

A Characterization of Markov Equivalence Classes for Acyclic Digraphs[†]

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25 April 2001

Abstract

Undirected graphs and acyclic digraphs (ADGs), as well as their mutual extension to chain graphs, are widely used to describe dependencies among variables in multivariate distributions. In particular, the likelihood functions of ADG models admit convenient recursive factorizations that often allow explicit maximum likelihood estimates and that are well suited to building Bayesian networks for expert systems. Whereas the undirected graph associated with a dependence model is uniquely determined, there may, however, be many ADGs that determine the same dependence (= Markov) model. Thus, the family of all ADGs with a given set of vertices is naturally partitioned into Markov-equivalence classes, each class being associated with a unique statistical model. Statistical procedures, such as model selection or model averaging, that fail to take into account these equivalence classes, may incur substantial computational or other inefficiencies. Here it is shown that each Markov-equivalence class is uniquely determined by a single chain graph, the *essential graph*, that is itself simultaneously Markov equivalent to all ADGs in the equivalence class. Essential graphs are characterized, a polynomial-time algorithm for their construction is given, and their applications to model selection and other statistical questions are described.

1. Introduction.

The use of directed graphs to represent possible dependencies among statistical variables dates back to Wright (1921) and has generated considerable research activity in the social and natural sciences. Since 1980, particular attention has been directed to graphical Markov models specified by conditional independence relations among the variables, i.e., by the Markov properties determined by the graph. Both directed and undirected graphs have found extensive applications, the latter in such areas as spatial statistics and image analysis. The recent books by Whittaker (1990) and Lauritzen (1996) conveniently summarize the statistical perspective on these developments.

[†]Research supported in part by the U. S. National Science Foundation and the U. S. National Security Agency.

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Graphical Markov models determined by acyclic directed graphs (ADGs) admit especially simple statistical analyses. In particular, ADG models admit convenient recursive factorizations of their joint probability density functions (Lauritzen *et al* (1990)), provide an elegant framework for Bayesian analysis (Spiegelhalter and Lauritzen (1990)), and, in expert system applications, allow simple causal interpretations (Lauritzen and Spiegelhalter (1988)). In the multinomial and multivariate normal cases, the likelihood function (i.e., both the joint probability density function and the parameter space) factorizes and admits explicit maximum likelihood estimates, which exist with probability one (Lauritzen (1996), Andersson and Perlman (1996)). Furthermore, the only undirected graphical (UDG) models with these properties are the *decomposable* models, i.e., the UDG models that have the same Markov properties as ADG models (Dawid and Lauritzen (1993), Andersson *et al* (1996a)).

For these reasons, ADG models have become popular across an extraordinary range of applications; see, for example, Lauritzen and Spiegelhalter (1988), Pearl (1988), Neapolitan (1990), Spiegelhalter and Lauritzen (1990), Spiegelhalter *et al* (1993), Madigan and Raftery (1994), and York *et al* (1995). Indeed, the vibrant “Uncertainty in Artificial Intelligence” community focuses much of its effort on ADG models.

Much of this applied work has adopted a Bayesian perspective: “experts” specify a prior distribution on competing ADG models. These prior distributions are combined with likelihoods (typically integrated over parameters) to give posterior model probabilities. Model selection algorithms then seek out the ADG models with highest posterior probability, and subsequent inference proceeds conditionally on these selected models (Cooper and Herskovits (1990), Buntine (1994), Spiegelhalter *et al* (1993), Heckerman *et al* (1994), Madigan and Raftery (1994)). Non-Bayesian model selection methods proceed in a similar manner, replacing posterior model probabilities by, for example, penalized maximum likelihoods (Chickering (1995)).

Heckerman *et al* (1994) highlighted a fundamental problem with this general approach. Because several different ADGs may determine the *same* statistical model, i.e., may determine the same set of conditional independence restrictions among a given set of random variates, the collection of all possible ADGs for these variates naturally coalesces into one or more classes of *Markov-equivalent* ADGs, where all ADGs within a Markov-equivalence class determine the *same* statistical model. Model selection algorithms that ignore these equivalence classes face three main difficulties:

1. Repeating analyses for equivalent ADGs leads to significant computational inefficiencies.

2. Ensuring that equivalent ADGs have equal posterior probabilities imposes severe constraints on prior distributions.
3. Weighting individual ADGs in Bayesian model averaging procedures to achieve specified weights for all Markov-equivalence classes is impractical without an explicit representation of these classes.

Treating each Markov-equivalence class as a single model would overcome these difficulties. As Heckerman *et al* (1994) have pointed out, however, a tractable characterization of these equivalence classes has not been available. In the present paper we show that for every ADG D , the equivalence class $[D]$ can be uniquely represented by a certain Markov-equivalent *chain graph* D^* (Note 1), the *essential graph* associated with the equivalence class (Note 2). Furthermore, we present an explicit characterization of those graphs G such that $G = D^*$ for some ADG D , then we apply this characterization to obtain a polynomial-time algorithm for constructing D^* from D . This characterization and construction lead to more efficient model selection and model averaging procedures for ADG models, based on essential graphs. Such procedures are discussed briefly in Section 7 and at greater length in Madigan *et al* (1996).

We suggest, therefore, that graphical modelers, both Bayesian and non-Bayesian, may wish to focus their attention on the class of essential graphs rather than ADGs.

Some basic definitions, terminology, and results concerning graphs, graphical Markov models, and their Markov equivalence are summarized in Appendices A and B, which the reader might review first. In Section 2 the essential graph D^* associated with an ADG D is formally defined and illustrated. Section 3 introduces the notions of *irreversible*, *protected*, and *strongly protected arrows* and relates these to the *essential arrows* of D , i.e. the arrows of D^* .

In Section 4 we show first that D^* is a chain graph, each of whose chain components induces a chordal UDG (Proposition 4.1). Every $D' \in [D]$ can be recovered from D^* by orienting the edges of each (chordal) chain component of D^* in all possible “perfect” ways (Proposition 4.2). The chain graph D^* is itself Markov equivalent to D (Proposition 4.3).

Theorem 4.1, the main result of Section 4, applies Proposition 4.1 to obtain an explicit characterization of those graphs G that can occur as the essential graph D^* for some ADG D . Corollaries 4.1 and 4.2 characterize those UDGs and digraphs that can occur as essential graphs D^* for some ADG D . These results in turn lead to Proposition 4.5, which can be applied to establish the irreducibility of certain Markov chains used for Monte Carlo search procedures over the space of essential graphs (see Section 7).

A polynomial-time algorithm for constructing D^* from D is presented in Section 5 (Note 3). Its validity is established in Theorem 5.1 by means of our characterization of essential graphs. In Section 6 we exhibit all essential graphs on four or fewer vertices and note that the number of essential graphs is substantially smaller than the number of ADGs.

In Section 7 we indicate how the Markov-equivalence classes and their associated essential graphs can be used to overcome the three difficulties listed above that complicate model selection and model averaging for ADG models. We also briefly discuss model-search procedures based on equivalence classes and essential graphs.

Markov dependence models determined by chain graphs recently were introduced and developed by Frydenberg and Lauritzen (1989), Lauritzen and Wermuth (1989), and Frydenberg (1990); also see Andersson *et al* (1996a). The introduction of chain graphs followed earlier work in this direction by Goodman (1973), Asmussen and Edwards (1983) and Kiiveri *et al* (1984). Chain graphs provide much of the focus for current research on modeling statistical dependence; see, for example, Wermuth and Lauritzen (1990) and Cox and Wermuth (1993, 1996). The fact that the essential graph D^* associated with an ADG D is a chain graph that is Markov equivalent to D allows us to conduct statistical inference in the space of essential graphs, rather than in the larger space of individual ADGs - see Section 7, especially (7.2).

2. Markov Equivalence of Acyclic Digraphs; the Essential Graph D^* .

Our development begins with a well-known graph-theoretic criterion for the Markov equivalence of ADGs, given in Theorem 2.1. This was discovered by Verma and Pearl (1990, Theorem 1; 1992, Corollary 3.2) and, independently, by Frydenberg (1990, Theorem 5.6) for the more general class of chain graphs - also see Andersson *et al* (1996a, Theorem 3.1). Frydenberg's result is stated as Theorem B.1 of our Appendix B. For completeness, in Appendix B we also present a direct proof of Theorem 2.1, different from that of Verma and Pearl.

Theorem 2.1. Two ADGs are Markov equivalent if and only if they have the same skeleton and the same immoralities (see Figure 2.1).

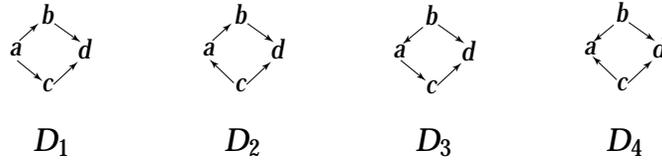


Figure 2.1: The four ADGs with the same skeleton as D_1 and the immorality (b, d, c) . The ADGs D_1 , D_2 , and D_3 have no other immoralities, hence are Markov equivalent by Theorem 2.1. The ADG D_4 has the additional immorality (b, a, c) , hence is not Markov equivalent to the others. Thus, $[D_1] = \{D_1, D_2, D_3\}$.

We say that two ADGs D_1 and D_2 are *graphically equivalent*, and write $D_1 \sim D_2$, if they have the same skeleton and the same immoralities. By Theorem 2.1, D_1 and D_2 are Markov equivalent if and only if they are graphically equivalent; thus we shall use the term *equivalent* for both notions. The equivalence class containing D is denoted by $[D]$.

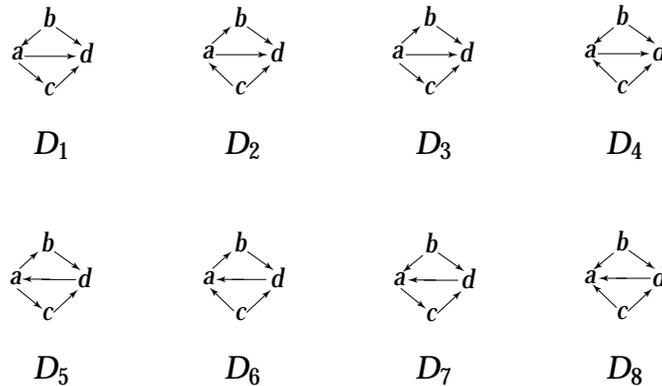


Figure 2.2: The $2^3 = 8$ possible digraphs with the same skeleton as D_1 and the immorality (b, d, c) . Of these 8, D_5 , D_6 , and D_7 are not acyclic, while D_4 and D_8 are acyclic but possess the additional immorality (b, a, c) , so $[D_1] = \{D_1, D_2, D_3\}$.

While Theorem 2.1 provides a practical criterion for deciding whether two given ADGs are Markov equivalent, it does not directly yield a characterization of the entire equivalence class $[D]$ for a given ADG D . Consider, for example, the following question regarding the non-transitive ADG D_1 in Figure 2.2: does $[D_1]$ contain a *transitive* ADG? (For the statistical relevance of this question, see Andersson *et al* (1995).) Theorem 2.1 does not allow us to answer this question by direct inspection of D_1 ; instead, we must first determine all members of $[D_1]$, then check each member for transitivity, as follows.

Since (b, d, c) is an immorality in D_1 , the arrows $b \rightarrow d$ and $c \rightarrow d$ are *essential* in D_1 , i.e., these arrows must occur in each member of $[D_1]$. The other three edges of D_1 can be oriented in $2^3 = 8$ possible ways, as shown in Figure 2.2; of these 8 digraphs, only 5 are acyclic, and of these 5, only three (D_1, D_2, D_3) possess the same immorality as D_1 and no other. Thus, $[D_1] = \{D_1, D_2, D_3\}$, hence $[D_1]$ does contain a transitive ADG, namely D_3 .

Since the number of possible orientations of all arrows that do not participate in any immorality of an ADG D grows exponentially with the number of such arrows, hence super-exponentially with the number of vertices, determination of the equivalence class $[D]$ by exhaustive enumeration of possibilities, as in the preceding example, rapidly becomes computationally infeasible as the size of D increases. A closer examination of this example reveals, however, that the arrow $a \rightarrow d$ occurs in every member of $[D_1]$, hence is an essential arrow of D_1 even though it is not involved in any immorality of D_1 . Had we been able to identify all 3 essential arrows of D_1 directly from D_1 itself, it would not have been necessary to consider $D_5 - D_8$ in order to determine $[D_1]$. On the other hand, it appears necessary to determine $[D_1]$ before we can identify the essential arrows of D_1 .

Fortunately, this is not the case. A main purpose of the present paper is to develop a polynomial-time algorithm (Section 5) for determining all essential arrows of an ADG D . This is done by introducing and characterizing the *essential graph* D^* associated with D . Furthermore, questions such as the existence of a transitive member of $[D]$ can be answered by a polynomial-time inspection of D^* itself, without the need for an exhaustive search of $[D]$ (Andersson *et al* (1996b)).

Definition 2.1. The *essential graph* D^* associated with D is the graph

$$D^* := \cup(D' \mid D' \sim D),$$

i.e., D^* is the smallest graph larger than every $D' \in [D]$.

