Graph Decompositions and Junction Trees

Lecture 3
Saint Flour Summerschool, July 6, 2006

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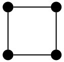
Overview of lectures

1. Conditional independence and Markov properties
2. More on Markov properties
3. Graph decompositions and junction trees
4. Probability propagation and similar algorithms
5. Log-linear and Gaussian graphical models
6. Conjugate prior families for graphical models
7. Hyper Markov laws
8. Structure learning and Bayes factors
9. More on structure learning.

Some motivation

- *Perfect DAGs* are simple, because their directions can be ignored as they are Markov equivalent to their skeleton;
- Undirected graphs which can occur as *skeletons of perfect DAGs* are therefore particularly simple;
- An n-cycle with $n \geq 4$ *cannot be oriented* to form a perfect DAG:



- The important simplifying idea is that of *graph decomposition* and *decomposability*.

Graph decomposition

Consider an *undirected* graph $\mathcal{G} = (V, E)$. A partitioning of V into a triple (A, B, S) of subsets of V forms a *decomposition* of $\mathcal{G}$ if

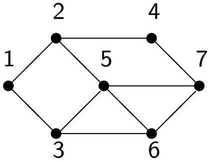
$$A \perp_{\mathcal{G}} B \mid S \text{ and } S \text{ is complete.}$$

The decomposition is *proper* if $A \neq \emptyset$ and $B \neq \emptyset$.

The *components* of $\mathcal{G}$ are the induced subgraphs $\mathcal{G}_{A \cup S}$ and $\mathcal{G}_{B \cup S}$.

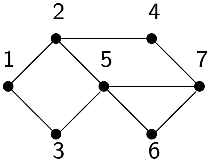
A graph is *prime* if no proper decomposition exists.

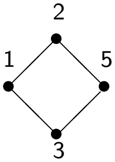
Examples

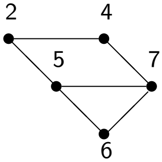


The graph to the left is prime

Decomposition with $A = \{1, 3\}$, $B = \{4, 6, 7\}$ and $S = \{2, 5\}$







Decomposition of Markov properties

Suppose P satisfies (F) w.r.t. $\mathcal{G}$ and (A, B, S) is a decomposition. Then

(i) *$P_{A\cup S}$ and $P_{B\cup S}$ satisfy (F) w.r.t. $\mathcal{G}_{A\cup S}$ and $\mathcal{G}_{B\cup S}$ respectively;*

(ii)
$$f(x)f_S(x_S) = f_{A\cup S}(x_{A\cup S})f_{B\cup S}(x_{B\cup S}).$$

The first part of the statement is true when (F) is replaced by (G).

The second is also true for (G) if the relevant densities exist.

Markov combination

Let Q and R be distributions on $\mathcal{X}_{A\cup S}$ and $\mathcal{X}_{B\cup S}$ resp. and assume Q and R are *consistent*, i.e. $Q_S = R_S$.

Then *there is a unique distribution* $P = Q * R$ so that

(i) $P_{A\cup S} = Q$ and $P_{B\cup S} = R$;

(ii) $A \perp\!\!\!\perp_P B \mid S$.

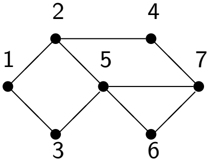
$Q * R$ is the *Markov combination* of Q and R. If Q and R have densities q and r, *so has* P and

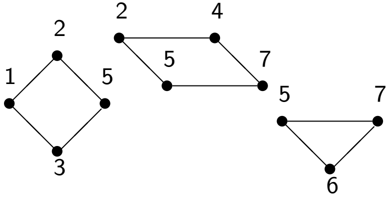
$$p(x)q_S(x_S) = p(x)r_S(x_S) = q(x_{A\cup S})r(x_{B\cup S}).$$

The Markov combination *maximizes entropy* among measures satisfying (i).

Decomposability

Any graph can be recursively decomposed into its maximal prime subgraphs:





A graph is *decomposable* (or rather fully decomposable) if it is complete or admits a proper decomposition into *decomposable* subgraphs.

