Log-linear models Maximum likelihood Decomposable models Graph decomposition Identifying chordal graphs

#### Decomposition of log-linear models

Steffen Lauritzen, University of Oxford

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A density f factorizes w.r.t. A if there exist functions  $\psi_a(x)$  which depend on  $x_a$  only so that

$$f(x) = \prod_{\mathsf{a} \in \mathcal{A}} \psi_{\mathsf{a}}(x).$$

The set of distributions  $\mathcal{P}_{\mathcal{A}}$  which factorize w.r.t.  $\mathcal{A}$  is the hierarchical log-linear model generated by  $\mathcal{A}$ .

 ${\cal A}$  is the *generating class* of the log–linear model.

For any generating class  $\mathcal A$  we construct the dependence graph  $G(\mathcal A)=G(\mathcal P_{\mathcal A})$  of the log–linear model  $\mathcal P_{\mathcal A}$ .

The dependence graph is determined by the relation

$$\alpha \sim \beta \iff \exists \mathbf{a} \in \mathcal{A} : \alpha, \beta \in \mathbf{a}.$$

For sets in A are clearly complete in G(A) and therefore distributions in  $\mathcal{P}_A$  do factorize according to G(A).

They are thus also global, local, and pairwise Markov w.r.t. G(A).

As a generating class defines a dependence graph G(A), the reverse is also true.

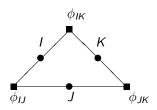
The set C(G) of *cliques* (maximal complete subsets) of G is a generating class for the log-linear model of distributions which factorize w.r.t. G.

If the dependence graph completely summarizes the restrictions imposed by  $\mathcal{A}$ , i.e. if

$$\mathcal{A}=\mathcal{C}(G(\mathcal{A})),$$

A is conformal.





The *factor graph* of  $\mathcal{A}$  is the bipartite graph with vertices  $V \cup \mathcal{A}$  and edges define by

$$\alpha \sim a \iff \alpha \in a$$
.

Using this graph even non-conformal log-linear models admit a simple visual representation.



The maximum likelihood estimate  $\hat{p}$  of p is the unique element of  $\overline{\mathcal{P}_{\mathcal{A}}}$  which satisfies the system of equations

$$n\hat{p}(x_a) = n(x_a), \forall a \in \mathcal{A}, x_a \in \mathcal{X}_a.$$
 (1)

Here  $g(x_a) = \sum_{y:y_a = x_a} g(y)$  is the *a-marginal* of the function g.

The system of equations (1) expresses the *fitting of the marginals* in  $\mathcal{A}$ .

There is a *convergent* algorithm which solves the likelihood equations. This cycles (repeatedly) through all the *a*-marginals in  $\mathcal{A}$  and fit them one by one.

For  $a \in \mathcal{A}$  define the following *scaling* operation on p:

$$(T_a p)(x) \leftarrow p(x) \frac{n(x_a)}{np(x_a)}, \quad x \in \mathcal{X}$$

where 0/0 = 0 and b/0 is undefined if  $b \neq 0$ .

Make an ordering of the generators  $A = \{a_1, \dots, a_k\}$ . Define S by a full cycle of scalings

$$Sp = T_{a_k} \cdots T_{a_2} T_{a_1}$$
.

Define the iteration

$$p_0(x) \leftarrow 1/|\mathcal{X}|, \quad p_n = Sp_{n-1}, n = 1, \ldots$$

It then holds that

$$\lim_{n\to\infty}p_n=\hat{p}$$

where  $\hat{p}$  is the unique maximum likelihood estimate of  $p \in \overline{\mathcal{P}_{\mathcal{A}}}$ , i.e. the solution of the equation system (1).

In some cases the IPS algorithm converges after a finite number of cycles. An explicit formula is then available for the MLE of  $p \in \mathcal{P}_{\mathcal{A}}$ .

