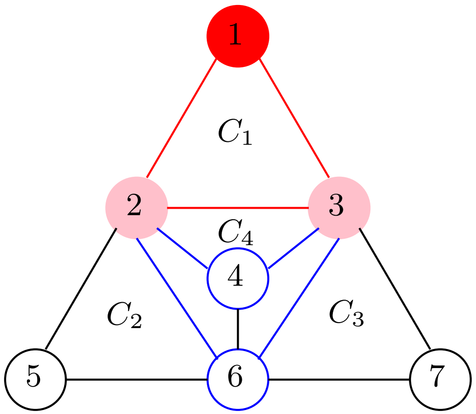


Boundary clique : $C_1$

Dominant clique : $C_4$

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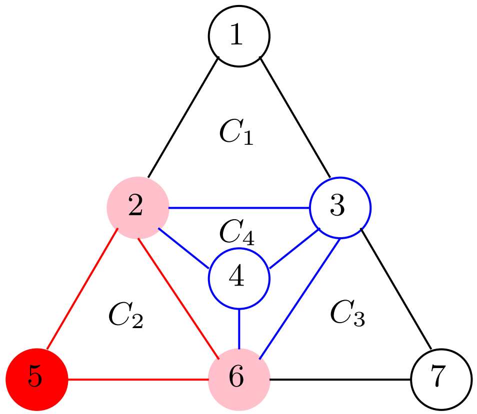


Boundary clique : $C_2$
Dominant clique : $C_4$

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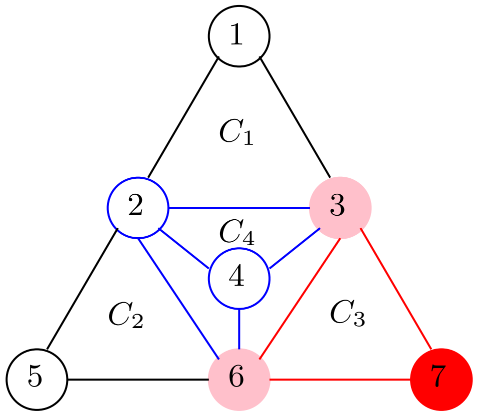


Boundary clique : $C_3$
Dominant clique : $C_4$

# Boundary cliques and endpoints in clique trees

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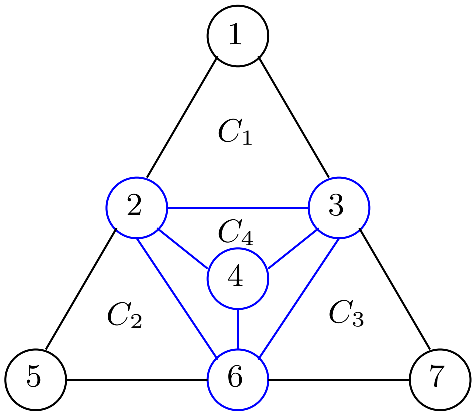


Dominant clique for all boundary cliques

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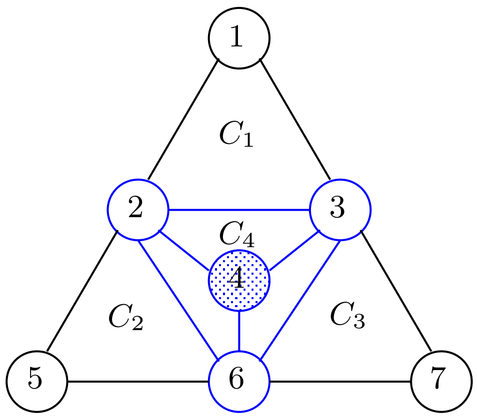


$\{4\}$ is a simplicial vertex, however,

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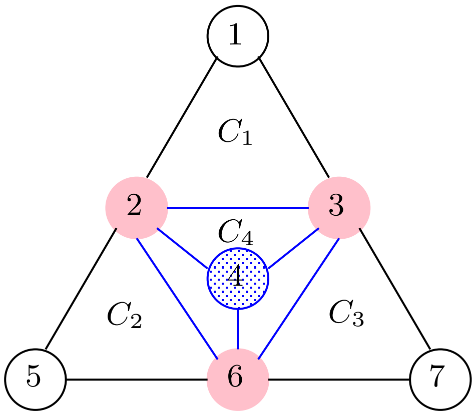


$\{4\}$ is a simplicial vertex, however,
there exists no dominant clique for this maximal clique

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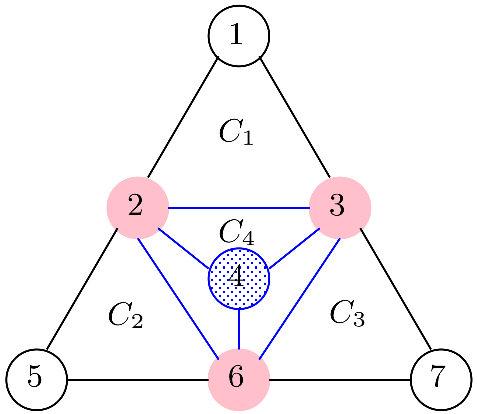