Definition is recursive. Alternatively this means that *all maximal prime subgraphs are cliques.*

Factorization of Markov distributions

Recursive decomposition of a decomposable graph into cliques yields the formula:

$$f(x)\prod_{S\in\mathcal{S}} f_S(x_S)^{\nu(S)} = \prod_{C\in\mathcal{C}} f_C(x_C).$$

Here $\mathcal{S}$ is the set of *minimal complete separators* occurring in the decomposition process and $\nu(S)$ the number of times such a separator appears in this process.

Combinatorial consequences

Note that if we let $\mathcal{X}_v = \{0, 1\}$ and f be uniform, this yields

$$2^{-|V|} \prod_{S \in \mathcal{S}} 2^{-|S|\nu(S)} = \prod_{C \in \mathcal{C}} 2^{-|C|}$$

and hence we must have

$$\sum_{C \in \mathcal{C}} |C| - \sum_{S \in \mathcal{S}} |S|\nu(S) = |V|.$$

It also holds that

$$\sum_{S \in \mathcal{S}} \nu(S) = |V| - 1.$$

Properties associated with decomposability

A numbering $V = \{1, \ldots, |V|\}$ of the vertices of an undirected graph is *perfect* if the induced oriented graph is a perfect DAG or, equivalently, if

$$\forall j = 2, \ldots, |V| : \mathrm{bd}(j) \cap \{1, \ldots, j-1\} \text{ is complete in } \mathcal{G}.$$

An undirected graph $\mathcal{G}$ is *chordal* if it has no chordless n-cycles with $n \geq 4$.

These graphs are also known as *rigid circuit* graphs or *triangulated* graphs.

A set S is an (α, β)*-separator* if $\alpha \perp_{\mathcal{G}} \beta \,|\, S$,

Characterizing chordal graphs

The following are equivalent for any undirected graph $\mathcal{G}$.

(i) *$\mathcal{G}$ is chordal;*

(ii) *$\mathcal{G}$ is decomposable;*

(iii) *All maximal prime subgraphs of $\mathcal{G}$ are cliques;*

(iv) *$\mathcal{G}$ admits a perfect numbering;*

(v) *Every minimal (α, β)-separator are complete.*

Trees are chordal graphs and thus decomposable.

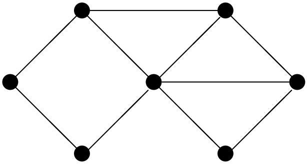
Identifying chordal graphs

Here is a (greedy) algorithm for checking chordality:

1. Look for a vertex v^* with $\mathrm{bd}(v^*)$ complete. *If no such vertex exists, the graph is not chordal.*
2. Form the subgraph $\mathcal{G}_{V \setminus v^*}$ and let $v^* = |V|$;
3. Repeat the process under 1;
4. *If the algorithm continues until only one vertex is left, the graph is chordal and the numbering is perfect.*

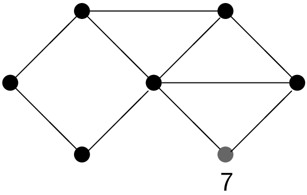
The complexity of this algorithm is $O(|V|^2)$.

Greedy algorithm



Is this graph chordal?

Greedy algorithm



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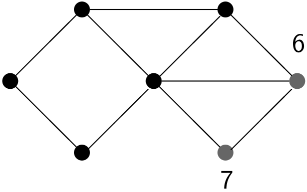

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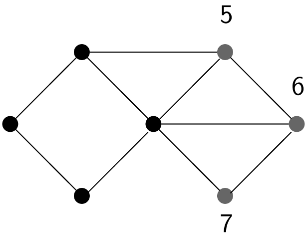

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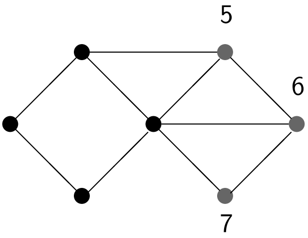
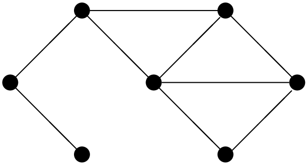


This graph is *not* chordal, as there is no candidate for number 4.