Thus, D^* is the graph with the same skeleton as D , but where an edge is directed in D^* iff it occurs as a directed edge (\equiv arrow) *with the same orientation in every* $D' \in [D]$; all other edges of D^* are undirected. (See Figure 2.3 for examples.) The directed edges (\equiv arrows) in D^* are called the *essential arrows* of D . Clearly, every arrow that participates in an immorality in D is essential, but D may contain other essential arrows as well, e.g., the arrow $a \rightarrow d$ in the second graph in Figure 2.3 and the arrows $a \rightarrow d$ and $b \rightarrow d$ (verify!) in the third graph in Figure 2.3 (Note 4). We will show that D^* is a chain graph (Proposition 4.1) that is itself Markov equivalent (Note 5) to D (Proposition 4.3), so that

D^* contains the same statistical information as D . (Note that D and D^* have the same skeleton and immoralities, so that $D_1 \sim D_2$ iff $D_1^* = D_2^*$.) The complete characterization of essential graphs in Theorem 4.1 involves further restrictions on the configurations of arrows and lines (\equiv undirected edges) that can occur in D^* .

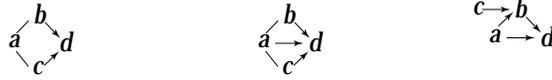


Figure 2.3: Three examples of essential graphs D^* . In the first example, D is the ADG D_1 of Figure 2.1. In the second example, D is the ADG D_1 of Figure 2.2. In the third example, $D = D^*$ (see Corollary 4.2).

3. First Characterization of the Essential Arrows of D .

By Definition 2.1, an arrow $a \rightarrow b$ in and ADG D is essential iff $a \rightarrow b \in D'$ for each $D' \in [D]$. Proposition 3.1 below shows that, in addition, $a \rightarrow b$ must be *protected* in each $D' \in [D]$, that is, must occur in each D' in at least one of the three configurations (a), (b), (c) shown below Definition 3.2.

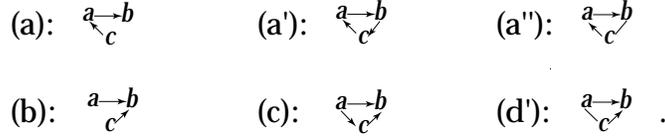
To begin, note that an essential arrow $a \rightarrow b$ must be *irreversible* in D :

Definition 3.1. Let G be a chain graph. An arrow $a \rightarrow b \in G$ is *irreversible* in G if changing $a \rightarrow b$ to $a \leftarrow b$ either creates or destroys an immorality or creates a directed cycle.

To determine whether an arrow $a \rightarrow b$ is irreversible in G according to Definition 3.1, global knowledge of G is required, since directed cycles of arbitrary length must be considered. For a characterization of irreversibility to be computationally feasible, however, it must be local, that is, must only require consideration of directed cycles of bounded length. For an ADG D , Lemma 3.1(i) shows that in fact only directed cycles of length 3 need be considered. The following definition is required.

Definition 3.2. Let G be a graph. An arrow $a \rightarrow b \in G$ is *protected* in G if $\text{pa}_G(a) \neq \text{pa}_G(b) \setminus \{a\}$.

It is easy to see that $a \rightarrow b$ is protected in G if and only if $a \rightarrow b$ occurs in at least one of the following six configurations as an induced subgraph of G :



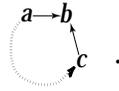
If G is a chain graph, then only (a), (b), (c), or (d') can occur; if $G \equiv D$ is an ADG, then only (a), (b), or (c) can occur. For a general graph G , $a \rightarrow b$ is protected in G iff $a \rightarrow b$ is protected in the directed graph $D(G)$ obtained by deleting all undirected edges (lines) in G (since $\text{pa}_G(a) = \text{pa}_{D(G)}(a)$).

The arrow $a \rightarrow b$ is irreversible in a chain graph G if and only if *either* $a \rightarrow b$ occurs in configuration (a) or (b) as an induced subgraph of G *or else* $a \rightarrow b$ blocks some directed cycle in G . If $a \rightarrow b$ is protected in a chain graph G , then clearly it is irreversible in G . If $G \equiv D$ is an ADG, then the converse is also true:

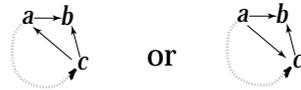
Lemma 3.1. Let D be an ADG.

- (i) An arrow $a \rightarrow b$ is irreversible in D if and only if it is protected in D .
- (ii) An arrow $a \rightarrow b$ is reversible in D if and only if the digraph D' obtained from D by replacing $a \rightarrow b$ by $a \leftarrow b$ is acyclic and $D' \sim D$.

Proof. (i) Suppose that $a \rightarrow b$ is irreversible in D by virtue of blocking some directed cycle in D :



If no edge $a \dots c$ is present in D then $a \rightarrow b$ already occurs in configuration (b) as an induced subgraph of D . If an edge $a \dots c$ is present in D then either



occurs in D . The first case is impossible since it contains a directed cycle. Thus the second must hold, so $a \rightarrow b$ occurs in configuration (c) in D . Thus $a \rightarrow b$ is protected in D .

- (ii) This assertion is immediate.

Lemma 3.1(i) is not true for a general chain graph G ; the following chain graph provides a counterexample:

$$\begin{array}{l} a \rightarrow b \\ c \rightarrow d \end{array}$$

Proposition 3.1. Let D be an ADG. An essential arrow $a \rightarrow b$ of D is protected in every $D' \in [D]$.

Proof. If $a \rightarrow b$ is an essential arrow of D then clearly $a \rightarrow b$ is irreversible in every $D' \in [D]$, hence, by Lemma 3.1(i), $a \rightarrow b$ is protected in every $D' \in [D]$.

In Proposition 3.1, it is possible *a priori* that the third vertex c in the “protecting” configuration (a), (b), or (c) for the essential arrow $a \rightarrow b \in D$ may vary with D' , i.e., $c = c(D')$. In fact this is not the case, but the notion of “protected” must be extended:

Definition 3.3. Let G be a graph. An arrow $a \rightarrow b \in G$ is *strongly protected* in G if $a \rightarrow b$ occurs in at least one of the following four configurations as an induced subgraph of G :

$$(a): \begin{array}{c} a \rightarrow b \\ \swarrow \\ c \end{array} \quad (b): \begin{array}{c} a \rightarrow b \\ \searrow \\ c \end{array} \quad (c): \begin{array}{c} a \rightarrow b \\ \swarrow \searrow \\ c \end{array} \quad (d): \begin{array}{c} c_1 \\ \swarrow \searrow \\ a \rightarrow b \\ \swarrow \searrow \\ c_2 \end{array} \quad (c_1 \neq c_2).$$

Since (d) \Rightarrow (d'), “strongly protected” \Rightarrow “protected”, while if $G \equiv D$ is an ADG, then “strongly protected” \Leftrightarrow “protected”. For a chain graph G , the definition of “strongly protected” differs from that of “protected” only in that (d) replaces (d'), but this difference is significant: by Theorem 4.1, every essential graph D^* must be a chain graph and every arrow in D^* (i.e., every essential arrow of D) must be *strongly protected* in D^* (see the examples in Figure 2.3). This characterization provides the basis for the polynomial-time algorithm in Section 5 for constructing D^* from D . (Also see Remark 5.1.)

In Corollary 4.2, it is shown that every arrow of an ADG D is essential (i.e., $D = D^*$) if and only if every arrow of D is protected in D . The third graph in Figure 2.3 provides an example.

The final lemma will be needed for the proof of Theorem 2.1 in Appendix B.

Lemma 3.2. Let D, D' be two ADGs such that $D \sim D'$ but $D \neq D'$. Then there exists a finite sequence $D \equiv D_1, \dots, D_k \equiv D'$ such that each $D_i \in [D]$ and each consecutive pair D_i, D_{i+1} differ in exactly one edge.

Proof. By the definition of equivalence, D and D' have the same vertex set V and the same skeleton. Let $F := \{a_1 \rightarrow b_1, \dots, a_n \rightarrow b_n\} \neq \emptyset$ denote the set of edges in D that occur

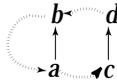
with the opposite orientation in D' . By Lemma 3.1(ii) and induction, it suffices to show that at least one $a_i \rightarrow b_j$ is reversible in D .

Suppose, to the contrary, that each $a \rightarrow b \in F$ is irreversible in D , hence by Lemma 3.1(i), is protected in D . Let b^* be a minimal element of $\{b_1, \dots, b_n\}$ with respect to the partial ordering (V, \leq) determined by the ADG D : $a \leq b$ if and only if $a = b$ or there exists a path from a to b in D . Let a^* be a maximal element of $\{a \in V \mid a \rightarrow b^* \in F\}$. Since $a^* \rightarrow b^* \in F$, $a^* \rightarrow b^*$ cannot occur in an immorality in D . Thus, because $a^* \rightarrow b^*$ is protected in D , $a^* \rightarrow b^* \in F$ must occur in D either in configuration (a) as an induced subgraph of D with $c \rightarrow a^* \in F$, or else in configuration (c) with either $a^* \rightarrow c \in F$ or $c \rightarrow b^* \in F$. But the first two possibilities violate the minimality of b^* , while the third violates the maximality of a^* . This completes the proof.

4. Characterization of the Essential Graph D^* .

Theorem 4.1, the main result of this section, gives necessary and sufficient conditions for a graph $G \equiv (V, E)$ to be the essential graph D^* for some ADG D . We begin by showing that such a G must be a chain graph. (Most proofs are deferred to the end of this section.)

Let D^{**} denote the *smallest chain graph larger than every* $D' \in [D]$. That is, D^{**} is the graph obtained from D^* by converting to undirected edges (\equiv lines) all those directed edges in D^* that participate in a directed cycle in D^* . Note that this can be done in a single step: suppose that the arrow $a \rightarrow b$ occurs in a directed cycle in D^* and that, after converting $a \rightarrow b$ into a line, a second arrow $c \rightarrow d \in D^*$ now becomes part of a directed cycle:



(possibly $a = c$ or $b = d$). Then $c \rightarrow d$ was already part of a directed cycle in D^* before $a \rightarrow b$ was converted to a line.

Clearly $D \subseteq D^* \subseteq D^{**}$. In fact, the second inclusion is an equality:

Proposition 4.1. (i) $D^* = D^{**}$, hence D^* is a chain graph.

(ii) For each chain component $\tau \in \mathbf{T}(D^*)$, the induced UDG $(D^*)_\tau$ is chordal.

Next, every ADG $D' \in [D]$ can be recovered from the essential graph D^* :

Proposition 4.2. A digraph D' is acyclic and equivalent to the ADG D if and only if D' is obtained from D^* by orienting the edges of each (chordal) chain component $(D^*)_\tau$ of D^* in any perfect way.

Proposition 4.3. Let D be an ADG and D^* its essential graph. Then D and D^* are Markov equivalent.

Theorem 4.1 (Characterization of D^*). A graph $G \equiv (V, E)$ is equal to D^* for some ADG D if and only if G satisfies the following four conditions:

- (i) G is a chain graph;
- (ii) for every chain component τ of G , G_τ is chordal;
- (iii) the configuration $a \rightarrow b - c$ does not occur as an induced subgraph of G ;
- (iv) every arrow $a \rightarrow b \in G$ is strongly protected in G .

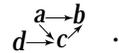
Since both UDGs and ADGs are chain graphs, Theorem 4.1 immediately yields the following two corollaries.

Corollary 4.1. Let G be a UDG. Then $G = D^*$ for some ADG D if and only if G is chordal.

Corollary 4.2. Let G be a digraph. Then $G = D^*$ for some ADG D if and only if G is an ADG and every arrow of G is protected in G ; in this case $G = D = D^*$.

Proof. Apply Theorem 4.1 and the fact that an arrow is protected in an ADG if and only if it is strongly protected in the ADG. (Note that the chain components of an ADG are just its vertices, hence trivially are chordal.)

The following is an example of an ADG D such that $D = D^*$:



Clearly, each arrow of D is protected in D .

Let $G \equiv (V, E)$ be a chain graph. An arrow $a \rightarrow b$ is an *initial arrow* of G if a is minimal in $\{a' \in V \mid \exists b \in V \ni a' \rightarrow b \in E\}$ with respect to the pre-ordering (V, \leq) determined by G . Note that G has no initial arrows iff G is a UDG. Clearly an initial arrow $a \rightarrow b$ cannot occur in configuration (a) in G , so, if $G = D^*$ for some ADG D , then Theorem 4.1 implies that $a \rightarrow b$ must occur in configuration (b), (c), or (d) as an induced subgraph of G .

Because D^* is determined by the immoralities of D , one might speculate that in this case, every initial arrow of G must in fact occur in configuration (b) or (d) as an induced subgraph of G , but this is not true in general: consider the initial arrow $a \rightarrow b$ of the chain graph (in fact, ADG) $G \equiv D \equiv D^*$ in the figure in the preceding paragraph. It is almost true, however, as seen by the following result, which provides a useful necessary condition for determining whether a given graph G is an essential graph.

