Junction Trees and Chordal Graphs

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Definition Decomposability Factorization of Markov distributions Explicit formula for MLE

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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. Graph decomposition

Identifying chordal graphs Junction trees Local computation Definition Decomposability Factorization of Markov distributions Explicit formula for MLE



The graph to the left is prime

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



 Graph decomposition
 Definition

 Identifying chordal graphs
 Decomposability

 Junction trees
 Factorization of Markov distributions

 Local computation
 Explicit formula for MLE

Any graph can be recursively decomposed into its maximal prime subgraphs: $2 \qquad 4$



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*.

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Definition Decomposability Factorization of Markov distributions Explicit formula for MLE

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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 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.

Definition Decomposability Factorization of Markov distributions Explicit formula for MLE

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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.

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

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

Trees are chordal graphs and thus decomposable.

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

- 1. Choose $v_0 \in V$ arbitrary and let $v_0 = 1$;
- 2. When vertices $\{1, 2, ..., j\}$ have been identified, choose v = j + 1 among $V \setminus \{1, 2, ..., j\}$ with highest cardinality of its numbered neighbours;
- 3. If $bd(j+1) \cap \{1, 2, \dots, j\}$ 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.

Characterizing chordal graphs Maximum cardinality search

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



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

Definition Characterizing chordal graphs Construction of junction tree Junction trees of prime components Decompositon formula for MLE

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

If the sets in an arbitrary A are pairwise incomparable, they can be arranged in a junction tree if and only if A = C where C are the cliques of a chordal graph

Definition Characterizing chordal graphs Construction of junction tree Junction trees of prime components Decompositon formula for MLE

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

- (i) \mathcal{G} is chordal;
- (ii) \mathcal{G} is decomposable;
- (iii) All prime components of G are cliques;
- (iv) *G* admits a perfect numbering;
- (v) Every minimal (α, β) -separator are complete.
- (vi) The cliques of \mathcal{G} can be arranged in a junction tree.

The junction tree can be *constructed directly from the MCS* ordering $C_{\lambda}, \lambda \in \Lambda$, where C_{λ} are the cliques: Since the MCS-numbering is perfect, $C_{\lambda}, \lambda > \lambda_{min}$ all satisfy

$$\mathcal{C}_{\lambda} \cap (\cup_{\lambda' < \lambda} \mathcal{C}_{\lambda'}) = \mathcal{C}_{\lambda} \cap \mathcal{C}_{\lambda^*} = \mathcal{S}_{\lambda}$$

for some $\lambda^* < \lambda$.

A junction tree is now easily constructed by attaching C_{λ} to any C_{λ^*} satisfying the above. Although λ^* may not be uniquely determined, S_{λ} is.

Indeed, the sets S_{λ} are the minimal complete separators and *the* numbers $\nu(S)$ are $\nu(S) = |\{\lambda \in \Lambda : S_{\lambda} = S\}|$.

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Definition Characterizing chordal graphs Construction of junction tree Junction trees of prime components Decompositon formula for MLE

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A chordal graph



Definition Characterizing chordal graphs Construction of junction tree Junction trees of prime components Decompositon formula for MLE

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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 .

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In general, the *prime components* of any undirected graph can be arranged in a junction tree in a similar way.

Then every pair of neighbours (C, D) in the junction tree represents a decomposition of \mathcal{G} into $\mathcal{G}_{\tilde{C}}$ and $\mathcal{G}_{\tilde{D}}$, where \tilde{C} is the set of vertices in cliques connected to C but separated from D in the junction tree, and similarly with \tilde{D} .

The corresponding algorithm is based on a slightly more sophisticated algorithm known as *Lexicographic Search* (LEX) which runs in $O(|V|^2)$ time.

Graph decomposition Identifying chordal graphs Junction trees Local computation Decompositon formula for MLE

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

$$\hat{p}(x) = \frac{\prod_{Q \in \mathcal{Q}} \hat{p}_Q(x_Q)}{\prod_{S \in \mathcal{S}} \{n(x_S)/n\}^{\nu(S)}}$$

where $\hat{p}_Q(x_Q)$ is the estimate of the marginal distrbution based on data from Q only and $\nu(S)$ is the number of times S appears as a separator in the decomposition of its dependence graph into prime components.

When the prime components are cliques it further holds that $\hat{p}_C(x_C) = n(x_C)/n$.

In fact, true also if if A is not conformal, but it holds that $S \in A$ for all separators of the dependence graph $\mathcal{G}(A)$.

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