THE GRAPHICAL CONDITION FOR IDENTIFYING ARROWS IN RECOVERING CAUSAL STRUCTURE

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This paper deals with problems of recovering a causal structure by using not only conditional independence relationships but also prior knowledge when data are generated according to the causal structure among variables. Although some algorithms for recovering a causal structure based on independencies have been developed, the influence of prior knowledge on the recovery algorithms has not been clarified. In this paper, a necessary and sufficient condition for the existence of unidentified arrows in a recovered diagram is given in terms of graph structure. Also, it is shown that a causal structure such that a recovered diagram is a forest can be recovered by recognizing exogenous variables in a causal diagram completely. The result enables us to elucidate enough prior information to determine a causal diagram uniquely.

Key words and phrases: exogenous variable, faithfulness, maximally oriented pattern, observational equivalence, orientation rules, pattern.

1. Introduction

The statistical causal analysis started with the pioneering work of Wright (1923, 1934) who introduced path analysis to statistics, and progressed to be the structural equation models (Wold (1954), Bollen (1989)).

The aim of the statistical causal analysis is to combine qualitative cause-effect information with statistical data in order to provide quantitative assessment of cause-effect relationships among variables of interest. At this time, prior knowledge of the causal relations is to be represented by a directed acyclic graph which is called a causal diagram. However, there are many cases where such prior information is not enough to make the causal diagram completely. As a course of matter, some theories and algorithms are developed in order to recover causal structure from partial prior information and conditional independence relationships among variables, assuming that observed data are generated according to an undisclosed causal diagram. When an ordering of variables is known beforehand, Wermuth and Lauritzen (1983) developed an algorithm which builds a directed independence graph by using this ordering. Verma and Pearl (1991) and Spirtes *et al.* (2000) gave algorithms for recovering the underlying causal diagram by using only conditional independencies without such an ordering knowledge. Also, Verma and Pearl (1992) gave orientation rules for identifying additional arrows

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in the undisclosed causal diagram. It is noted that the diagram recovered by the above algorithms may consist of not only arrows but also lines, although the undisclosed diagram is a directed acyclic graph. Such a relationship between the recovered diagrams and the undisclosed diagram is known as the observational equivalence. Meek (1995) showed that the rules by Verma and Pearl (1992) give the maximal set of arrows which can be identified. However, a condition for the existence of arrows which can not be identified is not clarified. In this paper, we will investigate the condition. For this purpose, this paper is structured in the following way. In section 2, we will give definitions for graph terminology and causal diagrams used in this paper. The basic theories for recovering causal structure will be introduced in section 3. In section 4, we will show a necessary and sufficient condition that arrows can not be identified by the recovery algorithms using only conditional independencies. Also, it is shown that a causal structure can be determined by recognizing exogenous variables in a causal diagram uniquely, when a recovered diagram has no lines between vertices which have common parents in the diagram and its subgraph induced by all vertices whose sets of parents in the diagram are empty is a forest.

2. Preliminaries

2.1. Graph terminology

A graph is a pair $G = (V, E)$, where V is a finite set of vertices and a set E of arrows is a subset of $V \times V$ of ordered pairs of distinct vertices. An arrow pointing from α to β indicates $(\alpha, \beta) \in E$ and $(\beta, \alpha) \notin E$. A line between α and β indicates $(\alpha, \beta) \in E$ and $(\beta, \alpha) \in E$. G is said to be a directed graph when all elements in E are arrows, and an undirected graph when all elements in E are lines.

If there is an arrow pointing from α to β , α is said to be a parent of β , and β a child of α . The set of parents of β is denoted as $pa(\beta)_G$ and the set of children of α as $ch(\alpha)_G$. If a line or an arrow between α and β is in E , α and β is said to be adjacent. A path of length n from α to β is a sequence $\alpha = \alpha_0, \alpha_1, \dots, \beta = \alpha_n$ of distinct vertices such that $(\alpha_{i-1}, \alpha_i) \in E$ or $(\alpha_i, \alpha_{i-1}) \in E$ for all $i = 1, \dots, n$. A directed path of length n from α to β is a sequence of distinct vertices such that $(\alpha_{i-1}, \alpha_i) \in E$ and $(\alpha_i, \alpha_{i-1}) \notin E$ for all $i = 1, \dots, n$. When there exists a directed path from α to β , α is said to be an ancestor of β and β a descendant of α . The set of ancestors of β is denoted as $an(\beta)_G$ and the set of descendants of α as $de(\alpha)_G$. Also, $nd(\alpha) = V \setminus de(\alpha)_G$.