Proposition 4.4. Suppose that $G = D^*$ for some ADG D . For every initial arrow $a \rightarrow b$ of G , there exists a vertex $c \in V$ such that $a \rightarrow c$ is also an initial arrow of G and $a \rightarrow c$ occurs in configuration (b) or (d) as an induced subgraph of G .

Corollary 4.3. An ADG D has no essential arrows (i.e., D^* is a UDG) if and only if D has no immoralities.

Proof. If D is moral then so is D^* , hence configurations (b) and (d) cannot occur in D^* . Proposition 4.4 implies that D^* has no initial arrows, hence D^* is a UDG. The converse is trivial.

Remark 4.1. An initial arrow in D^* need not be initial in D , nor vice versa. Consider the ADG

$$D := \begin{array}{c} d \rightarrow a \rightarrow b \\ \nearrow c \end{array} .$$

Then $a \rightarrow b$ is initial in

$$D^* \equiv \begin{array}{c} d \leftarrow a \rightarrow b \\ \nearrow c \end{array}$$

but not in D , whereas $d \rightarrow a$ is initial in D but does not occur in D^* .

The final result of this section can be applied to establish the irreducibility of certain Markov chains used for Monte Carlo search algorithms over the space of essential graphs - see Section 7.

Proposition 4.5. Let G and H be two essential graphs with the same vertex set V . Then there exists a finite sequence $G \equiv G_1, \dots, G_k \equiv H$ of essential graphs with vertex set V such that each consecutive pair G_i, G_{i+1} differ by either:

- (i) exactly one line $a \text{---} b$, or
- (ii) exactly one arrow $a \rightarrow b$, or
- (iii) exactly two arrows that form an immorality: $a \rightarrow b \leftarrow c$.

We turn to the proofs. The proof of Proposition 4.1 requires the following five Facts:

Fact 1. The configuration $a \rightarrow b \dashv c$ cannot occur as an induced subgraph of D^* .

Proof. If $a \rightarrow b \dashv c$ occurs as an induced subgraph in D^* (requiring that a and c are not linked), then $a \rightarrow b \leftarrow c$ must occur as an immorality in some $D' \sim D$, hence $b \leftarrow c$ must be an essential arrow, contradicting $b \dashv c \in D^*$.

Fact 2. If $\begin{array}{c} a \rightarrow b \\ \swarrow \searrow \\ c \end{array}$ occurs in D^* , then there exist $D_1, D_2 \in [D]$ such that $\begin{array}{c} a \rightarrow b \\ \swarrow \searrow \\ c \end{array}$ occurs in D_1 and $\begin{array}{c} a \rightarrow b \\ \swarrow \searrow \\ c \end{array}$ occurs in D_2 .

Proof. Any $D' \in [D]$ must contain either

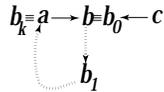
$$(1): \begin{array}{c} a \rightarrow b \\ \swarrow \searrow \\ c \end{array} \quad \text{or} \quad (2): \begin{array}{c} a \rightarrow b \\ \swarrow \searrow \\ c \end{array} \quad \text{or} \quad (3): \begin{array}{c} a \rightarrow b \\ \swarrow \searrow \\ c \end{array} .$$

If (1) were to occur in *no* $D' \in [D]$, then necessarily $c \rightarrow b \in D^*$, contradicting the hypothesis. Thus (1) must occur in some $D_1 \in [D]$. Similarly, (2) must occur in some $D_2 \in [D]$.

Fact 3. D^{**} has the same immoralities as D (hence, as D^*).

Proof. Recall that D^{**} is obtained by converting all arrows that occur in directed cycles in D^* into lines. It is evident that D^* has the same immoralities as D . Since $D^* \subseteq D^{**}$, D^{**} can have the same or fewer immoralities than D^* . We shall show it impossible that an immorality $a \rightarrow b \leftarrow c$ occurs in D^* while $a \dashv b \in D^{**}$.

If this were to happen, then $a \rightarrow b$ would be part of a directed cycle $(a, b \equiv b_0, b_1, \dots, b_k \equiv a)$ in D^* (see figure), where $k \geq 2$ and where each edge $b_{i-1} \rightarrow b_i$ in the cycle occurs as either $b_{i-1} \dashv b_i$ or $b_{i-1} \rightarrow b_i$, $1 \leq i \leq k$. (In particular, $b_1 \neq a, c$)

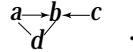


Case 1. Suppose that $b \dashv b_1 \in D^*$. Then there exist ADGs $D_1, D_2 \in [D]$ such that $b_1 \rightarrow b \in D_1$ and $b_1 \leftarrow b \in D_2$. Since $a \rightarrow b \leftarrow b_1$ cannot occur as an immorality in D_1 , there must be edges $a \rightarrow b_1$ and $c \rightarrow b_1$ in D_1 . To avoid a cycle, necessarily $a \rightarrow b_1 \in D_2$ and $c \rightarrow b_1 \in D_2$, so $a \rightarrow b_1 \leftarrow c$ forms an immorality in D_2 , hence also in D^* . Thus we have a *shorter*

directed cycle $(a, b_1, \dots, b_k \equiv a)$ in D^* such that the immorality $a \rightarrow b_1 \leftarrow c$ occurs in D^* but $a \rightarrow b_1 \in D^{**}$.

Case 2. Suppose that $b \rightarrow b_1 \in D^*$. Since D contains no directed cycles, at least one edge in the cycle $(a, b \equiv b_0, b_1, \dots, b_k \equiv a)$ must be undirected in D^* . Consider the smallest i such that $b_{i-1} \rightarrow b_i \in D^*$. This i satisfies $2 \leq i \leq k$ and $b_{i-2} \rightarrow b_{i-1} \rightarrow b_i$ occurs in D^* . By Fact 1, there must be an edge $b_{i-2} \rightarrow b_i$ in D^* . But $b_{i-2} \leftarrow b_i \notin D^*$, since there is some ADG $D' \in [D]$ containing $b_{i-1} \rightarrow b_i$ that consequently would contain a directed triangle. Therefore, either $b_{i-2} \rightarrow b_i \in D^*$ or $b_{i-2} \rightarrow b_i \in D^*$, again producing a *shorter* directed cycle $(a, b_0, \dots, b_{i-2}, b_i, \dots, b_k \equiv a)$ in D^* such that the immorality $a \rightarrow b_0 \leftarrow c$ occurs in D^* but $a \rightarrow b_0 \in D^{**}$.

Thus, Cases 1 and 2 together allow us to proceed by induction to reduce to the case where the immorality $a \rightarrow b \leftarrow c$ occurs in D^* but $a \rightarrow b$ occurs in a directed *triangle* (a, b, d) in D^* (necessarily, $d \neq c$). The only type of directed triangle (a, b, d) in D^* that does *not* imply the contradictory existence of an ADG $D' \in [D]$ such that (a, b, d) comprises a directed triangle in D' is pictured here:



By Fact 2, there exist ADGs $D_1, D_2 \in [D]$ with $a \rightarrow d, b \rightarrow d$ in D_1 and $a \leftarrow d, b \leftarrow d$ in D_2 . Thus there must be an edge $c \rightarrow d$ in D_2 . (Otherwise $d \rightarrow b \leftarrow c$ would form an immorality in D_2 , forcing $d \rightarrow b \in D^*$, contradicting the occurrence of the undirected edge $d \rightarrow b$ in D^*). Since the edge $c \rightarrow d$ must be present in D_1 also, it must be oriented there as $c \rightarrow d$ (otherwise (c, b, d) would form a directed triangle). Thus the configuration



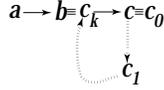
must occur in D_1 . This produces the immorality $a \rightarrow d \leftarrow c$ in D_1 , forcing $a \rightarrow d \in D^*$, contradicting the occurrence of $a \rightarrow d$ in D^* . This establishes Fact 3.

Fact 4. D^* and D^{**} have no undirected chordless k -cycles, $k \geq 4$.

Proof. If an undirected chordless k -cycle, $k \geq 4$, occurs in D^* or in D^{**} , then D must have at least one immorality in this cycle. This immorality must also occur in D^* , hence, by Fact 3, also in D^{**} , contradicting the assumption that the cycle is undirected.

Fact 5. The configuration $a \rightarrow b \rightarrow c$ cannot occur as an induced subgraph of D^{**} (i.e., a and c are not linked).

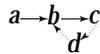
Proof. Suppose that $a \rightarrow b \rightarrow c$ occurs as an induced subgraph in D^{**} . Then $a \rightarrow b \in D^*$ and hence $a \rightarrow b \in D'$ for all $D' \in [D]$. Thus $b \leftarrow c \notin D'$ for all $D' \in [D]$ (otherwise $a \rightarrow b \leftarrow c$ forms an immorality in D' , hence in D^{**} by Fact 3), so $a \rightarrow b \rightarrow c$ occurs as an induced subgraph in all $D' \in [D]$, hence also in D^* . Therefore $b \rightarrow c$ must be part of a directed cycle $(b, c \equiv c_0, c_1, \dots, c_k \equiv b)$ in D^* (see figure), $k \geq 2$, where, for $1 \leq i \leq k$, the edge $c_{i-1} \dots c_i$ is either $c_{i-1} \rightarrow c_i$ or $c_{i-1} \leftarrow c_i$. (Note that $c_1 \neq a, b$)



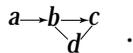
Case 1. Suppose that $c \rightarrow c_1 \in D^*$. Then there exist ADGs $D_1, D_2 \in [D]$ such that $c \rightarrow c_1 \in D_1$ and $c \leftarrow c_1 \in D_2$. Therefore there must be an edge $b \dots c_1$ in D_2 , (else $c \leftarrow c_1$ participates in an immorality), hence also in D_1 and D^* . To avoid a directed cycle, this edge must appear as $b \rightarrow c_1$ in D_1 . If there were an edge $a \dots c_1$ in D_1 , it must be $a \rightarrow c_1$ (otherwise (a, b, c_1) would comprise a directed triangle in D_1), which would imply the immorality $a \rightarrow c_1 \leftarrow c$ in D_1 , contradicting $c \rightarrow c_1 \in D^*$. Thus, there is no edge connecting a and c_1 in D_1 , hence none in D^* . Therefore the edge $b \dots c_1$ cannot occur in D^* as $b \rightarrow c_1$ (by Fact 1) or as $b \leftarrow c_1$ (since $b \rightarrow c_1 \in D_1$), hence $b \rightarrow c_1 \in D^*$. Thus $a \rightarrow b \rightarrow c_1$ also occurs as an induced subgraph in D^* , so $b \rightarrow c_1$ occurs in a *shorter* directed cycle $(b, c_1, \dots, c_k \equiv b)$ in D^* .

Case 2. Suppose that $c \rightarrow c_1 \in D^*$. Consider the smallest $i \geq 2$ such that $c_{i-1} \rightarrow c_i \in D^*$. Thus $c_{i-2} \rightarrow c_{i-1} \rightarrow c_i$ occurs in D^* , so by Fact 1, there must be an edge $c_{i-2} \dots c_i$ in D^* . As in Case 2 of Fact 3, either $c_{i-2} \rightarrow c_i \in D^*$ or $c_{i-2} \leftarrow c_i \in D^*$. Thus $a \rightarrow b \rightarrow c_0$ occurs as an induced subgraph in D^* , hence $b \rightarrow c_0$ occurs in a *shorter* directed cycle $(b, c_0, \dots, c_{i-2}, c_i, \dots, c_k \equiv b)$ in D^* .

Cases 1 and 2 together allow us to proceed by induction to reduce to the situation where $a \rightarrow b \rightarrow c$ occurs as an induced subgraph in D^* but $b \rightarrow c$ participates in a directed triangle (b, c, d) in D^* :



(necessarily, $d \neq a$). The only such directed triangle in D^* that does *not* imply the existence of an ADG $D' \in [D]$ such that (b, c, d) comprises a directed triangle in D' , is pictured here:



By Fact 2, there exist ADGs $D_1, D_2 \in [D]$ with $b \rightarrow d \leftarrow c$ in D_1 and $b \leftarrow d \rightarrow c$ in D_2 . Thus there must be an edge $a \cdots d$ in D_2 (otherwise $a \rightarrow b \leftarrow d$ would form an immorality in D_2 , forcing $b \leftarrow d \in D^*$, contradicting the occurrence of the undirected edge $b-d \in D^*$). The edge $a \cdots d$ also must be present in D_1 , where it must be oriented as $a \rightarrow d$ so that (a, b, d) does not form a directed triangle. Thus the configuration



must occur in D_1 . This produces the immorality $a \rightarrow d \leftarrow c$ in D_1 , forcing $d \leftarrow c \in D^*$, contradicting the occurrence of the undirected edge $d-c$ in D^* . Fact 5 is proved.

Proof of Proposition 4.1. (i) We know that $D^* \subseteq D^{**}$. To show that that $D^* = D^{**}$, it suffices to show that if an undirected edge $a-b \in D^{**}$, then also $a-b \in D^*$.

Let τ be the unique chain component of D^{**} such that $a-b \in (D^{**})_\tau$. By Fact 4, $(D^{**})_\tau$ is a chordal UDG. Therefore (see Appendix A) $(D^{**})_\tau$ admits two perfect directed versions, D_1 and D_2 , such that $a \rightarrow b \in D_1$ and $a \leftarrow b \in D_2$.

