Markov properties for directed graphs

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 $\mathcal{G}=(V,E)$ simple undirected graph; \perp_{σ} (semi)graphoid relation. Say \perp_{σ} satisfies

(P) the pairwise Markov property if

$$\alpha \not\sim \beta \Rightarrow \alpha \perp_{\sigma} \beta \mid V \setminus \{\alpha, \beta\};$$

(L) the local Markov property if

$$\forall \alpha \in V : \alpha \perp_{\sigma} V \setminus \mathsf{cl}(\alpha) \mid \mathsf{bd}(\alpha);$$

(G) the global Markov property if

$$A \perp_{\mathcal{G}} B \mid S \Rightarrow A \perp_{\sigma} B \mid S.$$

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For any semigraphoid it holds that

$$(\mathsf{G}) \Rightarrow (\mathsf{L}) \Rightarrow (\mathsf{P})$$

If \perp_{σ} satisfies graphoid axioms it further holds that

$$(\mathsf{P}) \Rightarrow (\mathsf{G})$$

so that in the graphoid case

$$(\mathsf{G})\iff (\mathsf{L})\iff (\mathsf{P}).$$

The latter holds in particular for $\perp \!\!\!\perp$, when f(x) > 0.

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Assume density f w.r.t. product measure on \mathcal{X} . For $a \subseteq V$, $\psi_a(x)$ denotes a function which depends on x_a only, i.e.

$$x_a = y_a \Rightarrow \psi_a(x) = \psi_a(y).$$

We can then write $\psi_a(x) = \psi_a(x_a)$ without ambiguity. The distribution of X factorizes w.r.t. \mathcal{G} or satisfies (F) if

$$f(x) = \prod_{a \in \mathcal{A}} \psi_a(x)$$

where \mathcal{A} are *complete* subsets of \mathcal{G} .

Complete subsets of a graph are sets with all elements pairwise neighbours.

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Factorization theorem

Let (F) denote the property that f factorizes w.r.t. \mathcal{G} and let (G), (L) and (P) denote Markov properties w.r.t. $\bot\!\!\!\bot$. It then holds that

$$(\mathsf{F}) \Rightarrow (\mathsf{G})$$

and further: If f(x) > 0 for all x, (P) \Rightarrow (F).

Thus in the case of positive density (but typically only then), *all the properties coincide:*

$$(\mathsf{F})\iff (\mathsf{G})\iff (\mathsf{L})\iff (\mathsf{P}).$$

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A *directed acyclic graph* \mathcal{D} over a finite set V is a simple graph with all edges directed and *no directed cycles*. We use DAG for brevity.

Absence of directed cycles means that, *following arrows in the graph, it is impossible to return to any point.*

Graphical models based on DAGs have proved fundamental and useful in a wealth of interesting applications, including expert systems, genetics, complex biomedical statistics, causal analysis, and machine learning.

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Example of a directed graphical model



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A semigraphoid relation \perp_{σ} satisfies *the local Markov property* (L) w.r.t. a directed acyclic graph \mathcal{D} if

$$\forall \alpha \in V : \alpha \perp_{\sigma} \{ \mathsf{nd}(\alpha) \setminus \mathsf{pa}(\alpha) \} \mid \mathsf{pa}(\alpha).$$

Here $nd(\alpha)$ are the *non-descendants* of α . A well-known example is a Markov chain:

with
$$X_{i+1} \perp (X_1, \dots, X_{i-1}) \mid X_i$$
 for $i = 3, \dots, n$.

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Local directed Markov property



For example, the local Markov property says $4 \perp_{\sigma} \{1, 3, 5, 6\} \mid 2, 5 \perp_{\sigma} \{1, 4\} \mid \{2, 3\} \\ 3 \perp_{\sigma} \{2, 4\} \mid 1.$

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Suppose the vertices V of a DAG D are *well-ordered* in the sense that they are linearly ordered in a way which is compatible with D, i.e. so that

 $\alpha \in \mathsf{pa}(\beta) \Rightarrow \alpha < \beta.$

We then say semigraphoid relation \perp_{σ} satisfies the *ordered Markov property* (O) w.r.t. a well-ordered DAG D if

 $\forall \alpha \in V : \alpha \perp_{\sigma} \{ \mathsf{pr}(\alpha) \setminus \mathsf{pa}(\alpha) \} \mid \mathsf{pa}(\alpha).$

Here $pr(\alpha)$ are the *predecessors* of α , i.e. those which are before α in the well-ordering..

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Ordered Markov property



The numbering corresponds to a well-ordering. The ordered Markov property says for example

$$\begin{array}{l} 4\perp_{\sigma}\{1,3\}\,|\,2,\\ 5\perp_{\sigma}\{1,4\}\,|\,\{2,3\}\\ 3\perp_{\sigma}\{2\}\,|\,1. \end{array}$$

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Separation in DAGs

A *trail* τ from vertex α to vertex β in a DAG D is *blocked* by *S* if it contains a vertex $\gamma \in \tau$ such that

- \blacktriangleright either $\gamma \in {\it S}$ and edges of τ do not meet head-to-head at $\gamma,$ or
- γ and all its descendants are not in S, and edges of τ meet head-to-head at γ.

A trail that is not blocked is *active*. Two subsets A and B of vertices are *d*-separated by S if all trails from A to B are blocked by S. We write $A \perp_{\mathcal{D}} B \mid S$.

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Separation by example



For $S = \{5\}$, the trail (4, 2, 5, 3, 6) is *active*, whereas the trails (4, 2, 5, 6) and (4, 7, 6) are *blocked*. For $S = \{3, 5\}$, they are all blocked.