Consider first the case of a generating class with only two elements:  $\mathcal{A}=\{a,b\}$  and thus  $V=a\cup b$ . Let  $c=a\cap b$ . Recall that the MLE is the unique solution to

$$n\hat{p}(x_a) = n(x_a), \forall a \in \mathcal{A}, x_a \in \mathcal{X}_a.$$

Let

$$p^*(x) = \frac{n(x_a)n(x_b)}{n(x_c)n}.$$

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This satisfies (1) since e.g.

$$np^{*}(x_{a}) = \sum_{y:y_{a}=x_{a}} \frac{n(y_{a})n(y_{b})}{n(y_{c})} = \sum_{y:y_{a}=x_{a}} \frac{n(x_{a})n(y_{b})}{n(x_{c})}$$
$$= \frac{n(x_{a})}{n(x_{c})} \sum_{y:y_{a}=x_{a}} n(y_{b}) = \frac{n(x_{a})}{n(x_{c})} n(x_{c}) = n(x_{a})$$

and similarly with the other marginal. Hence we have  $\hat{p} = p^*$ .

The generating class  $A = \{a, b\}$  is conformal. Its dependence graph G has exactly two cliques a and b.

The graph is *chordal*, meaning that any cycle of length  $\geq$  4 has a chord.

 $\mathcal A$  is called *decomposable* if  $\mathcal A$  is conformal, i.e.  $\mathcal A=\mathcal C(\mathcal G)$ , and  $\mathcal G$  is chordal.

The IPS-algorithm converges after a finite number of cycles (at most two) if and only if  $\mathcal{A}$  is decomposable.

# Chordal graphs Decomposition of Markov properties Factorization of Markov distributions Explicit formula for MLE Properties of decomposability

#### Non-decomposable generating classes

A generating class can be non-decomposable in different ways.

The generating class  $\mathcal{A} = \{\{1,2\},\{2,3\},\{1,3\}\}$  is the smallest non-decomposable generating class. This is non-conformal.

The graph below is the smallest non-chordal graph and its generating class is non-decomposable:



Chordal graphs
Decomposition of Markov properties
Factorization of Markov distributions
Explicit formula for MLE
Properties of decomposability

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

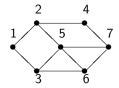
 $A \perp_{\mathcal{G}} B \mid S$  and S is complete.

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  $\mathcal{G}_{B \cup S}$ .

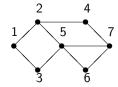
A graph is *prime* if no proper decomposition exists.

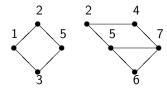
#### **Examples**



The graph to the left is prime

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





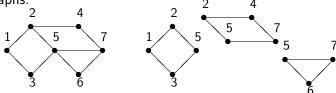
Suppose P satisfies (F) w.r.t.  $\mathcal G$  and (A,B,S) is a decomposition. Then

- (i)  $P_{A \cup S}$  and  $P_{B \cup S}$  satisfy (F) w.r.t.  $G_{A \cup S}$  and  $G_{B \cup S}$  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 converse also holds in the sense that if (i) and (ii) hold, and (A, B, S) is a decomposition of G, then P factorizes w.r.t. G.

#### 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*.



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.

As we have a particularly simple factorization of the density, we have a similar factorization of the maximum likelihood estimate for a decomposable log-linear model.

The MLE for p under the log-linear model with generating class  $\mathcal{A}=\mathcal{C}(\mathcal{G})$  for a chordal graph  $\mathcal{G}$  is

$$\hat{p}(x) = \frac{\prod_{C \in \mathcal{C}} n(x_C)}{n \prod_{S \in \mathcal{S}} n(x_S)^{\nu(S)}}$$

where  $\nu(S)$  is the number of times S appears as a separator in the total decomposition of its dependence graph.

#### Perfect numbering

A numbering  $V = \{1, \dots, |V|\}$  of the vertices of an undirected graph is *perfect* if

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

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

#### Characterizing chordal graphs

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

- (i) *G* is chordal;
- (ii) *G* is decomposable;
- (iii) All maximal prime subgraphs of G are cliques;
- (iv) G admits a perfect numbering;
- (v) Every minimal  $(\alpha, \beta)$ -separator are complete.