Now assign perfect orientations to the edges within all other chain components of D^{**} , obtaining two directed graphs, D' and D'' . These have the same skeleton as D, D^* , and D^{**} , and satisfy the following conditions:

- (1) All arrows in D^{**} also occur as arrows in D' and D'' .
- (2) $(D')_\tau = D_1$ and $(D'')_\tau = D_2$, so $a-b \in D' \cup D''$.

Both D' and D'' are acyclic. For, if D' or D'' has a directed cycle, at least one of the arrows in this cycle must be an arrow in D^{**} (otherwise the cycle must lie entirely within one chain component of D^{**} , hence cannot be directed). Thus if we convert back into lines all arrows in this cycle that came from lines in D^{**} , at least one arrow remains, giving a directed cycle in D^{**} , contradicting its chain graph property.

Next, D' and D'' have the same immoralities as D, D^* , and D^{**} , so D' and $D'' \in [D]$. To see this, begin by noting that, since D' and $D'' \subseteq D^{**}$, every immorality in D^{**} must also occur in D' and D'' . Suppose that $a \rightarrow b \leftarrow c$ is an immorality in D' or D'' . This immorality could not have arisen from the configuration $a-b-c$ in D^{**} , since the edges within each chain component of D^{**} are perfectly oriented in D' and D'' , nor, by Fact 5, could it have arisen from the configurations $a \rightarrow b-c$ or $a-b \leftarrow c$ in D^{**} . Thus the immorality $a \rightarrow b \leftarrow c$ must also occur in D^{**} .

Finally, since D' and $D'' \in [D]$, necessarily $D' \cup D'' \subseteq D^*$. But $a \rightarrow b \in D' \cup D''$, hence $a \rightarrow b \in D^*$. This completes the proof of (i). Part (ii) follows from Fact 4.

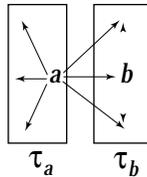
Proof of Proposition 4.2. Since $D^* = D^{**}$, the “if” assertion is established in the proof of Proposition 4.1. To verify “only if”, suppose that $D' \in [D]$. Then any arrow in D^* also occurs in D' , while D' can have no immoralities within any chain component of D^* (since D' and D^* have the same immoralities), hence the restriction of D' to each chain component of D^* is perfect.

Proof of Proposition 4.3. By Proposition 4.1, D^* is a chain graph. Since D and D^* have the same skeleton, by Theorem B.1 of Appendix B it suffices to show that D and D^* have the same minimal complexes. By Fact 3, they have the same immoralities. By Fact 1, D^* can have no minimal complexes other than immoralities; trivially, neither can D , since it is an ADG.

Proof of Theorem 4.1. (“only if”). Proposition 4.1 implies (i) and (ii), while (iii) follows from Fact 1. Property (iv) will be established by means of the following two Facts regarding the essential arrows of D : See Section 3 for the definitions of configurations (a) - (d) and (d').

Fact 6. Every essential arrow $a \rightarrow b$ of D occurs in at least one of the configurations (a), (b), (c), or (d') as an induced subgraph of D^* . Thus, $a \rightarrow b$ is irreversible in D^* .

Proof. Suppose that $a \rightarrow b \in D^*$ but satisfies neither (a), (b), (c), nor (d') in D^* . Consider the two (distinct) chain components τ_a and τ_b of D^* that contain a and b , respectively. By (ii), we can construct a directed graph D' from D^* by assigning arbitrary perfect orientations to the edges of $(D^*)_\tau$ for every chain component τ other than τ_a and τ_b , and by assigning perfect orientations *starting at* a (resp., b) to the edges within τ_a (resp., τ_b), so that all edges within τ_a (τ_b) that involve a (b) are oriented outward from a (b) (see figure). By Proposition 4.2, D' is an ADG and $D' \in [D]$.



Now construct another directed graph D'' , which is identical to D' except that $a \rightarrow b \in D'$ is changed to $a \leftarrow b$ in D'' . Then D'' is also acyclic, for if it were to contain a

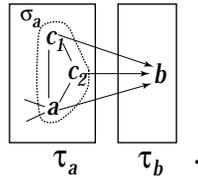
directed cycle, then this cycle must include $a \leftarrow b$, hence must include a subgraph $a \leftarrow b \leftarrow c$ of D'' with $c \neq a$. Necessarily $c \notin \tau_b$, since all arrows of D'' within τ_b are oriented outward from b , so $b \leftarrow c \in D^*$. Thus $a \rightarrow b \leftarrow c$ occurs in D^* , so, since $a \rightarrow b$ cannot satisfy (b) in D^* , there must be an edge $a \cdots c$ in D^* . This edge cannot be $a \rightarrow c$ or $a \leftarrow c$, otherwise $a \rightarrow b$ would satisfy (c) or (d') in D^* , hence must appear as $a \leftarrow c$ in D^* . Thus $a \leftarrow c$ must also occur in D'' , so the assumed directed cycle in D'' must have contained at least four vertices. Therefore, removing the vertex b from this cycle leaves another directed cycle in D'' , which must also occur in D' since D' and D'' coincide except for the edge $a \rightarrow b$. This is a contradiction, so we conclude that D'' is acyclic.

We shall show that D'' has the same immoralities as D' . If an immorality $c \rightarrow a \leftarrow b$ is created in D'' when $a \rightarrow b$ is changed to $a \leftarrow b$, necessarily $c \notin \tau_a$, since all arrows of D'' within τ_a are oriented outward from a . Therefore $c \rightarrow a \in D^*$, hence $c \rightarrow a \rightarrow b$ occurs as an induced subgraph in D^* , contradicting the assumed non-occurrence of (a) in D^* . Next, no immorality $a \rightarrow b \leftarrow c$ can occur in D' , since D' and $(D')^* = D^*$ have the same immoralities and (b) is assumed not to occur in D^* . Thus D' and D'' have the same immoralities.

It follows that $D'' \in [D]$, whereby $D' \cup D'' \subseteq D^*$. But $a \rightarrow b \in D' \cup D''$, hence $a \rightarrow b \in D^*$, contradicting the assumption that $a \rightarrow b \in D^*$ and thereby establishing Fact 6.

Fact 7. Every essential arrow of D is strongly protected in D^* .

Proof. Suppose that $a \rightarrow b \in D^*$ but satisfies neither (a), (b), (c), nor (d) in D^* . By Fact 6, $a \rightarrow b$ occurs in configuration (d') for some $c \neq a, b$. Define the chain components τ_a and τ_b as above, and define $\sigma_a = \{c' \in \tau_a \mid c' \rightarrow b \in D^*\}$:

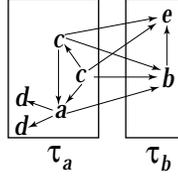


By (d'), a and $c \in \sigma_a$. We assert that G_{σ_a} is a complete subgraph of G_{τ_a} in $G \equiv D^*$.

Let c_1, c_2 be two distinct vertices in σ_a ; it must be shown that $c_1 \rightarrow c_2 \in D^*$. Suppose first that $c_2 = a$. Then an edge $a \cdots c_1$ must occur in D^* , or else $a \rightarrow b$ would satisfy (b) in D^* . Since $c_1 \in \sigma_a$, this edge must be $a \leftarrow c_1$. Next, suppose that $a \neq c_1, c_2$. By the first case, $a \leftarrow c_1 \in D^*$ and $a \leftarrow c_2 \in D^*$. Therefore an edge $c_1 \cdots c_2$ must occur in D^* , else $a \rightarrow b$ would satisfy (d) in D^* . Since $c_1, c_2 \in \tau_a$, this edge must be $c_1 \rightarrow c_2$.

Construct a directed graph D' from D^* as follows (see the following figure):

- (1) For each chain component τ of $G \equiv D^*$ other than τ_a or τ_b , orient the edges of G_τ perfectly.
- (2) Assign a perfect orientation to the edges of G_{τ_b} starting at b .
- (3) Assign a perfect orientation to the edges of G_{τ_a} so that:
 - (α) any edge $a-c$ with $c \in \sigma_a$ becomes $a \leftarrow c$, and
 - (β) any edge $a-d$ with $d \in \tau_a \setminus \sigma_a$ becomes $a \rightarrow d$.



It must be shown that such an orientation exists for G_{τ_a} . Let $c_1, \dots, c_q \equiv a$ be any ordering of the vertices in σ_a such that a occurs last. Starting at c_1 , order the edges of G_{τ_a} by applying Maximum Cardinality Search. The completeness of G_{σ_a} ensures that MCS can reproduce the initial sequence c_1, \dots, c_q . The resulting perfect orientation of the edges within G_{τ_a} determined by this perfect ordering clearly satisfies (α) and (β).

By Proposition 4.2, D' is an ADG and $D' \in [D]$. Now construct a directed graph D'' which is identical to D' except that $a \rightarrow b \in D'$ is changed to $a \leftarrow b$ in D'' . If D'' were to contain a directed cycle, then this cycle must include $a \leftarrow b$, hence must include a subgraph $a \leftarrow b \leftarrow c$ of D'' with $c \neq a$. By (2), $c \notin \tau_b$, so $b \leftarrow c \in D^*$. Thus $a \rightarrow b \leftarrow c$ occurs in D^* , so, since $a \rightarrow b$ cannot satisfy (b) in D^* , there must be an edge $a \dots c$ in D^* . This edge cannot be $a \rightarrow c$, otherwise $a \rightarrow b$ would satisfy (c) in D^* , hence must appear as either $a \rightarrow c$ or $a \leftarrow c$ in D^* . If $a \rightarrow c \in D^*$ then $c \in \tau_a$, hence $c \in \sigma_a$; by (α), this implies that $a \leftarrow c \in D'$ and therefore $a \leftarrow c \in D''$. If $a \leftarrow c \in D^*$, then again $a \leftarrow c$ must occur in both D' and D'' . In either case, the assumed directed cycle in D'' cannot consist of the three vertices a, b, c alone, hence must have at least four distinct vertices. Furthermore, since $a \leftarrow c \in D''$, removing b from this directed cycle leaves a shorter directed cycle in D'' which must also occur in D' since D' and D'' coincide except for the edge $a \dots b$, contradicting the acyclicity of D' . Thus D'' is acyclic.

Now we show that D'' has the same immoralities as D' . If a new immorality $c \rightarrow a \leftarrow b$ is created in D'' when $a \rightarrow b$ is changed to $a \leftarrow b$, then $c \rightarrow a \rightarrow b$ occurs in D' . Necessarily $c \notin \sigma_a$, for otherwise an edge $c \dots b$ would occur in D^* . Also $c \notin \tau_a \setminus \sigma_a$ otherwise, by (β), $c \leftarrow a \in D'$. Thus $c \notin \tau_a$, so $c \rightarrow a \in D^*$. Therefore $c \rightarrow a \rightarrow b$ occurs in D^* as an induced

subgraph of D^* , contradicting the assumed non-occurrence of (a). Next, no immorality $a \rightarrow b \leftarrow c$ can occur in D' , since D' and $(D')^* = D^*$ have the same immoralities and (b) is assumed not to occur in D^* . Thus D' and D'' have the same immoralities, so $D' \sim D''$.

It follows that $D'' \in [D]$, hence $D' \cup D'' \subseteq D^*$. But $a \rightarrow b \in D' \cup D''$, hence $a \rightarrow b \in D^*$, contradicting the assumed occurrence of $a \rightarrow b$ in D^* . This establishes Fact 7 and thereby completes the proof of the “only if” assertion of Theorem 4.1.

(“if”) Let $G \equiv (V, E)$ be a graph that satisfies conditions (i) - (iv). It must be shown that $G = D^*$ for some ADG D . Let D be a digraph obtained from G by assigning arbitrary perfect orientations to the edges within each (chordal) chain component of G . Note that $D \subseteq G$. We shall show that D is an ADG and that $G = D^*$.

Suppose first that D contains a directed cycle. It cannot lie entirely within one chain component of G , hence at least one of its arrows is also an arrow in G . Therefore it determines a directed cycle in G , contradicting (i). Thus D is an ADG.

To show that $G \subseteq D^*$, let $\mathbf{D}(G)$ be the collection of *all* ADGs D' constructed from G by assigning perfect orientations to the edges within each chain component of G (that is, all ADGs D' constructed in the same manner as D). Clearly $G \supseteq D'$, so $G \supseteq \cup(D' \mid D' \in \mathbf{D}(G))$. Furthermore, any line $a \rightarrow b \in G$ lies in G_τ for some chain component τ of G . By (ii), there exist two perfect orientations of the edges in G_τ , one with $a \rightarrow b$ and one with $a \leftarrow b$, so $G = \cup(D' \mid D' \in \mathbf{D}(G))$. By (ii) and (iii), no immorality in D' or D can involve an arrow that had been a line in G , i.e., an arrow that lies within a chain component of G . Thus any immorality in D' or D is an immorality in G and conversely, so $D' \sim D$. Therefore $\cup(D' \mid D' \in \mathbf{D}(G)) \subseteq \cup(D' \mid D' \sim D) \equiv D^*$, so $G \subseteq D^*$. It remains to show that $G = D^*$.