A directed path which begins and ends in the same point is said to be a cycle. If a directed graph has no cycles, the graph is said to be a directed acyclic graph. A graph is connected if it has paths between every pair of vertices in it. A maximal connected subgraph is a connected component. A tree is an undirected graph in which there is only one path between every pair of distinct vertices. A forest is an undirected graph where all connected components are trees.

Figure 1. Causal Diagram (1).

2.2. Causal diagram

In this paper, consider a pair $(G, f(x_1, \dots, x_n))$ for which $G = (V, E)$ is a directed acyclic graph and $f(x_1, \dots, x_n)$ is a strictly positive joint distribution of V such that (i) for any vertex X in V and every subset S of V that are not descendants or parents of X , X is conditionally independent of S given the parents $pa(X)_G$ of X , that is $X \perp\!\!\!\perp S \mid pa(X)_G$; and (ii) every independence in $f(x_1, \dots, x_n)$ is a consequence of the independencies in (i). In statistical causal analysis, a pair $(G, f(x_1, \dots, x_n))$ satisfying these conditions is said to be faithful and can be considered as causal structure in which causal dependencies generate statistical dependencies. The directed acyclic graph is said to be a causal diagram.

For example, consider a causal diagram shown in Figure 1. From Figure 1, we can judge that X_1 is a direct cause of X_2 and X_3 , that X_2 is a direct cause of X_3 , X_4 and X_5 , and that X_3 and X_4 are direct causes of X_5 . Further, the following independencies can be obtained from Figure 1:

$$(2.1) \quad X_4 \perp\!\!\!\perp X_1 \mid X_2 \quad X_4 \perp\!\!\!\perp X_3 \mid X_2 \quad X_4 \perp\!\!\!\perp (X_1, X_3) \mid X_2 \quad X_5 \perp\!\!\!\perp X_1 \mid (X_2, X_3, X_4).$$

3. Basic theories for recovering causal structure

Verma and Pearl (1991) and Spirtes *et al.* (2000) gave algorithms for recovering causal structure by using the following proposition under the assumption that all independencies are identified from observations. The algorithms are called recovery algorithms in this paper.

PROPOSITION 1. (*Spirtes et al. (2000)*) (1) For any X and Y of G , X and Y are adjacent if and only if X and Y are dependent conditional on every set of vertices of G that does not include X or Y .

(2) For any X, Y and Z such that X is adjacent to Y but not to Z and Y is adjacent to Z , $X \rightarrow Y \leftarrow Z$ (it is called a *v-structure*) is a subgraph of G if and only if X and Z are dependent conditional on every set containing Y but not X or Z . $\square$

A graph obtained by the repeated application of Proposition 1 is called a pattern for G and denoted by $Pattern(G)$ (Verma and Pearl (1991)).

For example, letting $V = \{X_1, X_2, X_3, X_4, X_5\}$. Suppose that we have equations (2.1). From equations (2.1), the pairs (X_1, X_2) , (X_1, X_3) , (X_2, X_3) ,

Figure 2. Pattern.

Figure 3. Maximally Oriented Pattern (1).

(X_2, X_4) , (X_2, X_5) , (X_3, X_5) and (X_4, X_5) are adjacent respectively, however (X_1, X_4) , (X_1, X_5) and (X_3, X_4) are not adjacent from Proposition 1.(1). Further, since X_3 and X_4 are not adjacent and are dependent conditional on every set containing X_5 , we have $X_3 \rightarrow X_5 \leftarrow X_4$ from Proposition 1.(2). Therefore, $Pattern(G)$ constructed by equations (2.1) is given in Figure 2.

Assuming that the underlying causal diagram is a directed acyclic graph, Verma and Pearl (1992) gave the following proposition which is applicable to identifying additional arrows in a pattern for the directed acyclic graph. This proposition is called the orientation rule.