Greedy algorithm



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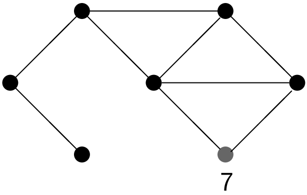

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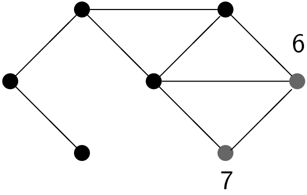

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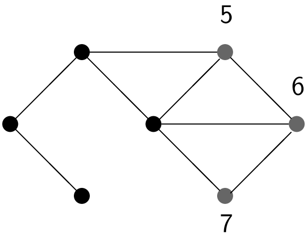

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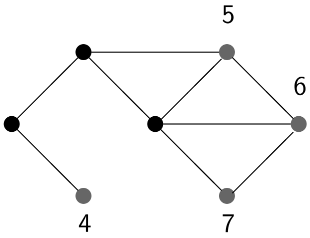

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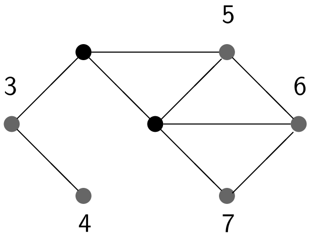

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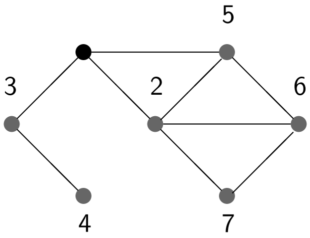

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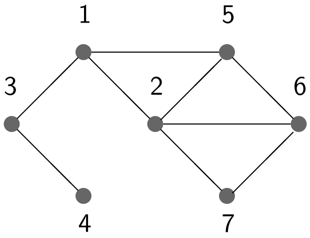


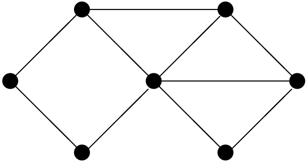
This graph is chordal!

Maximum cardinality search

This simple algorithm has complexity $O(|V| + |E|)$:

1. Choose $v_0 \in V$ arbitrary and let $v_0 = 1$;
2. When vertices $\{1, 2, \dots, j\}$ have been identified, choose $v = j + 1$ among $V \setminus \{1, 2, \dots, j\}$ with highest cardinality of its numbered neighbours;
3. *If* $\mathrm{bd}(j+1) \cap \{1, 2, \dots, j\}$ *is not complete,* $\mathcal{G}$ is not chordal;
4. Repeat from 2;
5. *If the algorithm continues until only one vertex is left, the graph is chordal and the numbering is perfect.*

Maximum Cardinality Search



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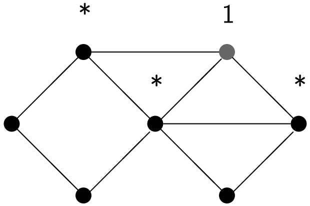
Maximum Cardinality Search



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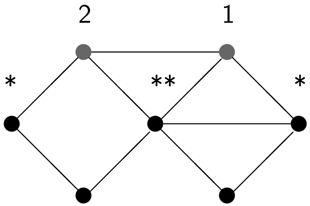

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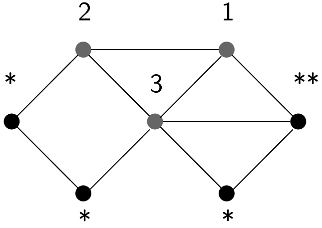
Maximum Cardinality Search



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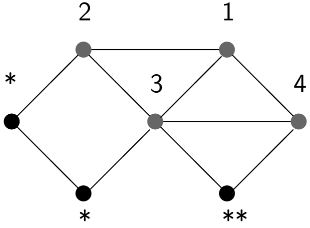
Maximum Cardinality Search