For this, it suffices to show that

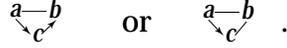
$$A := \{a \in V \mid \exists b \in V \ni a \rightarrow b \in G \text{ and } a \rightarrow b \in D^*\} = \emptyset.$$

If not, let a be a minimal element of A with respect to the pre-ordering (V, \leq) determined by the chain graph G . Since $a \in A$,

$$B := \{b \in V \mid a \rightarrow b \in G \text{ and } a \rightarrow b \in D^*\} \neq \emptyset.$$

Let b be a minimal element of B ; then $a \rightarrow b \in G$ and $a \rightarrow b \in D^*$. By (iv), $a \rightarrow b$ occurs in at least one of the configurations (a), (b), (c), or (d) as an induced subgraph of G . If (a) were to occur in G , then, since a is minimal in A , $c \rightarrow a \notin D^*$, hence $c \rightarrow a \in D^*$. But then $c \rightarrow a \rightarrow b$ occurs as an induced subgraph of D^* , which is impossible by Fact 1. If (b) were

to occur in G , then it must also occur in D , so $a \rightarrow b \in D^*$, which is also impossible. If (c) were to occur in G , then the minimality of b implies that $a \rightarrow c \notin D^*$. Since $G \subseteq D^*$, one of the following two directed triangles must occur in D^* , again impossible:



If (d) were to occur in G , then D^* would contain two directed triangles, also impossible. Thus $A = \emptyset$, hence $G = D^*$. The proof of Theorem 4.1 is complete.

Proof of Proposition 4.4. By hypothesis, the set

$$B := \{b' \in V \mid a \rightarrow b' \in G\}$$

is nonempty. Let c be any minimal element of B with respect to the pre-ordering (V, \leq) determined by the chain graph G . Since $a \rightarrow c$ is an initial arrow of G , it cannot occur in configuration (a) in G , nor can it occur in configuration (c), by the minimality of c . By Theorem 4.1(iv), therefore, $a \rightarrow c$ must occur in configuration (b) or (d) as an induced subgraph of G .

Proof of Proposition 4.5. It suffices to establish the result when H has *no* edges, i.e., $H = (V, \emptyset)$. First assume that G contains at least one line (\equiv undirected edge), so $G \equiv G_1$ has at least one chain component τ with at least two vertices. Since G_τ is chordal, it has at least one simplicial vertex a (cf. Blair and Peyton (1993, Lemma 2.2)); since G_τ is connected, $\text{bd}_{G_\tau}(a) \neq \emptyset$. Choose any $b \in \text{bd}_{G_\tau}(a)$, so that $a \rightarrow b \in G_\tau$, then remove the line connecting a and b to produce a graph G_2 . Since a was simplicial in G_τ , $(G_2)_\tau$ is also chordal. Because G_1 is an essential graph, it is now straightforward to verify that G_2 satisfies the conditions of Theorem 4.1, hence G_2 is also an essential graph. Continue this process (i) of single line removal until reaching an essential graph G_j with no lines. (A related argument appears in Lemma 5 of Frydenberg and Lauritzen (1989).)

If G_j has no arrows (\equiv directed edges), then $G_j = H$ and we are done. Otherwise, we can reach $H \equiv (V, \emptyset)$ by removing arrows from the ADG G_j according to (ii) or (iii) as follows. Let $B (\neq \emptyset)$ be the set of all *terminal* vertices of G_j , i.e., the set of all $b \in V$ such that b is maximal in V with respect to the ordering (V, \leq) determined by the ADG G_j . Since G_j has at least one arrow, there must exist at least one $b \in B$ such that $A := \{a \in V \mid a \rightarrow b \in G_j\} \neq \emptyset$. Define $A_0 := \{a \in V \mid a \text{ is minimal in } A\} (\neq \emptyset)$. By Corollary 4.2, every arrow in G_j is protected in G_j . If A_0 contains only one vertex a , the minimality of a and the maximality of b imply that removal of the arrow $a \rightarrow b$ cannot leave any other arrow

unprotected in the resulting ADG. If A_0 contains two or more vertices, their minimality implies that no two are adjacent in G_j . As in the first case, it follows that the arrows that these vertices form with b can be removed singly, until only two remain, and then either singly or as a pair (Note 6), in such a way that after each removal all remaining arrows are protected in the resulting ADG. Again by Corollary 4.2, each such ADG is an essential graph. This process can be continued until A_0 is exhausted, so that b becomes an isolated vertex in the resulting essential graph. Now consider the set of terminal vertices in this new essential graph and repeat the arrow removal process. Eventually all arrows can be removed and H will be reached. The proof is complete.

5. Construction of the Essential Graph D^* .

We now present a polynomial-time algorithm to construct the essential graph D^* from an ADG $D \equiv (V, E)$. This algorithm does *not* require an exhaustive search over the entire equivalence class $[D]$.

The Construction Algorithm. Define $G_0 := D$. For $i \geq 1$, convert every arrow $a \rightarrow b \in G_{i-1}$ that is *not* strongly protected in G_{i-1} into a line $a \text{---} b$, obtaining a graph G_i . Stop after k steps, where $k \geq 0$ is the smallest nonnegative integer such that $G_k = G_{k+1}$. Necessarily, $k \leq |E|$.

This algorithm produces a sequence G_0, \dots, G_k of graphs such that

$$(5.1) \quad D \equiv G_0 \subset \dots \subset G_k = G_{k+1}.$$

Since both arrows of an immorality are strongly protected, each G_i has the same immoralities as D and D^* . Let $n = |V|$. Because the determination of the set of arrows that are not strongly protected in G_{i-1} requires at most $O(n^4)$ operations and because $|E| = O(n^2)$, this algorithm requires at most $O(n^6)$ operations, although it can be implemented in a more efficient fashion.

Theorem 5.1 (Validity of the Construction Algorithm). $G_k = D^*$.

Proof. If $k = 0$ (i.e., if every arrow of D is protected in D) then the result follows from Corollary 4.2. Thus we may assume that $k \geq 1$.

We begin by showing that $G_k \subseteq D^*$. First, by (5.1), $a \rightarrow b \in G_k \Rightarrow a \rightarrow b \in D \Rightarrow a \leftarrow b \notin D^* \Rightarrow$ either $a \rightarrow b \in D^*$ or $a \leftarrow b \in D^*$. It remains to show that $a \leftarrow b \in G_k \Rightarrow a \leftarrow b \in D^*$. We shall accomplish this by proving that

$$B := \{b \in V \mid \exists a \in V \ni a \leftarrow b \in G_k \text{ and } a \rightarrow b \in D^*\} = \emptyset.$$

Suppose that $B \neq \emptyset$. Let b_0 be a minimal element of B with respect to the pre-ordering (V, \leq) determined by the chain graph D^* . Therefore

$$A := \{a \in V \mid a \leftarrow b_0 \in G_k \text{ and } a \rightarrow b_0 \in D^*\} \neq \emptyset.$$

For $a \in A$, let $i(a) \in \{1, \dots, k\}$ be the unique integer such that $a \rightarrow b_0 \in G_{i(a)-1}$ but $a \leftarrow b_0 \in G_{i(a)}$. Choose $a_0 \in A$ to minimize $i(a)$ over A . Thus, for no $a \in A$ is $a \rightarrow b_0$ converted to $a \leftarrow b_0$ before $a_0 \rightarrow b_0$ is converted to $a_0 \leftarrow b_0$ in the sequence G_0, G_1, \dots, G_k . Therefore, a_0 and b_0 satisfy the following four properties:

- (1) $a_0 \leftarrow b_0 \in G_k$ and $a_0 \rightarrow b_0 \in D^*$;
- (2) $a_0 \rightarrow b_0 \in G_{i(a_0)-1}$ but $a_0 \leftarrow b_0 \in G_{i(a_0)}$, i.e., $a_0 \rightarrow b_0$ is not strongly protected in $G_{i(a_0)-1}$;
- (3) if $a \rightarrow b_0 \in D^*$ but $a \leftarrow b_0 \in G_k$, then $a \rightarrow b_0 \in G_{i(a_0)-1}$;
- (4) if $b < b_0$ in D^* , then for every $a \in V$ either $a \leftarrow b \notin G_k$ or $a \rightarrow b \notin D^*$.

By Theorem 4.1(iv), $a_0 \rightarrow b_0 \in D^*$ must occur in at least one of the following four configurations as an induced subgraph of D^* :

$$(a): \begin{array}{c} a_0 \rightarrow b_0 \\ \searrow c \end{array} \quad (b): \begin{array}{c} a_0 \rightarrow b_0 \\ \nearrow c \end{array} \quad (c): \begin{array}{c} a_0 \rightarrow b_0 \\ \searrow c \nearrow \end{array} \quad (d): \begin{array}{c} c_1 \nearrow \\ a_0 \rightarrow b_0 \\ c_2 \searrow \end{array} \quad (c_1 \neq c_2).$$

However, each of these four possibilities leads to a contradiction:

(a): If $c \rightarrow a_0 \rightarrow b_0$ occurs as an induced subgraph of D^* , apply (4) with $b = a_0$ and $a = c$ to conclude that $c \leftarrow a_0 \notin G_k$. But $c \rightarrow a_0 \in D^* \Rightarrow c \rightarrow a_0 \in D \subset G_k$, hence $c \rightarrow a_0 \in G_k$. By (5.1), $c \rightarrow a_0 \in G_{i(a_0)-1}$, so by (2), $c \rightarrow a_0 \rightarrow b_0$ occurs as an induced subgraph of $G_{i(a_0)-1}$. This implies that $a_0 \rightarrow b_0$ is strongly protected in $G_{i(a_0)-1}$, which contradicts (2).

(b): The occurrence of the immorality $a_0 \rightarrow b_0 \leftarrow c$ in D^* implies its occurrence in $D \equiv G_0$. Thus both $a_0 \rightarrow b_0$ and $b_0 \leftarrow c$ are strongly protected in G_0 , hence in G_1, \dots, G_{k-1} . Therefore $a_0 \rightarrow b_0 \in G_k$, which contradicts (1).

(c): Here, necessarily $c \rightarrow b_0 \in D$. By (5.1), either $c \rightarrow b_0 \in G_k$ or $c \leftarrow b_0 \in G_k$. In the first case, $c \rightarrow b_0 \in G_{i(a_0)-1}$; in the second case, apply (3) with $a = c$ to reach the same conclusion. Together with (2), this implies that one of the following three configurations must occur in $G_{i(a_0)-1}$:

$$\begin{array}{c} a_0 \rightarrow b_0 \\ \swarrow \quad \searrow \\ \quad c \end{array} \quad \text{or} \quad \begin{array}{c} a_0 \rightarrow b_0 \\ \swarrow \quad \searrow \\ \quad c \end{array} \quad \text{or} \quad \begin{array}{c} a_0 \rightarrow b_0 \\ \swarrow \quad \searrow \\ \quad c \end{array} .$$

The first configuration is impossible, since $a_0 \rightarrow c \in D^* \Rightarrow a_0 \rightarrow c \in D \subseteq G_{i(a_0)-1}$. The second configuration is impossible, for otherwise $a_0 \rightarrow b_0$ is strongly protected in $G_{i(a_0)-1}$, contradicting (2). If the third configuration holds, apply (4) with $b = c$ and $a = a_0$ to deduce that $a_0 \leftarrow c \notin G_k$, which contradicts the fact that $a_0 \leftarrow c \in G_{i(a_0)-1}$ in this configuration.

(d): If this configuration occurs as an induced subgraph of D^* , then the immorality $c_1 \rightarrow b_0 \leftarrow c_2$ must occur in D and hence in G_1, \dots, G_k . Together with (2), this implies that



occurs in $G_{i(a_0)-1}$ but that $a_0 \rightarrow b_0$ is not strongly protected in $G_{i(a_0)-1}$. Therefore, one of the following three configurations must occur as an induced subgraph of $G_{i(a_0)-1}$:

$$\begin{array}{c} c_1 \rightarrow b_0 \\ \swarrow \quad \searrow \\ a_0 \rightarrow b_0 \\ \swarrow \quad \searrow \\ \quad c_2 \end{array} \quad \text{or} \quad \begin{array}{c} c_1 \rightarrow b_0 \\ \swarrow \quad \searrow \\ a_0 \rightarrow b_0 \\ \swarrow \quad \searrow \\ \quad c_2 \end{array} \quad \text{or} \quad \begin{array}{c} c_1 \rightarrow b_0 \\ \swarrow \quad \searrow \\ a_0 \rightarrow b_0 \\ \swarrow \quad \searrow \\ \quad c_2 \end{array} .$$

In the first case the immorality $c_1 \rightarrow a_0 \leftarrow c_2$ occurs in D and therefore in D^* , contradicting the assumed occurrence of $c_1 \leftarrow a_0 \leftarrow c_2$ in D^* . In the second case, either $c_1 \rightarrow a_0 \leftarrow c_2$ or $c_1 \rightarrow a_0 \rightarrow c_2$ must occur as an induced subgraph of D . As before, the immorality leads to a contradiction, so $c_1 \rightarrow a_0 \rightarrow c_2$ must occur as an induced subgraph of D and hence of $G_1, \dots, G_{i(a_0)-2}$. Therefore $a_0 \rightarrow c_2$ is strongly protected in $G_{i(a_0)-2}$, contradicting the occurrence of $a_0 \leftarrow c_2$ in $G_{i(a_0)-1}$ in this case. The third case is similar to the second.