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Returning to example



Hence $4 \perp_{\mathcal{D}} 6 \mid 3, 5$, but it is *not* true that $4 \perp_{\mathcal{D}} 6 \mid 5$ nor that $4 \perp_{\mathcal{D}} 6$.

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Equivalence of Markov properties

A semigraphoid relation \perp_{σ} satisfies the *global Markov property* (G) w.r.t. \mathcal{D} if

$$A \perp_{\mathcal{D}} B \mid S \Rightarrow A \perp_{\sigma} B \mid S.$$

It holds for any DAG D and any semigraphoid relation \perp_{σ} that all directed Markov properties are equivalent:

$$(\mathsf{G})\iff (\mathsf{L})\iff (\mathsf{O}).$$

There is also a pairwise property (P), but it is less natural than in the undirected case and it is weaker than the others.

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A probability distribution P over $\mathcal{X} = \mathcal{X}_V$ factorizes over a DAG \mathcal{D} if its density or probability mass function f has the form

(F):
$$f(x) = \prod_{v \in V} k_v(x_v | x_{pa(v)})$$

where $k_v \ge 0$ and $\int_{\mathcal{X}_v} k_v(x_v | x_{\mathsf{pa}(v)}) \mu_v(dx_v) = 1$. (F) *is equivalent to* (F^{*}), where

$$(\mathsf{F}^*): \quad f(x) = \prod_{v \in V} f(x_v \,|\, x_{\mathsf{pa}(v)}),$$

i.e. it follows from (F) that k_v in fact are conditional densities/pmf's. Proof by induction!

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Example of DAG factorization



The above graph corresponds to the factorization

$$\begin{array}{rcl} f(x) &=& f(x_1)f(x_2 \mid x_1)f(x_3 \mid x_1)f(x_4 \mid x_2) \\ & \times & f(x_5 \mid x_2, x_3)f(x_6 \mid x_3, x_5)f(x_7 \mid x_4, x_5, x_6). \end{array}$$

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Contrast with undirected factorization



Factors ψ are typically not normalized as conditional probabilities:

$$f(x) = \psi_{12}(x_1, x_2)\psi_{13}(x_1, x_3)\psi_{24}(x_2, x_4)\psi_{25}(x_2, x_5) \\ \times \quad \psi_{356}(x_3, x_5, x_6)\psi_{47}(x_4, x_7)\psi_{567}(x_5, x_6, x_7).$$

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Markov properties and factorization

In the directed case it is essentially always true that (F) holds if and only if \coprod_P satisfies (G),

so all directed Markov properties are equivalent to the factorization property!

$$(F)\iff (G)\iff (L)\iff (0).$$

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The moral graph \mathcal{D}^m of a DAG \mathcal{D} is obtained by adding undirected edges between unmarried parents and subsequently dropping directions, as in the example below:



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Undirected factorizations

If P factorizes w.r.t. D, it factorizes w.r.t. the moralised graph D^m . This is seen directly from the factorization:

$$f(x) = \prod_{v \in V} f(x_v \mid x_{\mathsf{pa}(v)}) = \prod_{v \in V} \psi_{\{v\} \cup \mathsf{pa}(v)}(x),$$

since $\{v\} \cup pa(v)$ are all complete in \mathcal{D}^m . Hence if *P* satisfies any of the directed Markov properties w.r.t. \mathcal{D} , it satisfies all Markov properties for \mathcal{D}^m .

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Alternative equivalent separation

To resolve query involving three sets A, B, S:

- 1. Reduce to subgraph induced by ancestral set $\mathcal{D}_{An(A\cup B\cup S)}$ of $A\cup B\cup S$;
- 2. Moralize to form $(\mathcal{D}_{An(A\cup B\cup S)})^m$;
- 3. Say that *S m*-separates *A* from *B* and write $A \perp_m B \mid S$ if and only if *S* separates *A* from *B* in this undirected graph.

It then holds that $A \perp_m B \mid S$ if and only if $A \perp_D B \mid S$. Proof in Lauritzen (1996) needs to allow self-intersecting paths to be correct.

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Forming ancestral set



The subgraph induced by all ancestors of nodes involved in the query $4 \perp_m 6 \mid 3, 5$?

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Adding links between unmarried parents



Adding an undirected edge between 2 and 3 with common child 5 in the subgraph induced by all ancestors of nodes involved in the query $4 \perp_m 6 \mid 3, 5$?

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Dropping directions



Since $\{3,5\}$ separates 4 from 6 in this graph, we can conclude that $4 \perp_m 6 \,|\, 3,5$

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Two DAGS \mathcal{D} and \mathcal{D}' are *Markov equivalent* if the separation relations $\perp_{\mathcal{D}}$ and $\perp_{\mathcal{D}'}$ are identical. \mathcal{D} and \mathcal{D}' are equivalent if and only if:

- 1. \mathcal{D} and \mathcal{D}' have same *skeleton* (ignoring directions)
- 2. \mathcal{D} and \mathcal{D}' have same unmarried parents





Contrast with undirected case, where *two undirected graphs are Markov equivalent if and only if they are identical.*

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Markov equivalence of directed and undirected graphs

A DAG \mathcal{D} is *Markov equivalent* to an undirected \mathcal{G} if the separation relations $\perp_{\mathcal{D}}$ and $\perp_{\mathcal{G}}$ are identical. This happens if and only if \mathcal{D} is perfect and $\mathcal{G} = \sigma(\mathcal{D})$. So, these are all equivalent

but not equivalent to