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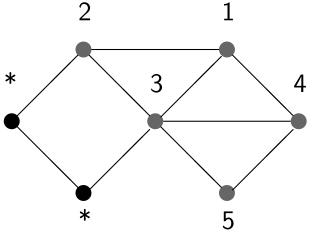
Maximum Cardinality Search



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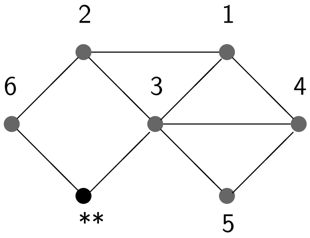
Maximum Cardinality Search



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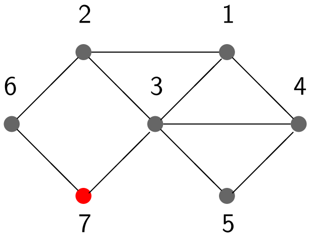
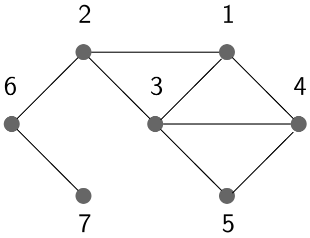
Maximum Cardinality Search



The graph is not chordal! because 7 does not have a complete boundary.

Maximum Cardinality Search



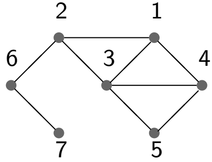
MCS numbering for the chordal graph. Algorithm runs essentially as before.

Finding the cliques of a chordal graph

From an MCS numbering $V = \{1, \ldots, |V|\}$, let

$$S_\lambda = \mathrm{bd}(\lambda) \cap \{1, \ldots, \lambda - 1\}$$

and $\pi_\lambda = |S_\lambda|$. Call λ a *ladder vertex* if $\lambda = |V|$ or if $\pi_{\lambda+1} < \pi_\lambda + 1$ and let Λ be the set of ladder vertices.



π_λ: 0,1,2,2,2,1,1. *The cliques are* $C_\lambda = \{\lambda\} \cup S_\lambda, \lambda \in \Lambda.$

Junction tree

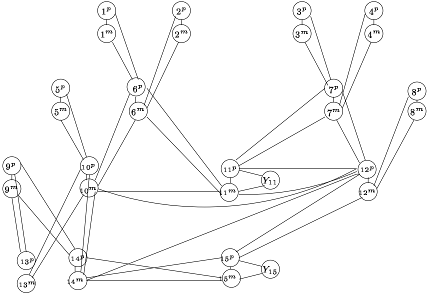
Let $\mathcal{A}$ be a collection of finite subsets of a set V. A *junction tree* $\mathcal{T}$ of sets in $\mathcal{A}$ is an undirected tree with $\mathcal{A}$ as a vertex set, satisfying the *junction tree property:*

If $A, B \in \mathcal{A}$ and C is on the unique path in $\mathcal{T}$ between A and B *it holds that* $A \cap B \subset C$.

If the sets in $\mathcal{A}$ are pairwise incomparable, *they can be arranged in a junction tree if and only if* $\mathcal{A} = \mathcal{C}$ *where* $\mathcal{C}$ *are the cliques of a chordal graph.*

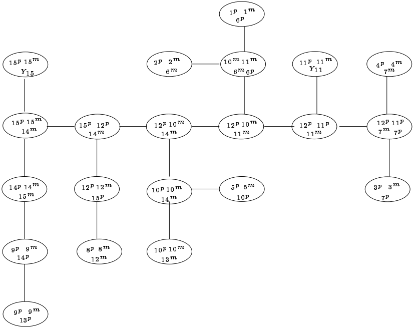
The junction tree can be *constructed directly from the MCS ordering* $C_\lambda, \lambda \in \Lambda$.

A chordal graph



This graph is chordal, but it might not be that easy to see. . . Maximum Cardinality Search is handy!

Junction tree



Cliques of graph arranged into a tree with $C_1 \cap C_2 \subseteq D$ for all cliques D on path between C_1 and C_2.