Thus, each of the four possible configurations (a), (b), (c), (d) leads to a contradiction, so $B = \emptyset$, hence $G_k \subseteq D^*$. It remains to show that $G_k = D^*$. For this purpose it suffices to show that

$$B' := \{b \in V \mid \exists a \in V \ni a \rightarrow b \in G_k \text{ and } a \leftarrow b \in D^*\} = \emptyset.$$

Suppose that $B' \neq \emptyset$. Let b_0 be a minimal element of B' with respect to the partial ordering (V, \leq) determined by the ADG D (not D^*). (Since $D \subseteq G_k$, this partial ordering

is compatible with arrows in G_k , i.e., $a \rightarrow b \in G_k \Rightarrow a < b \in D$.) Thus there exists $a \in V$ such that $a \rightarrow b_0 \in G_k$ and $a \dashv b_0 \in D^*$.

Since $a \rightarrow b_0 \in G_k$, $a \rightarrow b_0$ must be strongly protected in G_k , hence must occur in one of the following four configurations as an induced subgraph of G_k :

$$(a): \begin{array}{c} a \rightarrow b_0 \\ \swarrow \quad \searrow \\ c \end{array} \quad (b): \begin{array}{c} a \rightarrow b_0 \\ \swarrow \quad \searrow \\ c \end{array} \quad (c): \begin{array}{c} a \rightarrow b_0 \\ \swarrow \quad \searrow \\ c \end{array} \quad (d): \begin{array}{c} c_1 \rightarrow b_0 \\ \swarrow \quad \searrow \\ a \rightarrow b_0 \\ \swarrow \quad \searrow \\ c_2 \end{array} \quad (c_1 \neq c_2).$$

(a): If $c \rightarrow a \rightarrow b_0$ occurs as an induced subgraph of G_k , then it also occurs as such in D . The minimality of b_0 then implies that $c \rightarrow a \in D^*$, hence $c \rightarrow a \dashv b_0$ occurs as an induced subgraph of D^* , contradicting Fact 1.

(b): The occurrence of the immorality $a \rightarrow b_0 \leftarrow c$ in G_k implies its occurrence in D and hence in D^* , contradicting the fact that $a \dashv b_0 \in D^*$.

(c): If configuration (c) occurs in G_k , the minimality of b_0 implies that $a \rightarrow c \in D^*$. Since $G_k \subseteq D^*$ and $a \dashv b_0 \in D^*$, one of the following two directed triangles must occur in D^* , contradicting Proposition 4.1.

$$\begin{array}{c} a \rightarrow b_0 \\ \swarrow \quad \searrow \\ c \end{array} \quad \text{or} \quad \begin{array}{c} a \rightarrow b_0 \\ \swarrow \quad \searrow \\ c \end{array} .$$

(d): If configuration (d) occurs as an induced subgraph of G_k , then the configuration

$$\begin{array}{c} c_1 \rightarrow b_0 \\ \swarrow \quad \searrow \\ a \rightarrow b_0 \\ \swarrow \quad \searrow \\ c_2 \end{array}$$

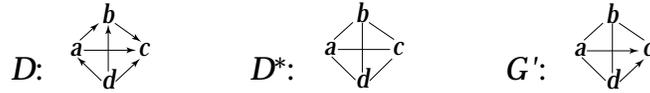
must occur as an induced subgraph of D^* . This forces the occurrence of the configuration

$$\begin{array}{c} c_1 \rightarrow b_0 \\ \swarrow \quad \searrow \\ a \rightarrow b_0 \\ \swarrow \quad \searrow \\ c_2 \end{array}$$

in D^* (otherwise D^* would contain a directed triangle). Since $D \subseteq D^*$, the immorality $c_1 \rightarrow a \leftarrow c_2$ must occur in D and therefore in G_k , contradicting the assumed occurrence of $c_1 \dashv a \dashv c_2$ in G_k .

Each of the four possible configurations (a), (b), (c), (d) has led to a contradiction, so $B' = \emptyset$. Therefore $G_k = D^*$ and the proof of Theorem 5.1 is complete.

Remark 5.1. The Construction Algorithm becomes invalid if “strongly protected” is replaced by “protected”. The following ADG D provides a counterexample:



The valid algorithm produces D^* from D after $k = 2$ steps, while the invalid version stops at G' after $k = 2$ steps.

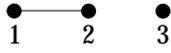
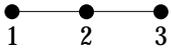
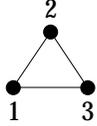
6. A Brief Catalog of Essential Graphs.

By Theorem 4.1, essential graphs may be viewed as generalizations of chordal graphs. Darroch *et al* (1980) give a brief catalog of chordal (\equiv decomposable) graphs; here we do the same for essential graphs with $n \leq 4$ vertices. In Table 6.1 we list all such *unlabelled* essential graphs (Note 7) together with their corresponding *global* Markov properties (Note 8), then we simply enumerate the corresponding *labelled* essential graphs D^* and the corresponding *labelled* ADGs D' in the equivalence class $[D]$. In applications, of course, different labelled essential graphs represent different statistical models, whereas different labelled ADGs D' corresponding to the same labelled essential graph represent the same statistical model.

Thus, for example, the second essential graph listed in Table 6.1 corresponds to one labelled D^* : $1-2$; and to two labelled D' : $1 \rightarrow 2$ and $1 \leftarrow 2$. The fifth essential graph in Table 6.1 corresponds to three labelled D^* : $1-2-3$, $1-3-2$, $2-3-1$, each representing a different statistical model; and to nine labelled D' : $1 \rightarrow 2 \rightarrow 3$, $1 \leftarrow 2 \leftarrow 3$, $1 \leftarrow 2 \rightarrow 3$, $1 \rightarrow 3 \rightarrow 2$, $1 \leftarrow 3 \leftarrow 2$, $1 \leftarrow 3 \rightarrow 2$, $2 \rightarrow 1 \rightarrow 3$, $2 \leftarrow 1 \leftarrow 3$, $2 \leftarrow 1 \rightarrow 3$, representing the same three models.

For $n = 5$ vertices, we have utilized a computer search to find that the total numbers of labelled essential graphs and labelled ADGs are 8,782 and 29,281, respectively. Robinson (1976) gives a recursive formula for the number of labelled ADGs, from which it follows that there are 3,781,503 labelled ADGs for $n = 6$ vertices, but at present no formula is available for the number of labelled essential graphs. It would be of interest to determine the asymptotic behavior of the ratio of these numbers as n approaches infinity.

Table 6.1: Essential graphs with $n = 2, 3,$ and 4 vertices.

| | <i>Essential graph</i> | <i>Markov property</i> | <i>No. of labelled essential graphs</i> | <i>No. of labelled ADGs</i> |
|----------------|---|------------------------|---|-----------------------------|
| $n=2$ |  | $1 \perp 2$ | 1 | 1 |
| |  | (None) | 1 | 2 |
| | Totals: | | 2 | 3 |
| $n=3$ |  | $1 \perp 2 \perp 3$ | 1 | 1 |
| |  | $(1,2) \perp 3$ | 3 | 6 |
| |  | $1 \perp 3 \mid 2$ | 3 | 9 |
| |  | $1 \perp 3$ | 3 | 3 |
| |  | (None) | 1 | 6 |
| Totals: | | 11 | 25 | |

$n=4$

| | | | |
|--|---|----|----|
| | $1 \perp 2 \perp 3 \perp 4$ | 1 | 1 |
| | $(1,2) \perp 3 \perp 4$ | 6 | 12 |
| | $(1,2) \perp (3,4)$ | 3 | 12 |
| | $1 \perp 3 \mid 2$ $(1,2,3) \perp 4$ | 12 | 36 |
| | $1 \perp 3$ $(1,2,3) \perp 4$ | 12 | 12 |

| | | | |
|--|-------------------|---|----|
| | $(1,2,3) \perp 4$ | 4 | 24 |
|--|-------------------|---|----|

| | | | |
|--|--|----|----|
| | $1 \perp 3 \mid 2$ $(1,2) \perp 4 \mid 3$ | 12 | 48 |
| | $1 \perp (3,4)$ $2 \perp 4 \mid 1,3$ | 24 | 48 |

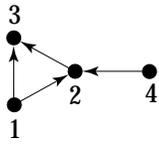
| | | | |
|--|--|---|----|
| | $1 \perp (3,4) \mid 2$ $(1,3) \perp 4 \mid 2$ | 4 | 16 |
|--|--|---|----|

| | | | |
|--|---------------------------------------|----|----|
| | $1 \perp 3$ $(1,3) \perp 4 \mid 2$ | 12 | 12 |
|--|---------------------------------------|----|----|

| | | | |
|--|---------------------|---|---|
| | $1 \perp 3 \perp 4$ | 4 | 4 |
|--|---------------------|---|---|

| | | | |
|--|------------------------|----|----|
| | $(1,3) \perp 4 \mid 2$ | 12 | 96 |
|--|------------------------|----|----|

| | | | |
|--|-----------------|----|----|
| | $(1,3) \perp 4$ | 12 | 24 |
|--|-----------------|----|----|

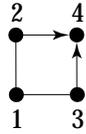


$$1 \perp 4$$

$$3 \perp 4 \mid 1,2$$

24

24

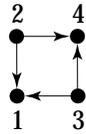


$$2 \perp 3 \mid 1$$

$$1 \perp 4 \mid 2,3$$

12

36

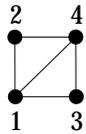


$$2 \perp 3$$

$$1 \perp 4 \mid 2,3$$

6

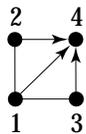
6



$$2 \perp 3 \mid 1,4$$

6

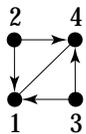
60



$$2 \perp 3 \mid 1$$

12

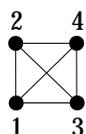
36



$$2 \perp 3$$

6

12



(None)

1

24

Totals:

185

543

7. Model Selection and Model Averaging for Acyclic Digraphs.

By focusing on Markov-equivalence classes of ADGs rather than on the individual ADGs themselves, data analysts and expert system builders can overcome several difficulties associated with ADG models. Three such difficulties were listed in Section 1 - here we examine these in more detail and indicate how the introduction of essential graphs can help to overcome them.

1. Heckerman *et al* (1994) and Chickering (1995) argue that statistical inference for ADG models should be “score equivalent”: in the absence of *a priori* causal knowledge, Markov-equivalent ADGs should have identical posterior model probabilities (Bayesian) or identical penalized likelihoods (non-Bayesian). Under this criterion, therefore, model selection and model averaging algorithms need visit each Markov-equivalence class only once. However, standard algorithms (e.g., Madigan and Raftery (1994), Madigan and York (1995), Heckerman *et al* (1994)) fail to treat each Markov-equivalence class of ADGs as a single statistical model and search in the space of ADGs, introducing considerable computational inefficiency. For example, an exhaustive search amongst all ADGs on four variables would require the calculation of posterior probabilities for all 543 such ADGs, whereas a search over the space of essential graphs (in 1-1 correspondence with the equivalence classes) would require only 185 such calculations. For five variables the numbers become 8,782 and 29,281, respectively.

2. For a Bayesian analysis over the space of all *individual* ADG models with a fixed vertex set V , score equivalence imposes severe restrictions on the prior distributions that may be used to represent prior knowledge about the parameters these models. For any individual ADG D , the joint pdf (if it exists) of a global D -Markovian distribution admits the factorization (cf. Lauritzen *et al* (1990, Theorem 1))

$$(7.1) \quad f(V) = \prod(f(a | \text{pa}_D(a)) | a \in V).$$

For categorical data (Note 9), where each conditional pdf $f(a | \text{pa}_D(a))$ is multinomial, Spiegelhalter and Lauritzen (1990) proposed the now-widely accepted conjugate family of Dirichlet prior distributions for the parameters occurring in these conditional multinomial distributions. However, Heckerman *et al* (1994) show that score equivalence *requires that the sum of the parameters of all the Dirichlet distributions associated with each $a \in V$ (ie, the Dirichlet distributions for each of the levels of $\text{pa}_D(a)$) be identical for all $a \in V$* . Since these sums behave as “equivalent sample sizes” in subsequent Bayesian

updating, this constraint severely restricts an “expert” with more prior knowledge about some variables than others - he must use a single equivalent sample size for *each* of the Dirichlet distributions occurring in the conjugate prior, and is therefore unable fully to utilize his prior knowledge.

