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A Polynomial Algorithm for Deciding Equivalence in Directed Cyclic Graphical Models

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# A Polynomial Algorithm for Deciding Equivalence in Directed Cyclic Graphical Models

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#### **1 Introduction:**

This paper is concerned with statistical dependence and independence in linear causal systems with feedback. Such systems can be represented by Directed Cyclic Graphical Models (DCGs), which are a generalization of DAG models (See Spirtes (1993), Koster (1994)). We give a feasible characterization of the class of Directed Cyclic Graphical models (DCGs) which entail, in virtue of their structure, the same conditional independencies. This problem was posed (independently) by Koster (1994), and similar questions have been considered by Basmann (1965), Stetzl (1986) and Lee (1987).

A greater understanding of the relationship between cyclic causal systems and statistical independencies will facilitate the construction of efficient discovery algorithms which will output the class of Directed Cyclic Graphical models compatible with data given as input, in situations where the underlying causal structure contains loops.

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#### 2 Systems with Feedback

In many physical processes the relation between cause and effect is not anti-symmetric: An event of type A can cause an event of type B, which can then subsequently cause an event of type A. As a consequence, in any given population, the number of occurrences of A, may be determined in part by the number of occurrences of B, while the number of occurrences of B is itself determined by the number of occurrences of A. There are examples of systems which display behaviour of this kind in many fields:

In economics, the price of a good in a market may be a function of the quantity either demanded or supplied, while these quantities themselves may be influenced by the price or the expectation of price that consumers or suppliers may have.

In **analogue electronics**, operational amplifiers provide a common example of a system in which feedback is exploited in order to carry out various operations, such as integration, differentiation, and digital to analogue conversion.

In **biology**, the concept of homeostasis, introduced by Bernard in the 19th century, provides many instances. Homeostasis occurs at every level in the natural world, from the molecular processes that control the enzymatic production of chemicals, to the predator-prey relationships which curb population growth among macro-fauna. Control systems that act to maintain 'dynamic equilibria' very often consist of feedback systems in which causal processes operate in contrary directions.

Other examples of systems in which causal influences propagate in opposite directions abound in fields as diverse as sociology, robotics and psychology, where some types of neural net are of this form.

#### 2.1 Non-Recursive Structural Equation Models

The numerous instances of systems with this structure motivate the construction of models to describe the underlying causal mechanisms. In engineering, economics, and the social sciences, when it has seemed reasonable to assume linearity, these systems have been modelled by a certain kind of linear structural equation model.

In a Structural Equation Model (SEM), the variables are divided into two disjoint sets, the error terms, and the non-error terms. Associated to each non-error variable V there is a unique error term ey. A linear SEM contains a set of equations in which each non-error random variable V is written as a linear function of other non-error random variables and ey- A *linear* SEM also specifies a joint distribution over the error terms.

In our discussion we will consider only linear SEMs. We shall also assume that the error terms are jointly independent, but as we shall see, in an important sense, the scope of our analysis is not limited by this assumption of independence. The following is an example of such a model:

X=EX
$$A = ai'X + arB + 8A$$
Y=8y $B = Pi-Y + p_2'A + 8_B$ 

In this model the Ey's are jointly independent standard normal error terms.

A structural equation model in which, for some ordering of the variables, the matrix of coefficients is in lower triangular form, is said to be *recursive*. If for no ordering of the variables is the matrix of coefficients lower triangular, then we say that the structural equation model is *nonrecursive*, (the model above is an example). This latter class, the *nonrecursive* SEMs have traditionally been used to simulate systems with feedback. The fact that the coefficient matrix cannot be written in lower triangular form means that given any ordering of the variables  $<X_{1v}..X_n >$  there will exist an ordered subset  $<X_{ii},...,X_{it} >$  (ir<ir+i) such that each variable X; is a linear function of X; (and other variables), and  $Xj_t$  is a linear function of X<sup>(and other variables)</sup>. In the example of a non-recursive model that we give above t=2, and  $\langle X_{i_t}, X_{i_2} \rangle = \langle A, B \rangle$ .