$\{4\}$ : weakly simplicial vertex

# Characterization of endpoints of clique tree

**Theorem**

$C$ is a boundary clique
$\Leftrightarrow \exists T \in \mathcal{T}$ s.t. $C \in \mathcal{C}$ is an endpoint of $T$

- $\Leftarrow$ : Shibata(1988)
- $\Rightarrow$ : Hara and Takemura(2006)

# Characterization of minimal Markov bases

- We consider Markov bases for decomposable models from the view point of minimality in terms of chordal graphs
  1. notations and terminologies
  2. a complete description of minimal Markov bases in terms of chordal graphs
  3. a necessary and sufficient condition that the minimal MB is unique
  4. The minimality of Dobra's MB

# Contingency table

- A survey on health care

  A. Drinking habit
  1. everyday, 2. a few times a week, 3. less than a times a week

  B. Smoking : 1. yes, 2. no

  C. Breakfast : 1. bread, 2. rice

  D. Exercise habit : 1. yes, 2. no

| | | $A_1$ | | $A_2$ | | $A_3$ | |
|---|---|---|---|---|---|---|---|
| | | $B_1$ | $B_2$ | $B_1$ | $B_2$ | $B_1$ | $B_2$ |
| $C_1$ | $D_1$ | 3 | 7 | 4 | 5 | 1 | 3 |
| | $D_2$ | 34 | 3 | 16 | 14 | 6 | 22 |
| $C_2$ | $D_1$ | 13 | 24 | 16 | 15 | 4 | 15 |
| | $D_2$ | 28 | 7 | 18 | 9 | 12 | 16 |

# Notation

- $\Delta$ : the set of variables $\Leftrightarrow \{A, B, C, D\}$
- $I_\delta$ : the number of levels of $\delta \in \Delta$
  $\Leftrightarrow I_A = 3,\ I_B = I_C = I_D = 2$
- $\mathcal{I}_\delta$ : the set of levels of $\delta$
  $\Leftrightarrow \mathcal{I}_A = \{A_1, A_2, A_3\}$
- a cell $\boldsymbol{i} \in \mathcal{I} = \prod_{\delta \in \Delta} \mathcal{I}_\delta$
  $\Leftrightarrow \boldsymbol{i} = (i_A, i_B, i_C, i_D) = (A_i, B_j, C_k, D_l)$
- $n(\boldsymbol{i})$ : the frequency of $\boldsymbol{i}$

# Notation

- a marginal cell for $D \subset \Delta$ :

  $\boldsymbol{i}_D \in \mathcal{I}_D = \prod_{\delta \in D} \mathcal{I}_\delta \Leftrightarrow \boldsymbol{i}_{AB} = (A_i, B_j)$

- a marginal frequency of $i_D$ :

  $n_D(\boldsymbol{i}_D) = \sum_{\boldsymbol{i}_{D^c} \in \mathcal{I}_{D^c}} n(\boldsymbol{i}_D, \boldsymbol{i}_{D^c})$

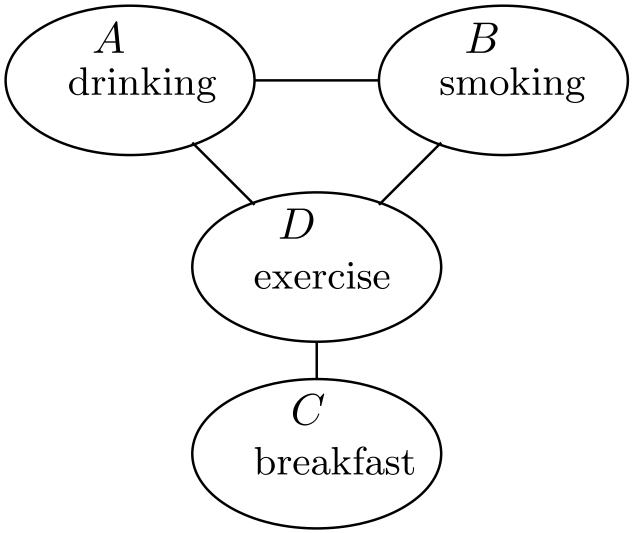
| | | $A_1$ | | $A_2$ | | $A_3$ | | |
|---|---|---|---|---|---|---|---|---|
| | | $B_1$ | $B_2$ | $B_1$ | $B_2$ | $B_1$ | $B_2$ | $\boldsymbol{i}_{CD}$ |
| $C_1$ | $D_1$ | 3 | 7 | 4 | 5 | 1 | 3 | 23 |
| | $D_2$ | 34 | 3 | 16 | 14 | 6 | 22 | 95 |
| $C_2$ | $D_1$ | 13 | 24 | 16 | 15 | 4 | 15 | 87 |
| | $D_2$ | 28 | 7 | 18 | 9 | 12 | 16 | 90 |
| | $\boldsymbol{i}_{AB}$ | 78 | 41 | 54 | 43 | 23 | 56 | 295 |