This difficulty can be overcome by constructing prior distributions over Markov-equivalence classes of ADG models, rather than over the individual ADG models themselves. To accomplish this, represent each equivalence class $[D]$ by its essential graph D^* , then select appropriate prior distributions for the parameters of the chain graph model determined by D^* . More precisely, by Theorem 4.1(ii) of Frydenberg (1990), the joint pdf (if it exists and is positive) of a global D^* -Markovian distribution P admits the factorization

$$(7.2) \quad f(V) = \prod(f(\tau | \text{bd}_{D^*}(\tau)) | \tau \in \mathbf{T}(D^*)),$$

where, further, each *marginal* pdf $f(\text{cl}_{D^*}(\tau))$ is global $[(D^*)_{\text{cl}_{D^*}(\tau)}]^m$ -Markovian. This in turn implies that each conditional pdf $f(\tau | \text{bd}_{D^*}(\tau))$ is global $(D^*)_{\tau}$ -Markovian (Note 10). But by our Theorem 4.1(ii), each $(D^*)_{\tau}$ is chordal (\equiv decomposable), so therefore we can utilize *hyper-Dirichlet* distributions as prior distributions for the parameters occurring in these conditional pdfs (Note 11). Since score equivalence is no longer an issue, *no constraints are required* on the parameters of these hyper-Dirichlet priors.

Furthermore, although the Dirichlet and hyper-Dirichlet families provide considerable flexibility for modelling prior knowledge in the Bayesian analysis of categorical data, more general priors, such as mixtures of Dirichlet distributions, sometimes may be needed to adequately reflect prior knowledge (Bernardo and Smith (1994), p.279). When working in the space of individual ADG models, however, Geiger and Heckerman (1995) show that the Dirichlet family is the *only family of prior distributions* that can be used to achieve score equivalence. Working in the space of Markov-equivalence classes, conveniently represented by essential graphs, eliminates the issue of score equivalence and therefore allows the adoption of *arbitrary* prior distributions on the associated parameters, at least in principle.

3. Madigan and Raftery (1994) and others have argued that basing inference on a single model ignores model uncertainty and leads to poorly calibrated predictions. Bayesian model averaging (BMA) provides a remedy: current BMA procedures average inferences or predictions over all models in the class under consideration, or at least over a subset of the models that receive substantial posterior weight (see Madigan and York (1995) for a review.) When applied naively to ADG models, however, BMA

assigns a weight to each Markov-equivalence class that is proportional to its size. Instead, averaging directly over equivalence classes overcomes this problem.

A stochastic search scheme over the space of ADGs based on the Metropolis-Hastings algorithm has been proposed for Bayesian model averaging by Madigan and York (1995) (Note 12). As suggested by the final paragraph of Section 6, the number of essential graphs on n vertices, although substantially smaller than the number of ADGs, will still be too large in most applications to allow an exhaustive analysis (Note 13), hence search procedures over the space of essential graphs also will be required.

Madigan *et al* (1996) describe several stochastic search procedures for model selection and model averaging, again based on the Metropolis-Hastings algorithm, that act directly on essential graphs rather than ADGs. Such procedures move through the space of essential graphs according to a Markov chain whose transition probabilities are chosen to achieve a desired stationary distribution. Convergence to the stationary distribution requires that the Markov chain be irreducible and aperiodic. By Proposition 4.5, irreducibility will hold whenever the chain has positive probability of moving to any essential graph that differs by *at most two edges* from the current essential graph. However, it follows from the proof of Proposition 4.5 that in fact irreducibility will hold whenever the chain has positive probability of moving from the current essential graph to each essential graph

- (a) that differs by *exactly one edge* from the current graph; or
- (b) that is obtained from the current graph by *deleting both arrows* in an immorality $a \rightarrow b \leftarrow c$, where b is a terminal vertex of the current graph and where a and c are the only parents of b in the current graph; or
- (c) that is obtained from the current graph by *adding two arrows* to form an immorality $a \rightarrow b \leftarrow c$, where b is an isolated vertex of the current graph and where a and c are not adjacent in the current graph.

Aperiodicity can be guaranteed, for example, by ensuring that the chain has positive probability of remaining in its current state.

Non-stochastic model selection and model averaging schemes based on essential graphs also can be developed, analogous to those proposed by Heckerman *et al* (1994) and Madigan and Raftery (1994) for ADGs.

Appendix A: Graphs.

Our terminology and notation closely follows those of Lauritzen *et al* (1990) and Frydenberg (1990), with one exception noted below. A *graph* G is a pair (V, E) , where V is a finite set of *vertices* and E , the set of *edges*, is a subset of $E^*(V) \equiv (V \times V) \setminus \{(a, a) \mid a \in V\}$, i.e., a set of ordered pairs of distinct vertices; thus our graphs include no loops or multiple edges. An edge $(a, b) \in E$ whose opposite $(b, a) \in E$ is called an *undirected* edge and appears as a *line* $a-b$ in our figures, whereas an edge $(a, b) \in E$ whose opposite $(b, a) \notin E$ is called a *directed* edge and appears as an *arrow*: $a \rightarrow b$ (Note 14). If G contains only undirected edges, it is an *undirected graph* (UDG); if G contains only directed edges it is a *directed graph* (*digraph*).

It shall be convenient to write “ $a \rightarrow b \in G$ ” to indicate that $(a, b) \in E$ but $(b, a) \notin E$; in this case we say that *the arrow* $a \rightarrow b$ *occurs in* G . Similarly, we write “ $a-b \in G$ ” to indicate that $(a, b) \in E$ and $(b, a) \in E$; in this case we say that *the line* $a-b$ *occurs in* G . We write “ $a \cdots b \in G$ ” to indicate that there is an edge of some type between a and b in G .

For each vertex $a \in V$, define $\text{pa}_G(a) := \{b \in V \mid b \rightarrow a \in G\}$, the set of *parents* of a in G . For any subset $A \subseteq V$, the *boundary* of A in G is the set $\text{bd}_G(A) := \{b \in V \setminus A \mid (b, a) \in E \text{ for some } a \in A\}$; the *closure* of A in G is the set $\text{cl}_G(A) := \text{bd}_G(A) \cup A$.

A subset $A \subseteq V$ *induces* the subgraph $G_A := (A, E_A)$, where $E_A := E \cap (A \times A)$.

The *skeleton* G^u of a graph $G \equiv (V, E)$ is its underlying undirected graph, i.e., $G^u := (V, E^u)$, where $E^u := \{(a, b) \mid (a, b) \in E \text{ or } (b, a) \in E\}$. Two vertices a, b are called *adjacent* in G if $(a, b) \in E^u$, or, equivalently, if $a \cdots b \in G$. A vertex a is *isolated* if it is not adjacent to any b .

Let a, b , and c be three distinct vertices of $G \equiv (V, E)$. The triple (a, b, c) is called an *immorality* of G if the induced subgraph $G_{\{a, b, c\}}$ is $a \rightarrow b \leftarrow c$; that is, if the “parents” a and c of b are “unmarried” (\equiv non-adjacent).

A graph $G_2 \equiv (V_2, E_2)$ is said to be *larger* than a graph $G_1 \equiv (V_1, E_1)$, denoted by $G_1 \subseteq G_2$, if $V_1 \subseteq V_2$ and $E_1 \subseteq E_2$. Thus, if $(G_1)^u = (G_2)^u$, then $G_1 \subseteq G_2$ iff G_1 and G_2 differ only in that some directed edges (arrows) in G_1 may be converted into undirected edges (lines) in G_2 . We write $G_1 \subset G_2$ if $G_1 \subseteq G_2$ but $G_1 \neq G_2$.

The *union* of a finite collection of subgraphs $\{G_i \equiv (V_i, E_i) \mid i = 1, \dots, n\}$, of $G \equiv (V, E)$ is the subgraph $\cup G_i := (\cup V_i, \cup E_i)$. Clearly, $\cup G_i$ is the smallest subgraph larger than each G_i , $i = 1, \dots, n$.

Let a, b be distinct vertices in $G \equiv (V, E)$. A *path* π of length $n \geq 1$ from a to b in G is a sequence $\pi \equiv \{a_0, a_1, \dots, a_n\} \subseteq V$ of distinct vertices such that $a_0 = a$, $a_n = b$, and either $a_{i-1} \rightarrow a_i \in G$ or $a_{i-1} - a_i \in G$ for every $i = 1, \dots, n$. If $a_{i-1} \rightarrow a_i \in G$ for at least one i , the path is *directed*; if this is not the case, the path is *undirected*. A (*directed*) *cycle* is a

(directed) path with the modification that $a_0 = a_n$. An arrow $a \rightarrow b \in G$ is said to *block a directed cycle in G* if there is a directed path from a to b in G other than $a \rightarrow b$ itself.

A UDG $G \equiv (V, E)$ is *complete* if all pairs of vertices are adjacent. Trivially, the empty graph is complete. A subset $A \subseteq V$ is *complete* if its induced subgraph G_A is complete. A complete subset that is maximal with respect to inclusion is called a *clique*. A vertex a is *simplicial* if its boundary $\text{bd}_G(a)$ is complete. A subset $A \subseteq V$ is *connected* in G if for every distinct pair $a, b \in A$, there is a path from a to b in G_A . For pairwise disjoint subsets $A (\neq \emptyset)$, $B (\neq \emptyset)$, and S of V , A and B are *separated* by S in G if all paths from vertices in A to vertices in B intersect S .

The UDG $G \equiv (V, E)$ is *chordal* if every cycle of length $n \geq 4$ possesses a *chord*, that is, two non-consecutive adjacent vertices. A total ordering of V is a *perfect ordering* of G if, when each edge of G is oriented in accordance with this ordering, the resulting ADG D is *perfect*, i.e., is *acyclic* and *moral* (without immoralities); D is called a *perfect directed version of G* . It is well-known that a UDG admits a perfect directed version if and only if it is chordal (cf. Blair and Peyton (1993)). Furthermore, such a perfect orientation of a chordal UDG G is not unique: in fact, by using *maximum cardinality search* (MCS) (cf. Blair and Peyton (1993)), the perfect ordering can be started at *any* vertex in G . Thus, for any distinct vertices $a, b \in V$, a chordal UDG G admits two perfect directed versions, say D_1 and D_2 , such that $a \rightarrow b \in D_1$ and $a \leftarrow b \in D_2$.

A graph $G \equiv (V, E)$ is called a *chain graph* (\equiv *adicyclic graph*) if it contains no directed cycles. Every induced subgraph G_A of G is also a chain graph. Any UDG is trivially a chain graph. A chain graph that is also a digraph is called an *acyclic digraph* (ADG).

An ADG D is *transitive* if $a \rightarrow c \in D$ whenever $a \rightarrow b \in D$ and $b \rightarrow c \in D$.

For the remainder of Appendix A, let $G \equiv (V, E)$ be a chain graph. Then G determines a pre-ordering (V, \leq) as follows: $a \leq b$ iff $a = b$ or there exists a path from a to b in G . A subset $A \subseteq V$ is an *anterior set* if $b \leq a \in A \Rightarrow b \in A$. For a subset $A \subseteq V$, $\text{An}(A)$ denotes the smallest anterior set containing A : $\text{An}(A) = \{b \in V \mid b \leq a \text{ for some } a \in A\}$.

If both $a \leq b$ and $b \leq a$ then we write $a \approx b$, which occurs iff $a = b$ or there is an *undirected* path from a to b in G . Frydenberg (1990) notes that \approx is an equivalence relation on V ; we denote the set of equivalence classes in V by $\mathbf{T}(G)$. Equivalently, $\mathbf{T}(G)$ is the set of connected components of the undirected graph obtained from G by removing all directed edges. Each $\tau \in \mathbf{T}(G)$ is called a *chain component* of G . A connected UDG has only one chain component, while for an ADG, every chain component consists of a single vertex.

We write $a < b$ if there exists a *directed* path from a to b . The *future* of a vertex $a \in V$ is the set $\phi(a) := \{b \in V \mid a < b\}$.

A triple (a, C, b) is called a *complex* in G if C is a connected subset of a chain component $\tau \in \mathbf{T}(G)$ and a and b are two non-adjacent vertices in $\text{bd}_G(\tau) \cap \text{bd}_G(C)$. A complex (a, C, b) is called a *minimal complex* in G if no proper subset $C' \subset C$ forms a complex (a, C', b) in G . Frydenberg(1990) notes that (a, C, b) is a minimal complex in G iff $G_{C \cup \{a, b\}}$ looks like the chain graph of Figure A.1. An immorality is the special case of a minimal complex where $|C| = 1$.

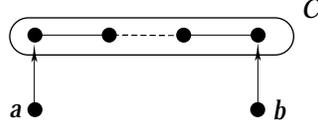


Figure A.1: A simple chain graph. Here (a, C, b) is a minimal complex.

The *moral graph* determined by G is the undirected graph $G^m \equiv (V, E^m)$, where $E^m := E^u \cup [\cup (E^*(\text{bd}_G(\tau)) \mid \tau \in \mathbf{T}(G))]$. That is, G^m is G^u augmented by all undirected edges needed to make $\text{bd}_G(\tau)$ complete in G^m for every chain component $\tau \in \mathbf{T}(G)$. Equivalently, G^m is obtained from G^u by adding a line $a-b$ whenever (a, C, b) is a minimal complex in G .

Appendix B: Graphical Markov Models and Markov Equivalence.

We consider multivariate probability distributions P on a product probability space $\mathbf{X} \equiv \times (\mathbf{X}_a \mid a \in V)$, where V is a finite index set and each \mathbf{X}_a is sufficiently regular to ensure the existence of regular conditional probabilities. Such distributions are conveniently represented by a random variate $X := (X_a \mid a \in V) \in \mathbf{X}$. For any subset $A \subseteq V$, we define $X_A := (X_a \mid a \in A)$. Often we abbreviate X_a and X_A by a and A , respectively, and define $X_\emptyset \equiv \text{constant}$.