#### 22 Graphs and DAG models

There is a directed graph, naturally associated with a given linear SEM, by the following rule:

X->Y in the graph if and only if the **coefficient** of **X**, in the **equation** for **Y**, is **non-zero** 

By convention we do not include error terms in the graph. Hence the graph relating to the model above is (here the error terms are omitted, being assumed jointly independent):

X\_\_\_\_\_\_ B ^\_\_\_\_Y

A linear SEM with a jointly independent distribution over the error terms defines a joint density function over the vertices in the associated graph.

It is easy to see that the linear SEM associated with an **acyclic** graph will be a recursive structural equation model. Likewise non-recursive SEMs are associated with **cyclic** graphs. (The set  $(x_{ll},...,X_{it})$  introduced above will be a cycle.) This is in keeping with the use of non-recursive SEMs to model processes in which feedback is present.

The *acyclic* graph associated with a *recursive* structural equation model is an example of a certain class of statistical models, known as directed acyclic graph (DAG) models, which encode independence, and conditional independence constraints. (See Pearl, 1988). Though the relationship between the graph and the SEM is straightforward - the graph represents explicitly the causal structure implicit in the SEM - this formalism has had fruitful results in many areas: there is now a relatively clear causal interpretation of these models, there are efficient procedures for determining the statistical indistinguishability of DAG's, reliable algorithms for generating a class of DAG models from sample data and background knowledge, etc. Two important elements in these investigations were:

• First, a purely graphical condition for calculating the conditional independence relations entailed by a DAG.

• Second, a 'local' characterization of equivalence between two graphs, in the sense that all of the same conditional independencies are entailed by each graph.

This local characterization was essential in allowing the construction of efficient algorithms which could search the whole class of DAG models to find those which fitted the given data.

The DAG formalism is very general: A gamut of more familiar constructs such as regression models, factor analytic models, path models, discrete latent variable models, and as we have seen, recursive linear SEMs with independent errors, can be represented as DAG models. However, as you might suspect from the name, directed acyclic graphs, DAG models do exclude non-recursive structural equation models. In this paper we will develop the theory of cyclic graphical models, thereby allowing the generalization of acyclic techniques and methods to the cyclic case.

#### **Definition: Linear Entailment**

A directed graph containing disjoint sets of variables X, Y, and  $Z^2$ linearly entails that X is independent of Y given Z if and only if X is independent of Y given Z for all values of the non-zero linear coefficients for which the model has a reduced form and all distributions of the exogenous variables in which they have positive variances and are jointly independent.

<sup>&</sup>lt;sup>2</sup>We use bold face letters (X) to denote sets of variables, and script letters (G) to denote graphs.

It is important to note that in any particular SEM with directed graph Q, there may be conditional independencies which hold even though they are not linearly entailed by Q. However, if a zero-correlation holds for some but not all parameterizations of Q, then the set of parameterizations in which this 'extra\* conditional independence holds, is of zero Lebesgue measure over the set of all parameter value assignments to the non-zero linear coefficients,

#### 23 Conditional Independencies and Equivalence in a graph.

In an acyclic graph Q, there is a graphical 'path' condition which holds between disjoint vertex sets X, Y and Z in the graph if and only if Qlinearly entails that X JL Y I Z.<sup>3</sup> Similarly, the same graphical 'path\* condition holds between X, Y and a set Z, not containing X or Y, if and only if in Q the partial correlation between X and Y controlling for Z, vanishes: PXY.Z - °- We can calculate the partial correlations that are zero in all linear parameterizations of Q in which X and Y have correlated errors in the following way. First, form a directed graph (# in which X and Y are the effects of a latent common cause T. The same graphical path condition holds in Qf iff in every parameter assignment to Q in which X and Y have correlated errors, PXY.Z - °•

This observation is central to the usefulness of the graphical method. The task of generalizing this result to the cyclic case has already been accomplished: Building on the work of Haavelmo(1943), Spirtes (1993) showed that the same graphical condition, the Geiger-Pearl-Verma d-separation criterion (defined in the Appendix) which determines whether a particular conditional independence relation or zero partial correlation is linearly entailed by a *recursive* structural equation model, can also be used with linear *non-recursive* models. Or equivalently, that the same

<sup>&</sup>lt;sup>3</sup>'X JL Y I Z' means that 'X is independent of Y given Z\

technique used for reading conditional independencies from an acyclic graph can be applied in the cyclic case.