# Notations and terminologies

- the generating class :
  $\mathcal{D} = \{D_1, \ldots, D_r\}$, $D_r \subset \Delta$ satisfying
  - no inclusion relation among $D_j$'s
  - $\bigcup_{j=1}^{r} D_j = \Delta$
- $D_i \in \mathcal{D}$ : a generating set
- the independence graph for $\mathcal{D}$:
  $\mathcal{G}^{\mathcal{D}} = (\Delta, E^{\mathcal{D}})$
  $(\delta, \delta') \in E^{\mathcal{D}} \Leftrightarrow \delta, \delta' \in \exists D \in \mathcal{D}$

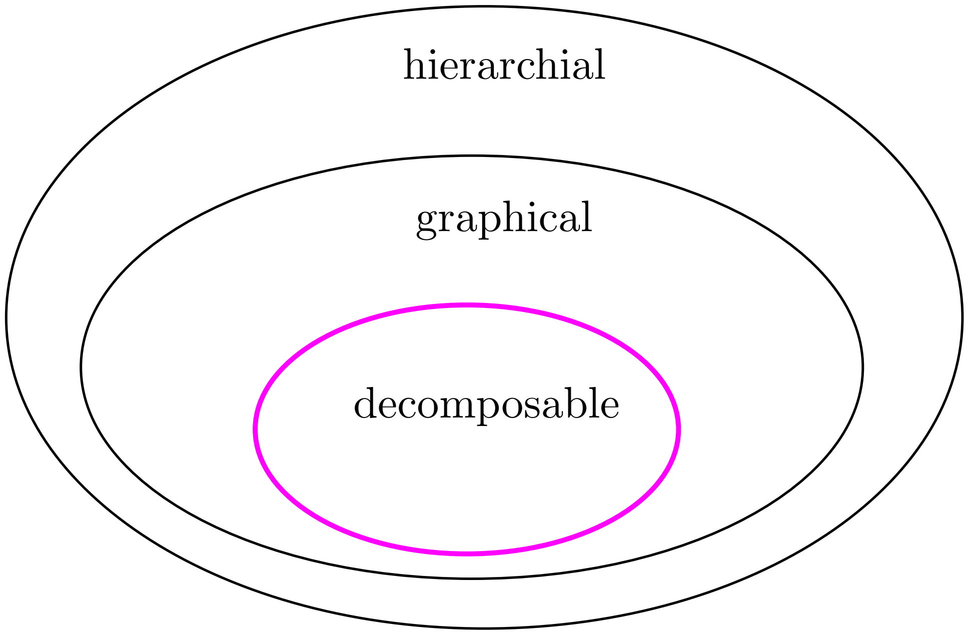
# Notations and terminologies

- $\mathcal{G}^{\mathcal{D}}$ with $\mathcal{D} = \{\{A, B, D\}, \{C, D\}\}$



# Decomposable models

- A decomposable model :
  $\mathcal{D}$ is the set of maximal clique of a chordal graph



# Notations and terminologies

- $\boldsymbol{b} = \{n_D(\boldsymbol{i}_D) \in \mathcal{I}_D, D \in \mathcal{D}\}$
- $\boldsymbol{b} = A\boldsymbol{n}$, $\quad A$ : the incidence matrix for $\mathcal{D}$
- $\boldsymbol{b}$-fiber : $\mathcal{F}_{\boldsymbol{b}} = \{\boldsymbol{n} \geq 0 \mid A\boldsymbol{n} = \boldsymbol{b}\}$
- $\mathcal{B}_{\text{nd}} = \{\boldsymbol{b} \mid |\mathcal{F}_{\boldsymbol{b}}| \geq 2\}$

# Degree two fibers

- $\boldsymbol{b} = \{n_D(\boldsymbol{i}_D) \in \mathcal{I}_D, D \in \mathcal{D}\}$
- deg $\boldsymbol{b}$ :

$$\deg \boldsymbol{b} = \sum_{D \in \mathcal{D}} \sum_{\boldsymbol{i}_D \in \mathcal{I}_D} n_D(\boldsymbol{i}_D)$$

- a degree two fiber : $\mathcal{F}_{\boldsymbol{b}}$ s.t. deg $\boldsymbol{b} = 2$

# Primitive move

- a move $\boldsymbol{z}$ : an integer array s.t. $\dim \boldsymbol{n} = \dim \boldsymbol{z}$ satisfying $A\boldsymbol{z} = 0$
- $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$, $\boldsymbol{z}^+ \geq 0$, $\boldsymbol{z}^- \geq 0$
- $\boldsymbol{z}^+ = \{z^+(\boldsymbol{i})\}_{\boldsymbol{i}\in\mathcal{I}}, \quad \boldsymbol{z}^- = \{z^-(\boldsymbol{i})\}_{\boldsymbol{i}\in\mathcal{I}}$
- Total frequencies of $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ are the same $z = \sum_{\boldsymbol{i}\in\mathcal{I}} z^+(\boldsymbol{i}) = \sum_{\boldsymbol{i}\in\mathcal{I}} z^-(\boldsymbol{i})$
- primitive move : a move $\boldsymbol{z}$ with $z = 2$