For three pairwise disjoint subsets A, B , and C of V , we write $A \perp B \mid C [P]$ to indicate that X_A and X_B are conditionally independent given X_C under P .

A graphical Markov model is defined by a collection of conditional independencies among the component random variates $(X_a \mid a \in V)$, which collection is represented by a chain graph $G \equiv (V, E)$ with vertex set V :

Definition B.1. A probability measure P on \mathbf{X} is said to be *local G -Markovian* if $a \perp [V \setminus \phi(a)] \setminus \text{cl}_G(a) \mid \text{bd}_G(a) [P] \forall a \in A$.

Definition B.2. A probability measure P on \mathbf{X} is said to be *global G -Markovian* if $A \perp B \mid S[P]$ whenever S separates A and B in $(G_{\text{An}(A \cup B \cup S)})^m$.

Frydenberg (1990, p.339) notes that global G -Markovian \Rightarrow local G -Markovian. The converse is not true in general, e.g, Andersson *et al* (1996a, Remark A.1), but Lauritzen *et al* (1990, Proposition 4) show that the converse is valid if G is an ADG.

We define the *graphical Markov model* on \mathbf{X} determined by a chain graph G to be the set of all *global G -Markovian* probability measures on \mathbf{X} . (In applications, an additional parametric assumption, such as multivariate normality, is often imposed.)

Definition B.3. Two chain graphs G_1 and G_2 are *Markov equivalent* on a product space \mathbf{X} indexed by V if the classes of global G_1 -Markovian and global G_2 -Markovian probability measures on \mathbf{X} coincide. If G_1 and G_2 are Markov equivalent on every such product space \mathbf{X} , G_1 and G_2 are called *Markov equivalent*.

The following basic result concerning Markov equivalence of chain graphs was first proved by Frydenberg (1990, Theorem 5.6) for a restricted class of probability measures and by Andersson *et al* (1996a, Theorem 3.1) for the general case. We shall say that two chain graphs are *graphically equivalent* if they have the same skeleton and the same minimal complexes.

Theorem B.1. Suppose that for each $a \in V$, the component space X_a of \mathbf{X} contains at least two points. Then two chain graphs G_1 and G_2 are Markov equivalent on \mathbf{X} if and only if they have the same skeleton and the same minimal complexes. Thus, G_1 and G_2 are Markov equivalent if and only if they are graphically equivalent.

Since the only possible minimal complexes in an ADG are immoralities, Theorem 2.1, the key equivalence theorem for ADGs, follows from Theorem B.1 as a special case. Because the proof of Theorem B.1 is quite complex, however, we present here a direct proof of Theorem 2.1, different from that of Verma and Pearl (1992) in that their notion of “d-separation” is not used.

We require the notion of a *well-numbering* (\equiv *topological sort*) of an ADG $D \equiv (V, E)$, namely, a 1-1 mapping $v: V \rightarrow \{1, \dots, n\}$, $n \equiv |V|$, such that $c \rightarrow d$ in $D \Rightarrow v(c) < v(d)$. A straightforward inductive argument shows that every ADG admits at least one well-numbering. Propositions 4 and 5 of Lauritzen *et al* (1990) together imply that a probability measure P on \mathbf{X} is global D -Markovian if and only if, for some (and, therefore, for every) well-numbering v of D ,

$$(B.1) \quad c \perp \{d \in V \mid v(d) < v(c)\} \setminus \text{pa}_D(c) \mid \text{pa}_D(c)[P] \quad \forall c \in V.$$

Proof of Theorem 2.1. (“if”) Suppose that D and D' are two ADGs with the same skeleton and same immoralities. In order to show that D and D' are Markov equivalent, by Lemma 3.2 we may assume in addition that D and D' differ in exactly one edge, say $a \rightarrow b \in D$ but $b \rightarrow a \in D'$. By Lemma 3.1(ii), $a \rightarrow b$ is reversible, and therefore unprotected, in D , i.e., $\text{pa}_D(a) = \text{pa}_D(b) \setminus \{a\}$. It follows that for some well-numbering¹ v of D , $v(b) = v(a) + 1$. This can then be applied to show² that $v': V \rightarrow \{1, \dots, n\}$ is a well-numbering of D' , where v' is defined as follows: $v'(a) = v(b)$, $v'(b) = v(a)$, $v'(c) = v(c)$ if $c \neq a, b$. Therefore, a probability measure P on \mathbf{X} is global D' -Markovian if and only if

$$(B.2) \quad c \perp \{d \in V \mid v'(d) < v'(c)\} \setminus \text{pa}_{D'}(c) \mid \text{pa}_{D'}(c)[P] \quad \forall c \in V.$$

Since D and D' differ only in the edge $a \rightarrow b$, $\text{pa}_D(c) = \text{pa}_{D'}(c)$ if $c \neq a, b$, so the conditions in (B.1) and (B.2) coincide when $c \neq a, b$. The remaining conditions in (B.1) and (B.2) are

$$(B.3) \quad a \perp \{d \in V \mid v(d) < v(a)\} \setminus \text{pa}_D(a) \mid \text{pa}_D(a)[P]$$

$$(B.4) \quad b \perp \{d \in V \mid v(d) < v(b)\} \setminus \text{pa}_D(b) \mid \text{pa}_D(b)[P]$$

and

$$(B.5) \quad a \perp \{d \in V \mid v'(d) < v'(a)\} \setminus \text{pa}_{D'}(a) \mid \text{pa}_{D'}(a)[P]$$

$$(B.6) \quad b \perp \{d \in V \mid v'(d) < v'(b)\} \setminus \text{pa}_{D'}(b) \mid \text{pa}_{D'}(b)[P],$$

respectively. Since $\text{pa}_{D'}(a) = \text{pa}_D(a) \cup \{b\}$ and $\text{pa}_{D'}(b) = \text{pa}_D(b) \setminus \{a\}$, (B.5) and (B.6) can be rewritten as

$$(B.7) \quad a \perp \{d \in V \mid v(d) < v(a)\} \setminus \text{pa}_D(a) \mid [\text{pa}_D(a) \cup \{b\}][P]$$

$$(B.8) \quad b \perp \{d \in V \mid v(d) < v(b)\} \setminus \text{pa}_D(b) \mid [\text{pa}_D(b) \setminus \{a\}][P].$$

¹Let γ be any well-numbering for D ; note that $\gamma(a) < \gamma(b)$. If $\gamma(b) > \gamma(a) + 1$, define $v(a) = \gamma(a)$, $v(b) = \gamma(a) + 1$, $v(c) = \gamma(c) + 1$ if $\gamma(a) < \gamma(c) < \gamma(b)$, and $v(c) = \gamma(c)$ otherwise. To verify that v is also a well-numbering for D , it suffices to show that if $\gamma(a) < \gamma(c) < \gamma(b)$ (so that $v(b) < v(c)$), then $c \rightarrow b \notin D$. But if $c \rightarrow b \in D$ then also $c \rightarrow a \in D$ (since $\text{pa}_D(a) = \text{pa}_D(b) \setminus \{a\}$), which contradicts $\gamma(a) < \gamma(c)$.

²It must be shown that if $v'(d) < v'(c)$ then $c \rightarrow d \notin D'$. Because D and D' differ only in the edge $a \rightarrow b$, only the case $(d, c) = (b, a)$ need be considered, but here clearly $c \rightarrow d \notin D'$.

Finally, use the relation $\text{pa}_D(b) = \text{pa}_D(a) \cup \{a\}$ and the following well-known property of conditional distributions to conclude that (B.3) and (B.4) are jointly equivalent to (B.7) and (B.8): for any four random variates $X, Y, Z,$ and $W,$

$$X \perp (Y, Z) | W \Leftrightarrow X \perp Y | W \text{ and } X \perp Z | W, Y \Leftrightarrow X \perp Z | W \text{ and } X \perp Y | W, Z.$$

Therefore (B.1) and (B.2) are equivalent, hence D and D' are Markov equivalent.

(“only if”) The proof given by Frydenberg (1990, pp. 347-8) for chain graphs applies without change to the special case of ADGs.

Acknowledgement: We are grateful to Julian Besag, Victor Klee, Michael Levitz, Colin Mallows, and Christopher Triggs for their helpful comments and encouragement, and especially to an anonymous referee for her/his extremely careful reading of this paper.

Notes

1. Chain graphs may have both directed and undirected edges but may contain no (partially) directed cycles; they include both ADGs and UDGs as special cases.
2. The essential graph associated with an (equivalence class of) ADG(s) was first introduced by Verma and Pearl (1990) as the *completed pattern* associated with the ADG.
3. Chickering (1995) and Meek (1995) also have obtained polynomial-time algorithms for constructing D^* from D .
4. Chickering (1995, Section 4) notes that, under certain additional assumptions, the essential arrows (= *compelled edges*) of an ADG may indicate causal influences.
5. This statement is valid because we have defined Markov equivalence of chain graphs in terms of the *global* Markov property - see Definition B.3 in Appendix B. If we were to replace the global Markov property by the *local* Markov property, then this statement is not valid in general: the local and global Markov properties of the chain graph D^* need not be equivalent, whereas those of the ADG D must be equivalent - see Appendix B and also the example in Remark 3.4 of Andersson *et al* (1996a).
6. This is not an arbitrary choice: removal of only one arrow may leave the other unprotected.
7. The vertices of the graphs in Table 6.1 are labelled only to allow us to describe the Markov properties.
8. In fact, we only present a parsimonious list of independencies that are *equivalent* to the global Markov properties of the essential graph. Recall from Note 5 that the local

and global Markov properties of the essential graph itself may not be equivalent, whereas the local and global Markov properties of any ADG in its equivalence class are equivalent to each other and to the *global* Markov properties of the essential graph. We use the *local* Markov properties of such ADGs, together with standard properties of conditional independence, to obtain our parsimonious lists.

9. In this case, the joint and conditional pdfs in (7.1) and (7.2) denote the pdfs for the classification of a *single individual*.

10. Since $f(\text{cl}_{D^*}(\tau))$ is global $[(D^*)_{\text{cl}_{D^*}(\tau)}]^m$ -Markovian, it admits a Gibbs factorization over the cliques χ_1, \dots, χ_k of $[(D^*)_{\text{cl}_{D^*}(\tau)}]^m$ (cf. Frydenberg (1990, p. 344)). Because each intersection $\chi_i \cap \tau$ is complete in $(D^*)_\tau$ it is contained in at least one clique of $(D^*)_\tau$. Thus, each conditional pdf $f(\tau | \text{bd}_{D^*}(\tau))$ admits a Gibbs factorization over the cliques of $(D^*)_\tau$, hence each conditional pdf is global $(D^*)_\tau$ -Markovian.

11. Dawid and Lauritzen (1993) introduced hyper-Dirichlet distributions as natural conjugate priors in decomposable models for categorical data. As in the case of Dirichlet priors for multinomial data, hyper-Dirichlet priors allow explicit expressions for posterior model probabilities.

12. George and McCulloch (1994) discuss similar stochastic search procedures for Bayesian model selection in regression analysis.

13. For example, Spiegelhalter *et al* (1993, Section 3) and Heckerman *et al* (1992) model dependencies in biomedical data by means of ADGs with $n = 20$ and $n = 108$ vertices, respectively.

14. Our notation differs from Frydenberg's in this regard: he uses the notation $a \Rightarrow b$ rather than $a \rightarrow b$ in his text, although not in his figures.

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CORRECTION

A CHARACTERIZATION OF MARKOV EQUIVALENCE CLASSES FOR ACYCLIC DIGRAPHS

By Steen A. Andersson, David Madigan, and Michael D. Perlman

Annals of Statistics (1997) 25 505-541

p. 513: In Lemma 3.2, D and D' are assumed to be *graphically* equivalent (p. 508).

p. 524-5. The proof of Proposition 4.5 contains two gaps. The complete proof appears in Remark 1 of the technical report "Graphical model search via essential graphs," available at the following URL:

<http://www.stat.washington.edu/www/research/reports/2000/tr367.pdf>

p. 538: In the sixth line of the proof of Theorem 2.1, replace "any well-numbering ν " by "some well-numbering ν ". The well-numbering ν can be constructed as follows. Begin with an arbitrary well-numbering $\gamma: V \rightarrow \{1, \dots, n\}$; necessarily $\gamma(a) < \gamma(b)$. Define $\nu(a) = \gamma(a)$, $\nu(b) = \gamma(a) + 1$, $\nu(c) = \gamma(c) + 1$ if $\gamma(a) < \gamma(c) < \gamma(b)$, and $\nu(c) = \gamma(c)$ otherwise. Since $\text{pa}_D(a) = \text{pa}_D(b) \setminus \{a\}$, it can be verified that ν is also a well-numbering for D . A brief additional argument then shows that ν' is also a well-numbering for D' . **[see footnotes]**

p. 538: In (B.7) and (B.8), $\nu(b)$ and $\nu(a)$ should be interchanged. **[corrections made]**

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