#### **Definition:** Equivalence for Graphs (Cyclic or Acyclic)

Graphs  $G_1$  and  $G_2$  are *equivalent* if they both linearly entail the same set of conditional independencies.

It is important to be clear what we are establishing when we work out the conditional independencies linearly entailed by a given model: we are calculating the conditional independence consequences of having a certain **form** of linear equations, i.e. having linear equations in which certain coefficients are zero. We are **not** trying to estimate parameters, we are **not** making any distinction between latent and measured variables, and we are **not** constructing a model from data; though the development of efficient procedures for determining the equivalence of cyclic models will facilitate the construction of computer aids for model specification and updating.

#### **3 Characterizations of Equivalence**

We begin with the following preliminary result which is a corollary of the Equivalence Theorem for cyclic graphs:

#### 3.1 The Orientation of cycles<sup>4</sup>

Given a graph G with a cycle C, there is an equivalent graph  $G^*$ , in which C is replaced by another cycle  $C^*$ , having the opposite orientation to C. Thus if C is clockwise,  $C^*$  is anti-clockwise, and vice-versa.



Fig. 1

<sup>&</sup>lt;sup>4</sup>By a cycle we mean a directed path  $X_0 \rightarrow X_2 \dots \rightarrow X_{n-1} \rightarrow X_0$  of n distinct vertices.

In Fig.1, in  $G_1$ , the cycle <C,B,D,E> has anti-clockwise orientation, while in the equivalent graph  $G_2$ , the corresponding cycle <C,B,D,E> has clockwise orientation. One important consequence of this result is that it is not possible to orient a cycle merely using conditional independence information.

#### **3.2 Equivalence in the Acyclic Case**

In the acyclic case there is a relatively simple characterization of the equivalence class that leads directly to an  $O(n^3)$  algorithm. We first require two definitions:

#### **Definition:** Adjacent (for acyclic graphs)

In an acyclic graph G, if there is an edge from A to B or from B to A in the graph, then we say that A and B are *adjacent* in G.

**Definition: Unshielded Collider and Non-Collider (acyclic graphs)** 

In an acyclic graph G, the triple  $\langle A,B,C \rangle$  forms an unshielded collider in G, if A and C are not adjacent, but  $A \rightarrow B \leftarrow C$ . If A and C are not adjacent, but  $\langle A,B,C \rangle$  is not an unshielded collider, then we say it is an unshielded non-collider, i.e.  $A \rightarrow B \rightarrow C$ ,  $A \leftarrow B \rightarrow C$ , or  $A \leftarrow B \leftarrow C$ .

Equivalence Theorem for Acyclic Graphs (Verma and Pearl 1990, Frydenberg 1990)

Two directed acyclic graphs,  $G_1$  and  $G_2$  are equivalent if and only if

(a)  $G_1$  and  $G_2$  have the same adjacencies

(b)  $\mathcal{G}_1$  and  $\mathcal{G}_2$  have the same unshielded colliders

Conditions (a) and (b) logically entail a third condition:

(c)  $G_1$  and  $G_2$  have the same unshielded non-colliders

Below we show three examples of acyclic equivalence classes:



Conditions (a) and (b) above lead to an  $O(n^3)$  algorithm for checking the equivalence of two acyclic graphs on n variables; this follows from the fact that (a) mentions pairs of variables, while (b) mentions triples. Although d-separation allows us to check any given conditional independence, there are  $O(2^n)$ -many conditional independencies, thus d-separation alone does not provide a feasible test for equivalence.

#### 33 Equivalence in the Cyclic Case

This raises the question of whether conditions similar to (a) and (b) exist for the cyclic case. The answer is that such a set of conditions do exist. The conditions are considerably more complicated, but still lead to a polynomial algorithm though of  $O(n^9)$ .<sup>5</sup> See Richardson (1994). This result provides criteria for detecting feedback: it gives sets of conditional independencies that are not linearly entailed by any acylic graph, with or without latent variables. It is also a first step towards a discovery algorithm which will construct models from conditional independencies present in data; the output of such a discovery algorithm is an equivalence class of models.

