Undirected Graphical Models: Chordal Graphs, Decomposable Graphs, Junction Trees, and Factorizations

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These notes present some properties of chordal graphs, a set of undirected graphs that are important for undirected graphical models.

Definitions

We consider *undirected graphs* $G = (V, E)$, where V is the vertex set and the edge set E is a set of unordered distinct pairs from V. We say that vertices $u, v \in V$ are *neighbors* if $\{u, v\} \in E$.

A *cycle* in a graph is a vertex sequence $v_1, \ldots, v_n$ where $v_1 = v_n$ but all other pairs are distinct, and $\{v_i, v_{i+1}\} \in E$. A cycle is *chordless* if all pairs of vertices that are not adjacent in the cycle are not neighbors (that is, any $\{v_a, v_b\}$ with $|a - b| \neq 1$ is not in E). That is, there is no *chord*, or shortcut, for the cycle.

A graph is *chordal* (also called *triangulated*) if it contains no chordless cycles of length greater than 3.

A graph is *complete* if E contains all pairs of distinct elements of V.

A graph $G = (V, E)$ is *decomposable* if either

1. G is complete, or
2. We can express V as $V = A \cup B \cup C$ where
   (a) A, B and C are disjoint,
   (b) A and C are non-empty,
   (c) B is complete,
   (d) B separates A and C in G, and
   (e) $A \cup B$ and $B \cup C$ are decomposable.

A *path* is a sequence $v_1, \ldots, v_n$ of distinct vertices for which all $\{v_i, v_{i+1}\} \in E$. A *tree* is an undirected graph for which every pair of vertices is connected by precisely one path. A *clique* of a graph G is a subset of vertices that are completely connected. A *maximal clique* of G is a clique for which every superset of vertices of G is not a clique.

A *clique tree* for a graph $G = (V, E)$ is a tree $T = (V_T, E_T)$ where V_T is a set of cliques of G that contains all maximal cliques of G.

We'll label each edge $e = (C_1, C_2)$ of a clique tree with the corresponding *separator set*, $C_1 \cap C_2$. (But notice that these labels might not uniquely specify an edge.)

A *junction tree* for a graph G is a clique tree for G that satisfies the following condition. For any cliques C_1 and C_2 in the tree, every clique on the path connecting C_1 and C_2 contains $C_1 \cap C_2$.

A vertex is *simplicial* in a graph if its neighbors form a complete subgraph. A graph is *recursively simplicial* if it contains a simplicial vertex v and when v is removed the subgraph that remains is recursively simplicial.

Equivalence Theorem

Theorem 1. *The following properties of G are equivalent.*

1. *G is chordal.*
2. *G is decomposable.*
3. *G is recursively simplicial.*
4. *G has a junction tree.*

We shall present the proof as a series of lemmas ($1 \implies 2 \implies 3 \implies 4 \implies 1$).

Lemma 1. *G is chordal implies G is decomposable.*

Proof. We prove by induction that every chordal graph with n vertices is decomposable. This is trivially true for $n = 1$. If it is true for any n, then the following argument shows that it is true for a graph G with $n + 1$ vertices.

Step 1: If G is complete, it is decomposable. So suppose that G is not complete.

Step 2: We can express V as the disjoint union $V = A \cup B \cup S$, where S separates A from B in G and A, B are nonempty. Indeed, since G is not complete, V contains a, b that are not neighbors. Let $S \subset V$ be a minimal set that separates a from b. (Notice that S might be empty). Let A be the subset of $V - S$ connected to a by some path in $V - S$, and let B be the remainder, $B = V - S - A$. Clearly, S separates A from B in G.

Step 3: S is complete.

3a: We may assume that S has cardinality at least 2, for otherwise it is trivially complete.

3b: For any two distinct nodes u, v in S, there are paths $u, a_1, \ldots, a_n, v$ and $u, b_1, \ldots, b_m, v$ with $a_i \in A$, $b_i \in B$ and $n, m \geq 1$. Indeed, since S was a minimal set that separates a from b, there must be a path from a to u and from a to v, since the absence of one of these paths would imply that S was not minimal.