# Markov bases of decomposable models

- Dobra(2003), Hoşten and Sullivant(2002)
  For decomposable models there exists a Markov basis consisting of primitive moves
- Takemura and Aoki(2004)
  The union of sets of moves which connect each degree two fiber is a MB

$$\Downarrow$$

The clarification of the structure of deg 2 fibers $\mathcal{F}_{\boldsymbol{b}}$ s.t. $|\mathcal{F}_{\boldsymbol{b}}| \geq 2$ is essential

# Degree 2 fibers

- There exist at most two levels with positive one dimensional marginal
  $\Rightarrow$ it suffices to consider the table with
  $$I_\delta = 2, \quad \delta \in \Delta, \; \mathcal{I} = \{0,1\}^{|\Delta|}$$
- $\mathcal{I}_\delta = (i_\delta, i_\delta^*) = (0, 1), \quad i_\delta^* = 1 - i_\delta$
- $\boldsymbol{i}_{\Delta'}^* = (i_\delta^*)_{\{\delta \in \Delta'\}}$

# Nondegenerate variables

- $\boldsymbol{b}$ s.t. $\deg \boldsymbol{b} = 2$ is given
- $\delta \in \Delta$ is degenerate :
  there exist a unique levels $i_\delta$ s.t. $n_\delta(i_\delta) = 2$
  i.e. $n_\delta(i_\delta^*) = 0$
- $\delta \in \Delta$ is nondegenerate :
  $n_\delta(i_\delta) = n_\delta(i_\delta^*) = 1$
- $\bar{\Delta}_{\boldsymbol{b}}$ : the set of nondegenerate variable
- $\mathcal{G}(\bar{\Delta}_{\boldsymbol{b}})$ : The subgraph of $\mathcal{G}^{\mathcal{D}}$ induced by $\bar{\Delta}_{\boldsymbol{b}}$

# Structure of degree 2 fibers

**Theorem** (Hara, Aoki and Takemura(2007))

$\mathcal{F}_{\boldsymbol{b}}$ : a degree two fiber s.t. $\bar{\Delta}_{\boldsymbol{b}} \neq \emptyset$
$c(\boldsymbol{b})$ : # of connected components of $\mathcal{G}(\bar{\Delta}_{\boldsymbol{b}})$
Then

$$|\mathcal{F}_{\boldsymbol{b}}| = 2^{c(\boldsymbol{b})-1}$$

- This theorem holds for general hierarchical models
- $\forall \Delta' \subset \Delta$ s.t. $\mathcal{G}^{\mathcal{D}}(\Delta')$ is disconnected
  $\exists \boldsymbol{b} \in \mathcal{B}_{\text{nd}}$ s.t. $\bar{\Delta}_{\boldsymbol{b}} = \Delta'$

# Notations

- $(\boldsymbol{i})(\boldsymbol{j})$ : the element of degree 2 fiber s.t.

$$n(\boldsymbol{i}') = \begin{cases} 1 & \text{if } \boldsymbol{i}' = \boldsymbol{i} \text{ or } \boldsymbol{i}' = \boldsymbol{j} \\ 0 & \text{otherwise} \end{cases}$$

- Example

| | |
|---|---|
| 1 | 0 |
| 0 | 1 |

(00)(11)

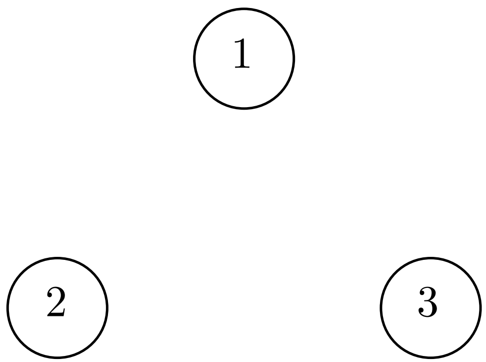
| | |
|---|---|
| 0 | 1 |
| 1 | 0 |

(01)(10)

# Example : 3way complete independence model

- $\mathcal{D} = \{\{1\},\{2\},\{3\}\}$
- Let $\boldsymbol{b} \in \mathcal{B}_{\text{nd}}$ satisfy $\bar{\Delta}_{\boldsymbol{b}} = \{1,2,3\}$
- $\bar{\Delta}_{\boldsymbol{b}} = \{1,2,3\}$

$$\Rightarrow \quad c(\boldsymbol{b}) = 3$$
$$\Rightarrow \quad |\mathcal{F}_{\boldsymbol{b}}| = 2^{(3-1)} = 4$$