#### 3.4 Real & Virtual Adjacencies

In the cyclic case the condition (a) which we gave above ( $\S2.2$ ) is no longer a necessary condition for equivalence.<sup>6</sup> This can be seen by considering the following two equivalent models:



Fig. 2

<sup>&</sup>lt;sup>^</sup>It should be stressed that this is a worst case complexity bound, the expected case may be much lower.

<sup>&</sup>lt;sup>6</sup>A similar point is made in Whittaker (1989).

In the model on the left A and C are adjacent, but not on the right. We introduce the following definition:

#### **Definition: Virtually Adjacent (Cyclic Graphs)**

A and C are said to be virtually adjacent in cyclic G if and only if A

and C have a common child B such that B is an ancestor of A or C.<sup>7</sup> We incorporate the notion of adjacency from acyclic graphs by saying that if there is an edge between A and C ( $A \rightarrow C$  or  $A \leftarrow C$ ) then A and C are *really adjacent*.

Thus in Fig. 2 in the graph on the right A and C are virtually adjacent. Virtual adjacencies can only occur in cyclic graphs (since B is in a cycle with A or C). Condition (a) is necessary for equivalence in the acyclic case since an acyclic graph linearly entails no conditional independencies between a pair of vertices  $(A,B)^8$  if and only if A and B are (really) adjacent. In the cyclic case no conditional independencies are linearly entailed if and only if A and B are either really or virtually adjacent. It follows that given two equivalent cyclic graphs  $G_1$ ,  $G_2$ , the following is true:

(1) If A and B are either virtually or really adjacent in  $\mathcal{G}_1$ , then A and B are either virtually or really adjacent in  $\mathcal{G}_2$ .

In fact, if a cyclic graph contains a virtual adjacency then there is always an equivalent cyclic graph in which that adjacency is real. In the rest of this paper the term 'adjacency' will mean 'real or virtual adjacency'.

 $<sup>^7</sup>$  The terms 'ancestor', 'child' etc., are defined in the appendix. Note that every vertex is its own descendant and ancestor.

<sup>&</sup>lt;sup>8</sup>By 'an independence between A and B' we mean an independence relation of the form  $A \perp B \mid S$ , with  $A,B \notin S$ .

#### 25 'Conductors'

In the cyclic case, the condition (c) given above (§2.2) is no longer necessary for equivalence. This can be seen from the following equivalent graphs  $\pounds_i$ , and  $Qi^2$ 



 $\langle A3,G \rangle$  forms an unshielded non-collider in  $Q \setminus$  but not in Q%. We make the following definition:

## **Definition: Unshielded Conductor and Unshielded Non-Conductor** (for Cyclic graphs)

In a cyclic graph Q, we say triple of vertices  $\langle A,B,C \rangle$  forms an *unshielded conductor* if:

- (i) A and B, and, B and C are adjacent, A and C are not adjacent
- (ii) B is an ancestor of A or C

If  $\langle A3, C \rangle$  satisfies (i), but B is not an ancestor of A or C, we say  $\langle A3, C \rangle$  is an *unshielded non-conductor*.

In the acyclic case condition (c) was necessary for equivalence, since there is a set of conditional independencies between a triple  $\langle A3,G \rangle$  which are linearly entailed by an acyclic graph if and only if  $\langle A3,C \rangle$  is an unshielded non-collider. In the cyclic case the same set of conditional independencies are linearly entailed by a graph iff  $\langle A3,G \rangle$  is an unshielded conductor. Thus if cyclic graphs  $Q \setminus Q\%$  are equivalent then:

(II)  $\langle A3, C \rangle$  is an unshielded conductor in  $Q \setminus if$  and only if  $\langle A3, C \rangle$  is an unshielded conductor in Qz

Thus an unshielded conductor is the cyclic analogue of the unshielded non-collider; in an acyclic graph every unshielded conductor will be an unshielded non-collider.

#### 3.6 'Perfect Non-Conductors'

Condition (b) given above is also no longer a necessary condition for equivalence. This can be seen by considering the triple  $\langle A,D,B \rangle$  in Fig. 3. In  $G_2 \langle A,B,D \rangle$  is an unshielded collider, but this is not the case in  $G_1$ .