PROPOSITION 2. (Verma and Pearl (1992)) Rule.1. Orient $Y - Z$ into $Y \rightarrow Z$ whenever there is an arrow $X \rightarrow Y$ such that X and Z are nonadjacent in $Pattern(G)$.

Rule.2. Orient $X - Z$ into $X \rightarrow Z$ whenever there is a path $X \rightarrow Y \rightarrow Z$ in $Pattern(G)$.

Rule.3. Orient $X - W$ into $X \rightarrow W$ whenever there are two paths $X - Y \rightarrow W$ and $X - Z \rightarrow W$ such that Y and Z are nonadjacent in $Pattern(G)$. $\square$

A graph obtained by Propositions 1 and 2 consists of all arrows and adjacent pairs that are common to any other causal diagrams that have the same conditional independencies as the underlying causal diagram G . In this sense, the graph is said to be a maximally oriented pattern for $Pattern(G)$, denoted as $Max(G)$.

For example, consider a pattern shown in Figure 2. Since there are two paths

$X_2 - X_3 \rightarrow X_5$ and $X_2 - X_4 \rightarrow X_5$ such that X_3 is not adjacent to X_4 , we can orient $X_2 - X_5$ into $X_2 \rightarrow X_5$ by using Rule.3. The graph obtained by Propositions 1 and 2 is given in Figure 3.

4. Identification of causal structure by prior knowledge

4.1. Selection of prior knowledge for recovering causal structure

As seen from section 3, there are many cases where a causal diagram can not be determined by using Propositions 1 and 2 without prior knowledge. Therefore, we need to clarify minimal prior knowledge to determine a causal diagram uniquely. For this purpose, it is important to recognize unidentified arrows in the causal diagram.

Suppose that we can recognize all arrows emerging from some vertices in a directed acyclic graph G as prior knowledge. Let $Result(G)$ be a graph obtained by applying both such prior knowledge and Proposition 2 to $Max(G)$. The following theorem can be developed in order to recognize unidentified arrows.

THEOREM 1. *For an adjacent pair (X, Y) in $Result(G)$, $X - Y$ in $Result(G)$ if and only if $pa(X)_{Result(G)} = pa(Y)_{Result(G)}$, where $pa(X)_{Result(G)}$ is a set of parents of X in $Result(G)$. $\square$*

In order to prove Theorem 1, we will introduce the following proposition:

PROPOSITION 3. (Meek (1995)) *In $Max(G)$, if $X \rightarrow Y$ and $Y - Z$, then $X \rightarrow Z$. $\square$*

Note that $X \rightarrow Y$ in Proposition 3 is an arrow identified by repeated application of Propositions 1 and 2 without prior knowledge.

We can obtain the following lemma, whose proof is obvious from the proof of Proposition 3 (see Meek (1995)) and is omitted.

LEMMA 1. *In $Result(G)$, if $X \rightarrow Y$ and $Y - Z$, then $X \rightarrow Z$. $\square$*

$X \rightarrow Y$ in the above lemma is an arrow identified by repeated application of Propositions 1 and 2 or the prior knowledge.

Our result can be proved by using Lemma 1.

PROOF OF THEOREM 1. For an adjacent pair (X, Y) in $Result(G)$, suppose that $pa(X)_{Result(G)} = pa(Y)_{Result(G)}$ but $X \rightarrow Y$. Since $X \in pa(Y)_{Result(G)}$ and $X \notin pa(X)_{Result(G)}$, we have $pa(X)_{Result(G)} \neq pa(Y)_{Result(G)}$. Contradiction. It means that if $pa(X)_{Result(G)} = pa(Y)_{Result(G)}$ then $X - Y$ in $Result(G)$.