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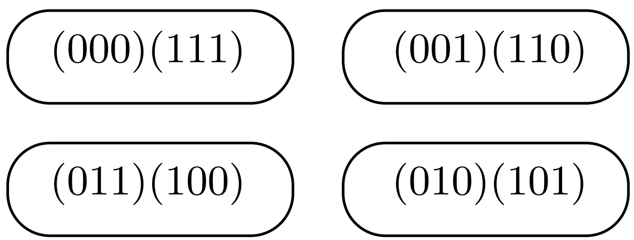
- $\bar{\Delta}_{\boldsymbol{b}} = \{1, 2, 3\}$
$$\Rightarrow \quad c(\boldsymbol{b}) = 3$$
$$\Rightarrow \quad |\mathcal{F}_{\boldsymbol{b}}| = 2^{(3-1)} = 4$$
- $\mathcal{F}_{\boldsymbol{b}} = \{(000)(111), (001)(110), (010)(101), (011)(100)\}$

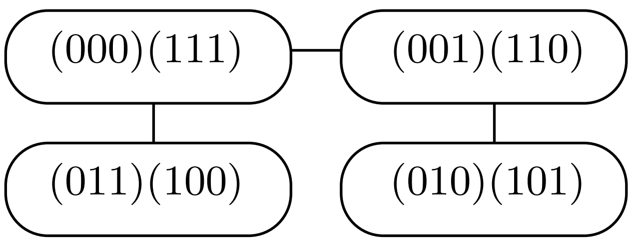
# Construction of a minimal MB

- For each fiber $\mathcal{F}_b$



# Construction of a minimal MB

- For each fiber $\mathcal{F}_{\boldsymbol{b}}$
- Construct a tree $\mathcal{T}_{\boldsymbol{b}} = (\mathcal{F}_{\boldsymbol{b}}, \mathcal{M}^0_{\boldsymbol{b}})$
  $\mathcal{M}^0_{\boldsymbol{b}}$ : a set of edges $\Leftrightarrow$ a set of moves



# Construction of a minimal MB

- For each fiber $\mathcal{F}_{\boldsymbol{b}}$
- Construct a tree $\mathcal{T}_{\boldsymbol{b}} = (\mathcal{F}_{\boldsymbol{b}}, \mathcal{M}^0_{\boldsymbol{b}})$
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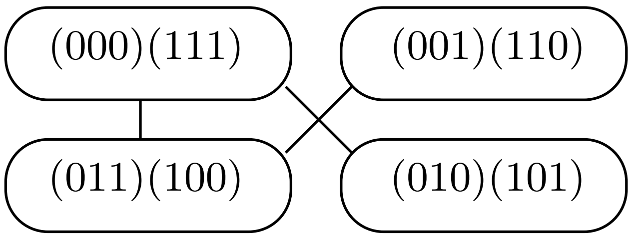

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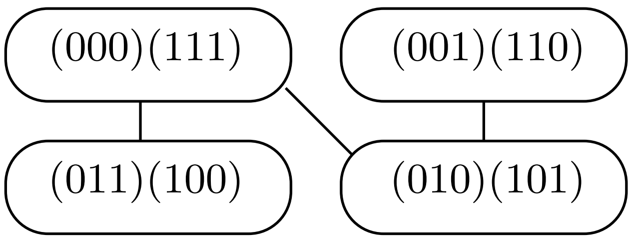

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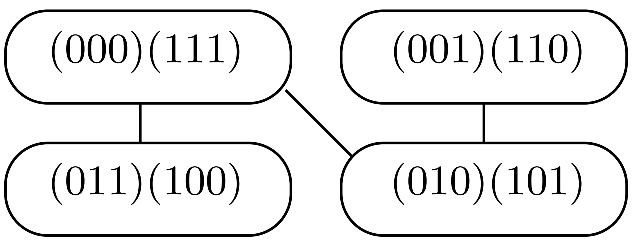
  $\mathcal{M}^0_{\boldsymbol{b}}$ : a set of edges $\Leftrightarrow$ a set of moves
- Dobra(2003), Takemura and Aoki(2004)
  $\mathcal{M}^0 = \bigcup_{\boldsymbol{b} \in \mathcal{B}_{\text{nd}}} \mathcal{M}^0_{\boldsymbol{b}} \quad \Rightarrow \quad$ a minimal MB



# The uniqueness of minimal MB

- $|\mathcal{F}_{\boldsymbol{b}}| = 2^{c(\boldsymbol{b})-1}$
- $c(\boldsymbol{b}) \geq 3 \quad \Rightarrow \quad \mathcal{T}_{\boldsymbol{b}}$ is not uniquely defined
  $\Rightarrow$ minimal MB are not unique
- In the case of decomposable models

> $c(\boldsymbol{b}) = 2$ for all $\boldsymbol{b} \in \mathcal{B}_{\mathrm{nd}}$
> $\Leftrightarrow$ minimal MB is unique

# The unique minimal Markov basis

**Lemma**(HAT(2007))

A decomposable model has the unique minimal MB if and only if the number of connected components in any induced subgraphs of $\mathcal{G}^{\mathcal{D}}$ is less than three.