Definition: Unshielded Perfect Non-Conductor (for Cyclic graphs)

In a cyclic graph G, we say triple of vertices  $\langle A,B,C \rangle$  is an unshielded perfect non-conductor if:

- (i) A and B, and, B and C are adjacent, A and C are not adjacent
- (ii) B is not an ancestor of A or C
- (iii) B is a descendant of a common child<sup>9</sup> of A and C

If <A,B,C> satisfies (i) and (ii) but B is not a descendant of a common child of A and C, we say <A,B,C> is an unshielded imperfect non-conductor.

As in the previous cases condition (b) was necessary for equivalence in the acyclic case because there is a set of conditional independencies which are linearly entailed by an acyclic graph if and only if that triple is an unshielded collider. In a cyclic graph the same set of independencies are linearly entailed, if and only if  $\langle A,B,C \rangle$  is an unshielded perfect non-conductor. Hence the following is also necessary for equivalence:

(III) <A,B,C> is an unshielded perfect non-conductor in  $G_1$  iff it is also an unshielded perfect non-conductor in  $G_2$ 

Thus unshielded perfect non-conductors are the cyclic analogue to unshielded colliders in the acyclic case. However, in an acyclic graph every unshielded triple is either an unshielded collider or non-collider, whereas it is not the case that in a cyclic graph every unshielded triple is either an unshielded conductor or an unshielded perfect non-conductor. A triple may form an unshielded *imperfect* non-conductor. It follows from

<sup>&</sup>lt;sup>9</sup> 'Child' refers to *real* adjacencies. Thus if D is a common child of A and C, then  $A \rightarrow D \leftarrow C$ . Virtual adjacencies are unoriented.

this that the conditional independencies linearly entailed by a graph among a triple which forms an unshielded imperfect non-conductor are not linearly entailed by any acyclic graph (even with latent variables). This provides a criterion for detecting the presence of feedback in linear systems.

#### 3/7 Contrast with the Acyclic case: Non-locality

In the acyclic case, if two graphs are *not* equivalent then there will be some conditional independence between vertices separated by at most two edges, linearly entailed by one graph, and not by the other. This means that we need only look at the structure of triples of adjacent vertices in order to establish that two graphs are equivalent. This is not true for the cyclic case, as the following two graphs which are not equivalent show:



Although every independence linearly entailed by Qi, is also entailed by Qi, in Qi, A JL B, while in £2, A JLB. But A and B are separated by more than two edges in both graphs. Clearly these graphs could be extended by increasing the number of X's so that A and B were separated by arbitrarily many edges. This is also why the cyclic equivalence algorithm is of higher complexity; cyclic graphs cannot be compared by checking that all 'local' subgraphs are equivalent.  $Q \setminus and Qi$  also show that the conditions (I)-(III) are not sufficient since they are satisfied by these non-equivalent graphs. The full set of necessary and sufficient conditions is given in the appendix.

#### Appendix

An arrow from A to B (A-\*B) or from B to A (B-\*A) is called an *edge* between A and B. Given three vertices A, B and C such that there is an edge between A and B, and between B and C, then if the edges 'collide\* at B, then we say B is a *collider* between A and C, relative to these edges i.e.  $A-*B \ll C$ . Otherwise we will say that B is a non-collider between A and C, relative to these edges. i.e. A is a non-collider: A-\*B-\*C,  $A \ll -B-*C$ ,  $A \ll -B \ll -C$ .

If there is an arrow from A to B (A-»B), then we say that A is a parent of B, and B is a child of A. We define 'descendant' relation as the transitive reflexive closure of 'child', and similarly, 'ancestor' as the transitive reflexive closure of 'parent'. A sequence of distinct edges  $\langle E \rangle$ ,..., *JE*^> in *Q* is an *undirected path* if and only if there exists a sequences of vertices  $\langle Vi, ..., V_{n+}i \rangle$  s.t. for 1^ is n either  $\langle Vi+i, Vi \rangle = \pounds$  or  $\langle Vi, Vi+i \rangle = \pounds$ .

**Definition:** d-connection / d-separation for (cyclic or acyclic) graphs For disjoint sets, X, Y and Z, X is *d-connected to* Y given Z if for some XGX, and YGY, there is a path from X to Y, satisfying the following conditions:

(i) If A, B and C are adjacent vertices on the path, and BGZ, then B is a collider between A and C.