3c: u and v are neighbors. To see this, take the path from u to v through A that has minimal length, and similarly the path from u to v through B of minimal length. This pair of paths forms a cycle, which must have a chord. To see that the chord must be between u and v, notice that the minimality of the paths implies that the chord cannot be between vertices that are both in A, nor can it be between vertices that are both in B. In addition, the fact that S separates A from B implies the chord cannot be between a vertex in A and one in B.

Step 4: The subgraphs induced by $A \cup S$ and $B \cup S$ are chordal. Indeed, if one of these subgraphs contains a chordless cycle, then so does G.

Step 5: By the inductive hypothesis, these subgraphs are strictly smaller than G and hence decomposable.

□

Lemma 2. *G decomposable implies G is recursively simplicial.*

Proof. We prove by induction that every decomposable graph with n vertices is recursively simplicial. This is trivially true for $n = 1$.

Step 1: G decomposable implies that G contains a simplicial vertex. To see this, we prove by induction the stronger statement that any decomposable graph is either complete or has two nonadjacent simplicial vertices. This is trivially true for graphs with $|V| = 1$, and for the induction step, we notice that any decomposable G is either complete, or V can be decomposed as sets A, B, C. If $A \cup B$ is complete, then any $a \in A$ is simplicial. Otherwise, the subgraph induced by $A \cup B$ has two non-adjacent simplicial nodes, by the inductive hypothesis. Since B is complete, one of these must be in A. Similarly, there is a simplicial $c \in C$.

Step 2: G decomposable implies that the subgraph corresponding to a subset of the vertices is decomposable. Again, we prove this by induction. It is trivially true for graphs with $|V| = 1$. For the induction step, the result is trivially true if G is complete, otherwise we consider the usual decomposition of V into A, B, C, where B is complete and $A \cup B$ and $B \cup C$ are decomposable. By the inductive hypothesis, removing a node from B leaves $A \cup B$ and $B \cup C$ decomposable. Removing a node from A leave $B \cup C$ unchanged, and either leaves A empty, in which case the remaining subgraph, $B \cup C$, is decomposable, or leaves $A \cup B$ decomposable by the inductive hypothesis.

Thus, the subgraph that remains when we remove a simplicial vertex v from a decomposable G is also decomposable. □

Lemma 3. *G recursively simplicial implies G has a junction tree.*

Proof. We prove by induction that every recursively simplicial graph with n vertices has a junction tree. This is trivially true for $n = 1$.

Consider a simplicial vertex v of G, and let G' be the subgraph that remains when we remove v. By the inductive hypothesis, G' has a junction tree T', and this can be extended to give a junction tree for G. To see this, let C' be a maximal clique in T' containing all neighbors of v in G. If C' is precisely the set of neighbors of v, then we can add v to C' to give a junction tree for G (it contains all maximal cliques, and v is not in any other clique, so the junction tree property is trivially satisfied). If not, that is, if C' contains the neighbors of v as a proper subset, then we add a new clique containing v and its neighbors to T', with an edge to C'. Since v is in no other clique and $C - \{v\}$ is a subset of C', this is a junction tree for G. □

Lemma 4. *If G has a junction tree then G is chordal.*

Proof. We prove by induction that the statement is true for junction trees with n nodes. If the clique tree has only one node, then G is complete, hence chordal.

Assuming that the statement is true for some value of n, consider a graph with a junction tree T containing $n+1$ nodes.

Fix a leaf C of T, and let C' be the neighbor of C in T, and let T' be the tree that remains when C is removed.

Step 1: If $C \subseteq C'$, then T' is a junction tree for G.

Step 2: On the other hand, if $C \cap C' \subset C$, removing the nonempty set $R = C - C'$ from V leaves a subgraph G' that is chordal. To see this, notice that R has an empty intersection with every clique in T'. It is easy to see that T' is a junction tree for G', and so G' is chordal.

Step 3: It follows that G contains no chordless cycles. Indeed, if a cycle is entirely in G', it is not chordless. If the cycle is entirely in the complete subgraph defined by C, it is not chordless. If the cycle intersects R, $C \cap C'$, and $V - C$, then since the subgraph defined by $C \cap C'$ is complete, the cycle has a chord. □

Undirected graphical models with chordal graphs

Theorem 2. *The following properties of G are equivalent.*

1. *G is chordal.*
2. *There is an elimination ordering for which the graph G is a fixed point of the* UndirectedGraphEliminate *algorithm.*
3. *There is an orientation of the edges of G that gives a directed acyclic graph whose moral graph is G.*
4. *There is a directed graphical model with conditional independencies identical to those implied by G.*

We sketch the proof of these implications.