# In terms of chordal graphs ...

**Theorem**(HAT(2007))

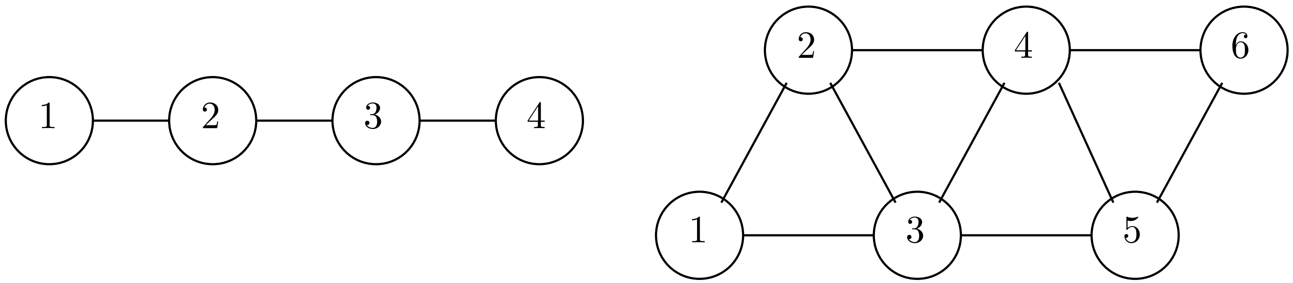
For a decomposable model, there exists the unique minimal MB if and only if

- $\mathcal{G}^{\mathcal{D}}$ has only two boundary cliques $D$, $D'$
- $D$ and $D'$ satisfy $D'' \subset D \cup D'$ for all $D'' \in \mathcal{D}$.

# Example

- $\mathcal{G}^{\mathcal{D}}$ with

$$\mathcal{D} = \{\{1,\ldots,r{-}1\},\{2,\ldots,r\},\ldots,\{r,\ldots,2r{-}2\}\}$$



# Markov basis for two maximal clique model

- $\mathcal{D} = \{D_1, D_2\}$
- $S = D_1 \cap D_2$ : the minimal vertex separator
- $D'_1 = D_1 \setminus S$, $D'_2 = D_2 \setminus S$
- $\mathcal{D}$ has the unique minimal MB $\mathcal{M}^0(D_1, D_2)$

$$\mathcal{M}^0(D_1, D_2)$$
$$= \{(i_{D'_1}\ j_S\ i_{D'_2})(i^*_{D'_1}\ j_S\ i^*_{D'_2}) - (i_{D'_1}\ j_S\ i^*_{D'_2})(i^*_{D'_1}\ j_S\ i_{D'_2}) \mid i_{D'_j} \in \mathcal{I}_{D'_j}, j_S \in \mathcal{I}_S\}$$

# Dobra's construction of Markov bases

- $\mathcal{D} = \{\{1\}, \{2\}, \{3\}, \{4\}\}$, $D_j = \{j\}$

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- $\mathcal{D} = \{\{1\}, \{2\}, \{3\}, \{4\}\}$, $D_j = \{j\}$
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  $V_{e_1} = \{1\}$, $V'_{e_1} = \{2, 3, 4\}$

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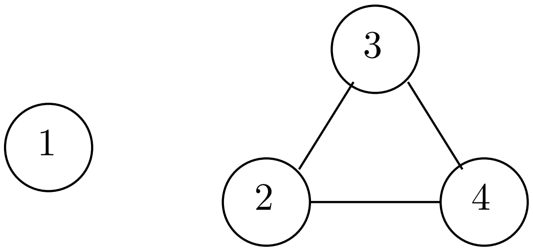
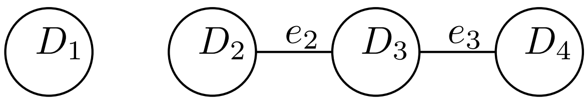



$$\Downarrow$$

$$\mathcal{M}^0(V_{e_1}, V'_{e_1})$$

$\mathcal{M}^0(V_{e_1}, V'_{e_1})$ : The set of primitive moves of the model $\mathcal{D}' = \{V_{e_1}, V'_{e_1}\}$

# Dobra's construction of Markov bases

- $\mathcal{D} = \{\{1\}, \{2\}, \{3\}, \{4\}\}$, $D_j = \{j\}$
- remove $e_2$
  $V_{e_2} = \{1, 2\}$, $V'_{e_2} = \{3, 4\}$