(ii) If B is a collider between A and C, then there is a descendant D, of CandDGZ.

If X and Y are not d-connected given Z then X and Y are said to be *d-separated* by Z.

The following important theorems give the relationship between d-separation and the linear entailment of conditional independencies, and partial correlations. Spirtes (1993) proved them for the cyclic case.

**Theorem** (Spirtes): In a (cyclic or acyclic) graph G, for disjoint sets, X, Y, Z, X and Y are d-separated given Z, if and only if G linearly entails  $X \perp Y \mid Z$ .

(This result was independently discovered by Koster(1994).

**Theorem** (Spirtes): In a (cyclic or acyclic) graph G, for any set Z, not containing X or Y, X and Y are d-separated given Z, if and only if G linearly entails  $\rho_{XY,Z} = 0$ .

We give below the Equivalence Theorem in full. However, this requires three more definitions:

#### **Definition: Itinerary**

If  $\langle X_0, X_1, ..., X_{n+1} \rangle$  is a sequence of distinct vertices s.t.  $\forall i \ 0 \le i \le n$ , X<sub>i</sub> and X<sub>i+1</sub> are really or virtually adjacent then we will refer to  $\langle X_0, X_1, ..., X_{n+1} \rangle$  as an *itinerary*.

# Definition: Mutually Exclusive Conductors with respect to a certain itinerary

If  $\langle X_0, \dots, X_{n+1} \rangle$  is a sequence of vertices such that:

(i)  $\forall t \ 1 \le t \le n$ ,  $\langle X_{t-1}, X_t, X_{t+1} \rangle$  is a conductor

(ii)  $\forall k \ 1 \le k \le n$ ,  $X_{k-1}$  is an ancestor of  $X_k$ , &  $X_{k+1}$  is an ancestor of  $X_k$ .

(iii)  $X_0$  is not a descendant of  $X_1$ , and  $X_n$  is not an ancestor of  $X_{n+1}$ then  $\langle X_0, X_1, X_2 \rangle$  and  $\langle X_{n-1}, X_n, X_{n+1} \rangle$  are mutually exclusive (m.e.) conductors on the itinerary  $\langle X_0, \dots, X_{n+1} \rangle$ .

#### **Definition: Uncovered itinerary**

If  $\langle X_0,...,X_{n+1} \rangle$  is an itinerary such that  $\forall i,j \ 0 \le i < j-1 < j \le n+1$  $\langle X_i,X_j \rangle$  is not an adjacency then we say that  $\langle X_0,...,X_{n+1} \rangle$  is an *uncovered itinerary*.

#### **Theorem: Equivalence in Cyclic Graphs** (Richardson 1994)

Cyclic graphs  $Q \setminus Q_i$  and  $Q_i$  are equivalent if and only if the following conditions hold:

(1) Q and Qi have the same adjacencies.

(2)  $Q \setminus and Qi$  the same unshielded conductors

(3) Qi and Qi the same unshielded perfect non-conductors

(4) If  $\langle A3, C \rangle$  and  $\langle X, Y, Z \rangle$  are m.e. conductors on some uncovered itinerary  $P = \langle A3, C, ..., X, Y, Z \rangle$  in  $Q \setminus$  if and only if  $\langle A3, C \rangle$  and  $\langle X, Y, Z \rangle$  are m.e. conductors on some uncovered itinerary  $Q = \langle A3, C, ..., X, Y, Z \rangle$  in &.

(5) If  $\langle A, X3 \rangle$ , and  $\langle A, Y3 \rangle$  are unshielded imperfect non-conductors, then X is an ancestor of Y in  $Q \setminus iff X$  is an ancestor of Y in Qi.

(6) If  $\langle A3, C \rangle$  and  $\langle X, Y, Z \rangle$  are m.e. conductors on some uncovered itinerary P= $\langle A, B, C, ..., X, Y, Z \rangle$  and  $\langle A, M, Z \rangle$  is an imperfect non-conductor, then M is a descendant of B in  $Q \setminus$  if and only if M is a descendant of B in Qi.

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