Define a *simplicial vertex sequence* as an ordering of the nodes of a recursively simplicial graph that exhibits the recursively simpliciality of the graph. That is, as we progressively remove the nodes in this order, the next node in the order is simplicial in the remaining subgraph.

Elimination ordering: Eliminating a node leaves the graph unchanged iff the node is simplicial. Thus, the existence of an elimination ordering that leaves the reconstituted graph identical is equivalent to the existence of a simplicial vertex sequence.

DAG with same moral graph: Given a recursively simplicial graph G, we can construct a DAG G_D as follows. Fix a simplicial vertex sequence $(v_1, \ldots, v_n)$ for G. Define $G_1 = G$. At step t, add v_t and its neighbors in G_t to G_D (if they are not already present), and add the corresponding edges to G_D so that they are directed towards v_t. Then set G_{t+1} to the subgraph of G_t that remains when v_t is removed.

It is clear that G_D is acyclic, since the edges are directed in a fixed order. Also, by construction, the moral graph requires no additional edges.

To see that the existence of a DAG G_D with moral graph G implies that G is recursively simplicial, fix a reverse topological order of the nodes in G_D (that is, children before parents). Set $G_0 = G$. At step t, remove v_t from G_{t-1} to give the subgraph G_t. The ordering ensures that the neighbors of v_t in G_{t-1} are its parents. Since the moral graph is the same, these parents must be connected in G_{t-1}. Hence, we have specified a simplicial vertex sequence.

Theorem 3. *Suppose G has a junction tree $T = (C, S)$. Fix some $s = \{c_1, c_2\} \in S$, and let $T_1 = (V_1, E_1)$ ($T_2 = (V_2, E_2)$) be the maximal subtree with root c_1 (c_2) that does not contain s. Then for*

$$\begin{aligned} A_1 &= V_1 - (c_1 \cap c_2) \\ B &= (c_1 \cap c_2) \\ A_2 &= V_2 - (c_1 \cap c_2), \end{aligned}$$

we have

$$A_1 \perp\!\!\!\perp A_2 | B.$$

Proof. Since T is a junction tree, any v in A_1 is not in A_2. Since C contains the maximal cliques, the neighbors of any v in A_1 are all in $A_1 \cup B$. It follows that A_1 is separated from A_2 by B. □

Theorem 4. *If G has a junction tree $T = (C, S)$, then any probability distribution that satisfies the conditional independencies implied by G can be factorized as*

$$p(x) = \frac{\prod_{c \in C} p(x_c)}{\prod_{s \in S} p(x_s)},$$

where if $s = \{c_1, c_2\}$ then x_s denotes $x_{c_1 \cap c_2}$.

Proof. Fix a root node of T and suppose that $C = \{c_1, \ldots, c_n\}$ is a topological ordering of the nodes of T (that is, each node's parent appears earlier in the ordering). Then we have

$$\begin{aligned} p(x) &= \prod_i p(x_{c_i} | x_{c_1}, \ldots, x_{c_{i-1}}) \\ &= \prod_i p(x_{c_i} | x_{c_{\pi(i)} \cap c_i}) \\ &= \prod_i \frac{p(x_{c_i})}{p(x_{c_{\pi(i)} \cap c_i})} \\ &= \frac{\prod_{c \in C} p(x_c)}{\prod_{s \in S} p(x_s)}, \end{aligned}$$

where the second equality follows from the previous theorem. □

References

The classic paper on the graph-theoretic equivalences presented here is C. Beeri, R. Fagin, D. Maier, and M. Yannakakis, On the desirability of acyclic database schemes, Journal of the ACM, 30(3):479–513, July 1983. See also J. Pearl, Probabilistic Reasoning in Intelligent Systems, Morgan Kaufmann, 1988. And Chapters 16 and 17 of the text, M. Jordan, An Introduction to Probabilistic Graphical Models.