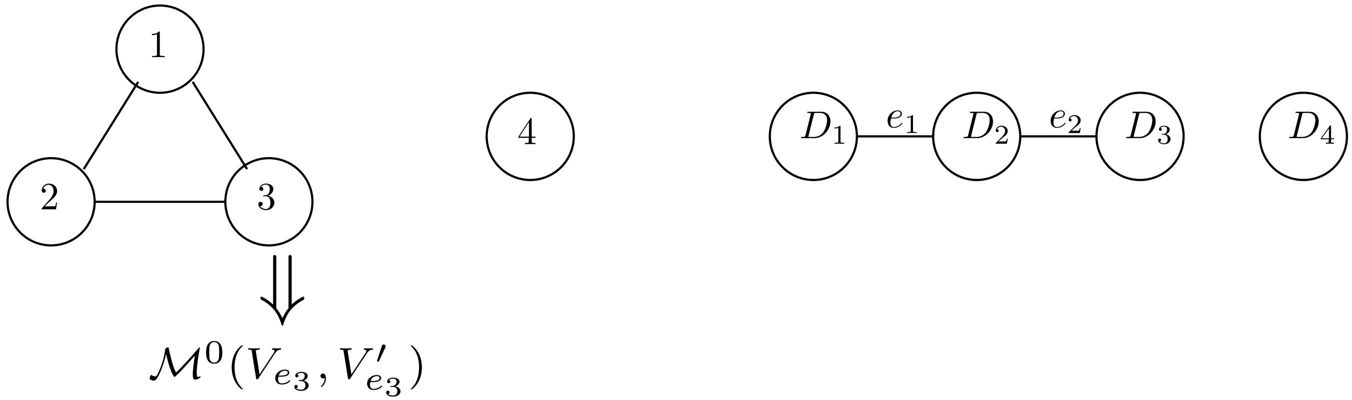

$$\Downarrow$$

$$\mathcal{M}^0(V_{e_2}, V'_{e_2})$$

$$\mathcal{M}^0(V_{e_1}, V'_{e_1}) \cup \mathcal{M}^0(V_{e_2}, V'_{e_2})$$

# Dobra's construction of Markov bases

- $\mathcal{D} = \{\{1\}, \{2\}, \{3\}, \{4\}\}$, $D_j = \{j\}$
- remove $e_3$
  $V_{e_3} = \{1, 2, 3\}$, $V'_{e_3} = \{4\}$




$\mathcal{M}^0(V_{e_1}, V'_{e_1}) \cup \mathcal{M}^0(V_{e_2}, V'_{e_2}) \cup \mathcal{M}^0(V_{e_3}, V'_{e_3}) \Rightarrow$ Markov basis

# Dobra's construction of Markov bases

- $\mathcal{D}$ : A decomposable model
  $\mathcal{T} = (\mathcal{D}, \mathcal{E})$ : A clique tree of $\mathcal{G}^{\mathcal{D}}$
- $\mathcal{T}_e = (\mathcal{D}_e, \mathcal{E}_e)$, $\mathcal{T}_e' = (\mathcal{D}_e', \mathcal{E}_e')$
  two subtree of $\mathcal{T}$ by removing $e \in \mathcal{E}$
- $V_e = \bigcup_{D \in \mathcal{D}_e} D$, $\quad V_e' = \bigcup_{D \in \mathcal{D}_e'} D$

$$\mathcal{M}^{\mathcal{T}} = \bigcup_e \mathcal{M}^0(V_e, V_e') \quad \Rightarrow \quad \text{Markov basis}$$

# Minimality of Dobra's Markov bases

**Theorem(HAT(2007))**

Dobra's MB $\mathcal{M}^{\mathcal{T}}$ is minimal if and only if the decomposable model has the unique minimal MB

- We can show that $\mathcal{M}^{\mathcal{T}}$ includes at least 4 moves for every $\mathcal{F}_{\boldsymbol{b}}$ s.t. $|\mathcal{F}_{\boldsymbol{b}}| = 4$

# Invariant Markov bases

- Suppose that move $z$ is included in a Markov basis.
- Then we also use a move where the levels of the moves are interchanged (invariance w.r.t. permutations of levels)

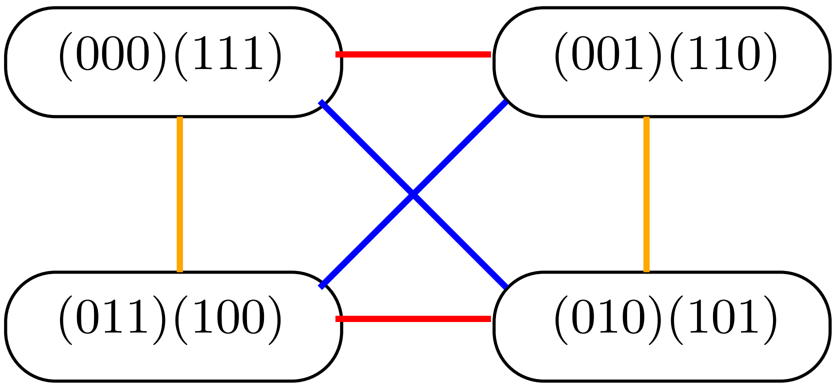
$$\boxed{\begin{matrix} +1 & -1 & 0 \\ -1 & +1 & 0 \\ 0 & 0 & 0 \end{matrix}} \Rightarrow \boxed{\begin{matrix} +1 & -1 & 0 \\ 0 & 0 & 0 \\ -1 & +1 & 0 \end{matrix}} \Rightarrow \boxed{\begin{matrix} +1 & 0 & -1 \\ -1 & 0 & +1 \\ 0 & 0 & 0 \end{matrix}}$$