On other hand, suppose that $X - Y$. $Z \in pa(X)_{Result(G)}$ implies $Z \rightarrow X$. Therefore, for any $Z \in pa(X)_{Result(G)}$, from $Z \rightarrow X$ and $X - Y$, $Z \rightarrow Y$ holds true by using Lemma 1. This implies $Z \in pa(Y)_{Result(G)}$. Therefore, $pa(X)_{Result(G)} \subset pa(Y)_{Result(G)}$ can be obtained. $pa(Y)_{Result(G)} \subset pa(X)_{Result(G)}$ can be deduced by the same procedure. It means that if $X - Y$ in $Result(G)$ then $pa(X)_{Result(G)} = pa(Y)_{Result(G)}$. *Q.E.D.*

Theorem 1 insists that an arrow (X, Y) such as $pa(X)_{Result(G)} = pa(Y)_{Result(G)}$ can be identified by prior knowledge such as a causal relation between X and Y . Also, from Theorem 1 and the argument which Meek (1995) gave for his Theorem 3, $Result(G)$ consists of all arrows and adjacent pairs that are common to any other causal diagrams consistent with the prior knowledge that have the same conditional independencies as the underlying causal diagram G . The graph is said to be a maximally oriented pattern for $Pattern(G)$ with respect to the prior knowledge.

The following corollary can be obtained by Proposition 3 and a trivial modification of the proof of Theorem 1.

COROLLARY 1. *For an adjacent pair (X, Y) in $Max(G)$, $X - Y$ in $Max(G)$ if and only if $pa(X)_{Max(G)} = pa(Y)_{Max(G)}$, where $pa(X)_{Max(G)}$ is a set of parents of X in $Max(G)$. $\square$*

For example, consider a graph shown in Figure 3. Since $pa(X_1)_{Max(G)}$, $pa(X_2)_{Max(G)}$, $pa(X_3)_{Max(G)}$ and $pa(X_4)_{Max(G)}$ are all empty sets, arrows (X_1, X_2) , (X_1, X_3) , (X_2, X_3) and (X_2, X_4) can be not identified without prior knowledge. Suppose that we have prior knowledge such that X_2 is a variable which has an arrow from X_1 to it and from it to X_3 , X_4 and X_5 . The causal structure is identified by the prior knowledge completely and the graph is given in Figure 1.

4.2. The role of exogenous variable in recovering causal structure

In passive observational studies, there are some cases where we can recognize which variables are exogenous, where “exogenous” means that a variable has no arrows into it in a causal diagram (e.g. Spirtes and Cooper (1999)).

In this section, consider the graph structure of $Max(G)$ where a causal structure can be determined uniquely by recognizing exogenous variables.

Let V^* be a set of all vertices that have no parents in $Max(G)$. Letting $Submax(G)$ be an undirected subgraph of $Max(G)$ induced by V^* , we have the following results:

THEOREM 2. *If $Max(G)$ satisfies the following conditions, then a directed acyclic graph G can be determined from $Max(G)$ uniquely by recognizing exogenous variables. Also, the result coincides with G .*

- (i) *There is no $X - Y$ in $Max(G)$ such as $pa(X)_{Max(G)} \neq \phi$ and $pa(Y)_{Max(G)} \neq \phi$.*
- (ii) *$Submax(G)$ is a forest.* $\square$

In order to establish Theorem 2, the following lemma shall be proved.

LEMMA 2. *Each connected component in $Submax(G)$ has only one exogenous variable in G .* $\square$

PROOF OF LEMMA 2. Without loss of generality, suppose that $Submax(G)$ is a connected component. Then, the proof of Lemma 2 consists of the following parts:

Case 1. The case where V^* has one vertex.

Case 2. The case where V^* has more than two vertices.

(i) The existence of exogenous variables.

(ii) The uniqueness of an exogenous variable.

Case 1: Suppose that V^* consists of one vertex. If the vertex is an endogenous variable, the vertex is connected to others not in V^* by lines or arrows entering it. However, that the vertex is connected to others not in V^* by lines contradicts with the definition of $Submax(G)$. Also, that the vertex is connected to others not in V^* by arrows contradicts with the definition of V^* . Therefore, the vertex is an exogenous variable in G .