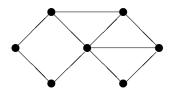
Trees are chordal graphs and thus decomposable.



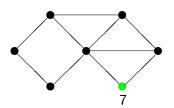
Here is a (greedy) algorithm for checking chordality:

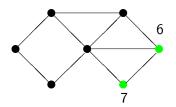
- 1. Look for a vertex  $v^*$  with  $bd(v^*)$  complete. If no such vertex exists, the graph is not chordal.
- 2. Form the subgraph  $\mathcal{G}_{V\setminus v^*}$  and let  $v^*=|V|$ ;
- 3. Repeat the process under 1;
- 4. If the algorithm continues until only one vertex is left, the graph is chordal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

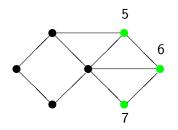
The complexity of this algorithm is  $O(|V|^2)$ .

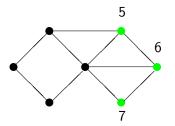




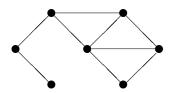


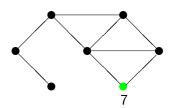


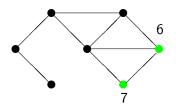


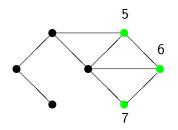


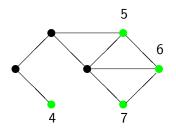
This graph is *not* chordal, as there is no candidate for number 4.

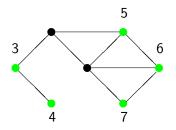


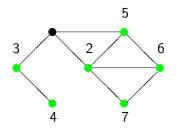


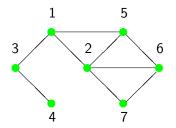








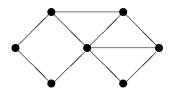


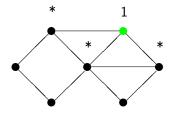


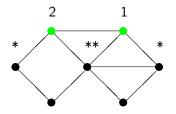
This graph is chordal!

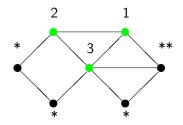
#### This simple algorithm has complexity O(|V| + |E|):

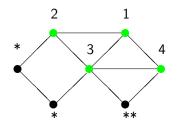
- 1. Choose  $v_0 \in V$  arbitrary and let  $v_0 = 1$ ;
- 2. When vertices  $\{1,2,\ldots,j\}$  have been identified, choose v=j+1 among  $V\setminus\{1,2,\ldots,j\}$  with highest cardinality of its numbered neighbours;
- 3. If  $bd(j+1) \cap \{1,2,\ldots,j\}$  is not complete,  $\mathcal{G}$  is not 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.

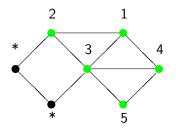


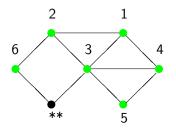


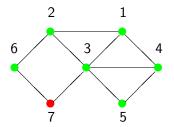




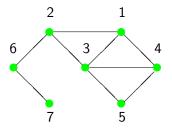






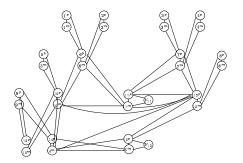


The graph is not chordal! because 7 does not have a complete boundary.



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

#### A chordal graph



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

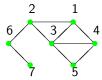


#### Finding the cliques of a chordal graph

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

$$B_{\lambda} = \mathsf{bd}(\lambda) \cap \{1, \dots, \lambda - 1\}$$

and  $\pi_{\lambda} = |B_{\lambda}|$ . Call  $\lambda$  a *ladder vertex* if  $\lambda = |V|$  or if  $\pi_{\lambda+1} < \pi_{\lambda} + 1$ . Let  $\Lambda$  be the set of ladder vertices.



 $\pi_{\lambda}$ : 0,1,2,2,2,1,1. The cliques are  $C_{\lambda} = {\lambda} \cup B_{\lambda}, \lambda \in \Lambda$ .