# Invariant Markov bases

**Theorem(HAT(2007))**

Minimal invariant Markov basis corresponds to a vector space basis of the vector space $\{0,1\}^{c-1}$ over $\mathrm{GF}(2)$ (in each relevant fiber)

3-way complete independence case:

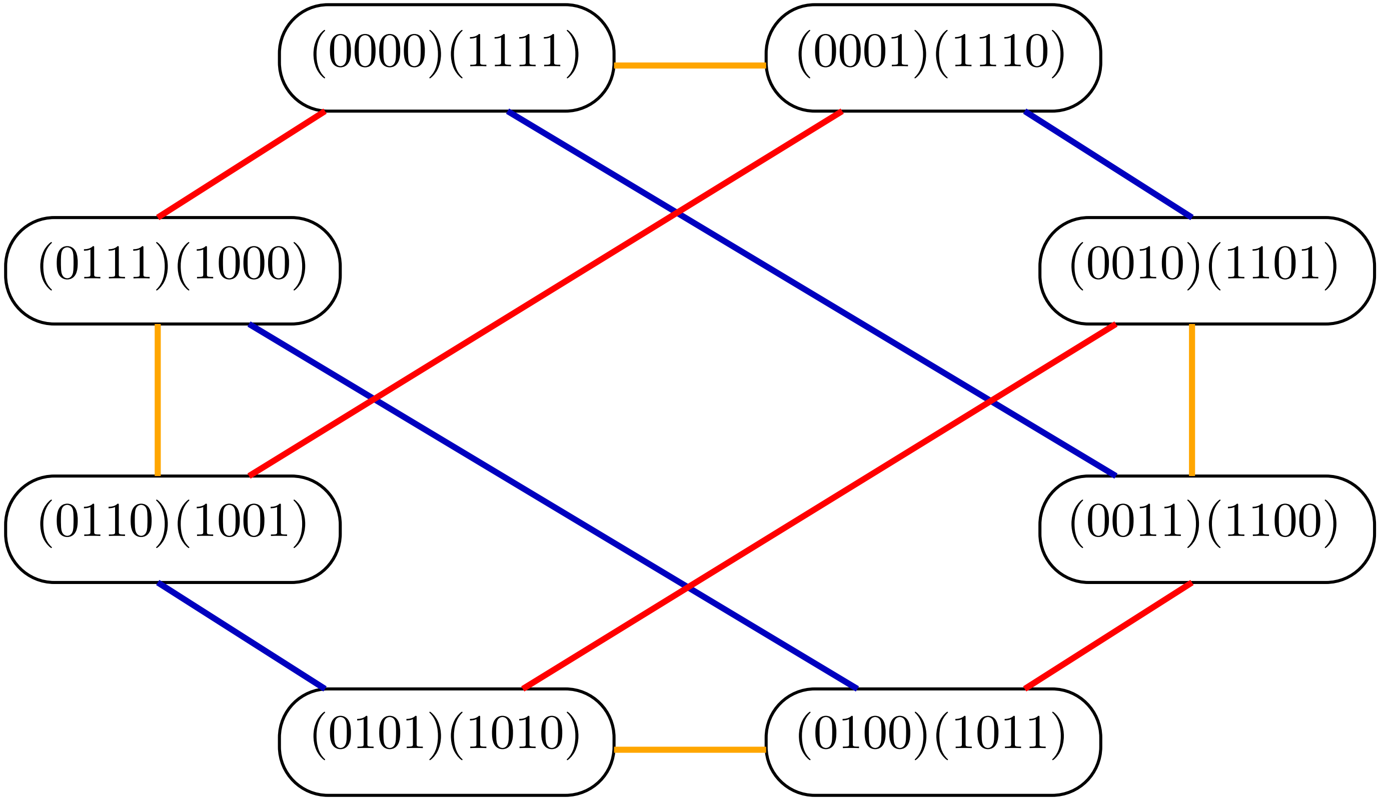


# Invariant Markov bases

- 3 orbits
- 2 orbits are enough to connect this fiber
- Corresponds to linear bases $\{(1,0),(0,1)\}$, $\{(1,0),(1,1)\}$, $\{(0,0),(1,1)\}$ of the vector space $\{0,1\}^2$.

# Invariant Markov bases

Four way case:



# Invariant Markov bases

- 3 orbits are enough (out of 7)
- In this picture we chose $\{(0,0,1),(0,1,1),$ $(1,1,1)\}$ as a linear basis of $\{0,1\}^3$.

# Conclusion

- We gave a brief review on chordal graphs and their clique trees
- We considered Markov bases from the viewpoint of minimality
  - a complete description of minimal MB in decomposable models
  - a necessary and sufficient condition that the unique minimal MB exists
  - the minimality of Dobra's Markov bases

# References


- Hara, H., Aoki, S and Takemura,A.(2007). Fibers of sample size two of hierarchical models and Markov bases of decomposable models for contingency tables. `arvix:math.ST/0701429`.
- Hara, H., Takemura, A.(2006). Boundary cliques, clique trees and perfect sequences of maximal cliques of a chordal graph. `arvix:cs.DM/0607055`.