Case 2: Suppose that V^* has more than two vertices. First, let us prove that V^* has exogenous variables in G . If an exogenous variable in G does not exist in $Submax(G)$, every variable in V^* is an endogenous variable in G . Suppose that all parents of every vertex of V^* in G are in V^* . Then, there exist vertices in $V_1^* \subset V^*$ whose descendants in G are in V^* . Here, every vertex in $V_1^* \subset V^*$ is endogenous in G and their ancestors in G are in V_1^* from the assumption of V_1^* . By repeating application of this procedure, we can obtain $V_n^* \subset V^*$ whose ancestors in G are not in V_n^* since G is a directed acyclic graph. It is contradictory to the definition of V^* . Therefore, there exist vertices in $Submax(G)$ whose parents in $Max(G)$ are not in V^* , or vertices in $Submax(G)$ are connected to others not in V^* by lines. They contradict with $pa(X)_{Max(G)} = \phi$ for any $X \in V^*$ or the assumption that $Submax(G)$ is a connected component. Therefore, $Submax(G)$ has one exogenous variable at least.

Second, let us prove that there exists only one exogenous variable in V^* . Suppose that $Submax(G)$ has exogenous variables X and Y in G . If X is adjacent to Y , we must have $X \rightarrow Y$ or $X \leftarrow Y$ since G is a directed acyclic graph. It contradicts that both of them are exogenous variables, which implies that X is not adjacent to Y .

Suppose that there exist undirected paths between X and Y in $Submax(G)$, since $Submax(G)$ is a connected component. Let P_G^* be the shortest undirected path between X and Y in $Submax(G)$. The shortest undirected paths are also the shortest undirected path in $Max(G)$. The path P_G in G corresponding to P_G^* is the shortest path in G that does not have v -structure, since if P_G has v -structure then the undirected path P_G^* must have v -structure by using Proposition 1.

Here, suppose that P_G^* has an endogenous variable W in G which has converging arrows in G and whose parents are connected in G . Therefore, let U_1 and U_2 be vertices in $pa(W)_G$ which are connected in G . Then, the length of the shortest path between U_1 and U_2 is 1, and the length of the shortest path between U_1 and U_2 via W is 2. Therefore, if P_G^* has U_1 and U_2 , then P_G^* does not have W or P_G^* has v -structure at U_1 or U_2 since P_G^* is the shortest path in $Max(G)$. Since P_G^* has W , P_G^* must have v -structure at U_1 or U_2 , which implies that either an arrow from U_1 to W or an arrow from U_2 to W can be identified from Proposition 2. It contradicts that P_G^* is an undirected path. Therefore, P_G^* does not have W which has converging arrow in G from the above discussion.

Suppose that P_G has $\leftarrow W \rightarrow$ and that W is nondescendant of X and Y . Since

Figure 4. Maximally Oriented Pattern (2).

W is an endogenous variable, every ancestor of W is the nondescendant of X and Y . Let $T \in an(W)_G$ be a vertex which does not have ancestor in $an(W)_G \setminus \{T\}$. Since X and Y are exogenous variables, T is an endogenous variable, which contradicts that T does not have ancestor in $an(W)_G \setminus \{T\}$ from the assumption of W . It implies that X or Y is an ancestor of W , $\leftarrow W \leftarrow$ or $\rightarrow W \rightarrow$. These discussion indicates that P_G is a directed path, which implies that either X or Y is an endogenous variable. Contradiction. Therefore, $Submax(G)$ has only one exogenous variable in G . *Q.E.D.*

PROOF OF THEOREM 2. Without loss of generality, suppose that $Submax(G)$ is a connected component and that $Submax(G) = Max(G)$, since $Max(G)$ does not have adjacent variables X and Y linked by lines such as $pa(X)_{Max(G)} \neq \emptyset$ from Condition (i). Then adjacent endogenous variables X and Y in G linked by lines in $Max(G)$ are connected to an exogenous variable W in G from Lemma 2. Therefore, consider whether we can orient all arrows in $Max(G)$ by Proposition 2 and recognizing an exogenous variable. If an arrow between X and Y can be not identified by Proposition 2 and the prior knowledge, we have $pa(X)_{Max(G)} = pa(Y)_{Max(G)}$. However, since $Max(G)$ is a tree structure and an exogenous variable is recognized, $pa(X)_{Max(G)} \neq pa(Y)_{Max(G)}$ holds by repeated application of Proposition 2, or X and Y are nondescendants of an exogenous variable W in G . Hence, from Corollary 1, $pa(X)_{Max(G)} \neq pa(Y)_{Max(G)}$ contradicts that an arrow between X and Y can be not identified by Proposition 2 and the prior knowledge. Suppose that X and Y are nondescendants of an exogenous variable W . Then, since X and Y are endogenous variables, it implies that there exist another exogenous variable in G , which is contradictory to Lemma 2 since $Submax(G)$ is a connected component. Therefore, X and Y are descendants of an exogenous variable W . From the above discussion, a directed acyclic graph can be determined from $Max(G)$ uniquely by recognizing an exogenous variable. That the result consists of G is obvious from the argument given by Meek (1995). *Q.E.D.*

Especially, when each component in $Submax(G)$ of Theorem 2 consists of one vertex, we can recover the causal diagram without prior knowledge.

For example, consider the graph shown in Figure 3. Provided that we have prior knowledge such that X_1 is an exogenous variable which has no arrows into

Figure 5. Causal Diagram and Maximally Oriented Pattern.

Table 1. Correlation Matrix Reproduced by Path Coefficients.

	X_1	X_2	X_3	X_4	X_5	X_6	X_7
X_1	1.000	0.000	0.620	0.250	0.174	0.229	0.309
X_2	0.000	1.000	0.000	0.000	0.000	0.410	0.172
X_3	0.620	0.000	1.000	0.155	0.280	0.201	0.244
X_4	0.250	0.000	0.155	1.000	0.043	0.170	0.331
X_5	0.174	0.000	0.280	0.043	1.000	0.370	0.347
X_6	0.229	0.410	0.201	0.170	0.370	1.000	0.546
X_7	0.309	0.172	0.244	0.331	0.347	0.546	1.000

it, the following graph can be obtained and an arrow (X_2, X_3) is not identified by the prior knowledge.

4.3. Example

We will apply the above results to analysis of data taken from a study on the causes of academic productivity drawn from sociology, economics, and psychology, reported by Rodgers and Maranto (1989). They were interested in why some academic psychologists publish more than others. The size of a sample is 162, and the following seven variables are considered:

Ability(X_1), Gender(X_2), Graduate program quality(X_3), Publications in graduate school(X_4), Quality of first job(X_5), Publication rate(X_6), Citation rate(X_7)

Rodgers and Maranto obtained a linear structural equation model that fits the data well, which causal diagram is shown in Figure 5 (a). By using the path coefficients given by Rodgers and Maranto, we will calculate the correlation matrix corresponding to the causal diagram, which is shown in Table 1.

We will recover a causal structure by applying the reproduced correlation matrix to a software for suggesting causal structures from data, TETRAD 2 (Scheines *et al.* (1994)), in which PC algorithm is used as a recovery algorithm based on Proposition 1. The result is shown in Figure 5 (b), which has the same adjacent relations and v -structures as a causal diagram shown in Figure 5 (a).

Figure 6. Maximally Oriented Pattern (4).

In Figure 5 (b) created by TETRAD 2, since parents of X_1 , X_3 , X_4 and X_5 are empty sets respectively, arrows (X_1, X_3) , (X_1, X_4) and (X_3, X_5) can not be identified without prior knowledge such as their causal relations from Corollary 1.

Suppose that all arrows emerging from and entering into X_3 can be recognized. Then, since an arrow (X_1, X_4) can not be identified by the prior knowledge from Theorem 1 as seen from Figure 6, adding a causal relation between X_1 and X_4 to the prior knowledge is sufficient to determine the causal diagram uniquely,

On the other hand, since an undirected subgraph induced by $V^* = \{X_1, X_3, X_4, X_5\}$ is a tree, the causal diagram can be recovered completely by recognizing that X_1 is an exogenous variable from Theorem 2, which consists with Figure 5 (a).

5. Conclusion

In this paper, we showed a necessary and sufficient condition for identifying arrows by the recovery algorithms and graph structure of the maximally oriented pattern where the causal diagram is determined uniquely by recognizing exogenous variables. The result in this paper is useful to give enough prior knowledge to recover causal structure completely.

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