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A Recursive Method for Structural Learning of Directed Acyclic Graphs

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Abstract

In this paper, we propose a recursive method for structural learning of directed acyclic graphs (DAGs), in which a problem of structural learning for a large DAG is first decomposed into two problems of structural learning for two small vertex subsets, each of which is then decomposed recursively into two problems of smaller subsets until none subset can be decomposed further. In our approach, search for separators of a pair of variables in a large DAG is localized to small subsets, and thus the approach can improve the efficiency of searches and the power of statistical tests for structural learning. We show how the recent advances in the learning of undirected graphical models can be employed to facilitate the decomposition. Simulations are given to demonstrate the performance of the proposed method.

Keywords: Bayesian network, conditional independence, decomposition, directed acyclic graph, structural learning

1. Introduction

Directed acyclic graphs (DAGs), also known as Bayesian networks, are frequently used to represent independencies, conditional independencies and causal relationships in a complex system with a large number of random variables (Lauritzen, 1996; Cowell et al., 1999; Pearl, 2000; Spirtes et al., 2000). Structural learning of DAGs from data is very important in applications to various fields, such as medicine, artificial intelligence and bioinformatics (Jordan, 2004; Engelhardt et al., 2006).

There have been two primary methods for learning the structures of DAGs from data. The search-and-score method defines a score for each possible structure based on the goodness-of-fit of the structure to data and the complexity of the structure, and then it tries to search the best structure over all possible structures (Cooper and Herskovits, 1992; Heckerman et al., 1995; Chickering, 2002; Friedman and Koller, 2003). The constraint-based method evaluates the presence or absence of an edge by testing conditional independencies among variables from data. The tests are usually done by using statistical or information-theoretic measures (Pearl, 2000; Spirtes et al., 2000; Cheng et al., 2002). There have also been hybrid methods. For example, Tsamardinos et al. (2006) takes advantage of both approaches. In a constraint-based method, search for separators of vertex pairs is a key issue for orientation of edges and for recovering DAG structures and causal relationships among variables. To recover structures of DAGs, Verma and Pearl (1990) presented the inductive causation (IC) algorithm which searches for a separator S of two variables, say u and v, from all possible

variable subsets such that u and v are independent conditionally on S. A systematic way of searching for separators in increasing order of cardinality was proposed by Spirtes and Glymour (1991). The PC algorithm limits possible separators to vertices that are adjacent to u and v (Pearl, 2000; Spirtes et al., 2000). Kalisch and Bühlmann (2007) showed that the PC algorithm is asymptotically consistent even when the number of vertices in a DAG grows at a certain rate as the sample size increases.

In this paper, we propose a recursive algorithm in which a problem of structural learning for a large DAG is split recursively into problems of structural learning for small vertex subsets. Our algorithm can be depicted as a binary tree whose top node is the full set of all vertices or variables and whose other nodes are proper subsets of the vertex set at its parent node. The algorithm mainly consists of two steps: the top-down step and the bottom-up step. First at the top-down step, the full set of all variables at the top is decomposed into two small subsets, each of which is decomposed recursively into two smaller subsets until each node cannot be decomposed further at the bottom of the tree. At each step, the decomposition is achieved by learning an undirected graph known as independence graph for a variable subset. Next at the bottom-up step, subgraphs (called skeletons) of leaf nodes are first constructed, and then a pair of child subgraphs are combined together into a large subgraph at their parent node until the entire graph is constructed at the top of the tree. In the algorithm, search for separators in a large graph is localized to small subgraphs. Statistical test is used to determine a skeleton as in the IC algorithm (Verma and Pearl, 1990) and the PC algorithm (Spirtes, 2000). By recursively decomposing the full variable set into small subsets, this algorithm can improve the efficiency of search for separators in structural learning, and it can also make statistical tests more powerful. We also discuss that several methods of learning undirected graphical models (Castelo and Roverato, 2006; Schmidt et al., 2007) can be used to facilitate the decomposition. Finally, we provide simulation results to show the performance of our method.

Section 2 gives notation and definitions. In Section 3, we first present the main theoretical results and then discuss the realization of the algorithm in detail, and we also introduce how the recent advances in various related fields can be used to improve the proposed method. In Section 4, we first use an example to illustrate our approach for learning the equivalence class of a DAG in detail, then we give numerical evaluations of its performance for several networks, and finally we discuss the computational complexity of our recursive algorithm. Conclusion is given in Section 5. The proofs of our main results are presented in Appendix.

2. Notation and Definitions

Let $\vec{G}_V = (V, \vec{E}_V)$ denote a DAG where $V = \{X_1, \ldots, X_n\}$ is the vertex set and $\vec{E}_V$ the set of directed edges. A directed edge from a vertex u to a vertex v is denoted by $\langle u, v \rangle$. We assume that there is no directed loop in $\vec{G}_V$. We say that u is a parent of v and v is a child of u if there is a directed edge $\langle u, v \rangle$, and denote the set of all parents of a vertex v by $pa(v)$ and the set of all children of v by $ch(v)$. We say that two vertices u and v are adjacent in $\vec{G}_V$ if there is an edge connecting them. A path l between two distinct vertices u and v is a sequence of distinct vertices in which the first vertex is u, the last one is v and two consecutive vertices are connected by an edge, that is, $l = (c_0 = u, c_1, \ldots, c_{m-1}, c_m = v)$ where $\langle c_{i-1}, c_i \rangle$ or $\langle c_i, c_{i-1} \rangle$ is contained in $\vec{E}_V$ for $i = 1, \ldots, m$ ($m \geq 1$), and $c_i \neq c_j$ for all $i \neq j$. We say that u is an ancestor of v and v is a descendant of u if there is a path between u and v in $\vec{G}_V$ and all edges on this path point at the direction toward v. The set of ancestors of v is denoted as $an(v)$, and we define $An(v) = an(v) \cup \{v\}$. A path l is said to be d-separated by a set of vertices Z if

(1) l contains a "chain": $u \to v \to w$ or a "fork" $u \leftarrow v \to w$ where v is in Z, or

(2) l contains a "collider" $u \to v \leftarrow w$ where v is not in Z and no descendant of v is in Z.

Two disjoint sets X and Y of vertices are d-separated by a set Z if Z d-separates every path from any vertex in X to any vertex in Y; We call Z a d-separator of X and Y. In $\vec{G}_V$, a collider $u \to v \leftarrow w$ is called a v-structure if u and w are non-adjacent in $\vec{G}_V$.

Let $\bar{G}_V = (V, \bar{E}_V)$ denote an undirected graph where $\bar{E}_V$ is a set of undirected edges. An undirected edge between two vertices u and v is denoted by (u,v). An undirected graph is called complete if any pair of vertices is connected by an edge. Define a moral graph $\bar{G}^m_V$ for a DAG $\vec{G}_V$ to be an undirected graph $\bar{G}^m_V = (V, \bar{E}_V)$ whose vertex set is V and whose edge set is constructed by marrying parents and dropping directions, that is, $\bar{E}_V = \{(u,v) : \langle u,v\rangle \text{ or } \langle v,u\rangle \in \vec{E}_V\} \cup \{(u,v) : (u,w,v) \text{ forms a } v\text{-structure}\}$ (Lauritzen, 1996). An undirected edge added for marrying parents is called a moral edge.

For an undirected graph, we say that vertices u and v are separated by a set of vertices Z if each path between u and v passes through Z. We say that two disjoint vertex sets X and Y are separated by Z if Z separates every pair of vertices u and v for any $u \in X$ and $v \in Y$. We call (A,B,C) a decomposition of $\bar{G}_V$ if

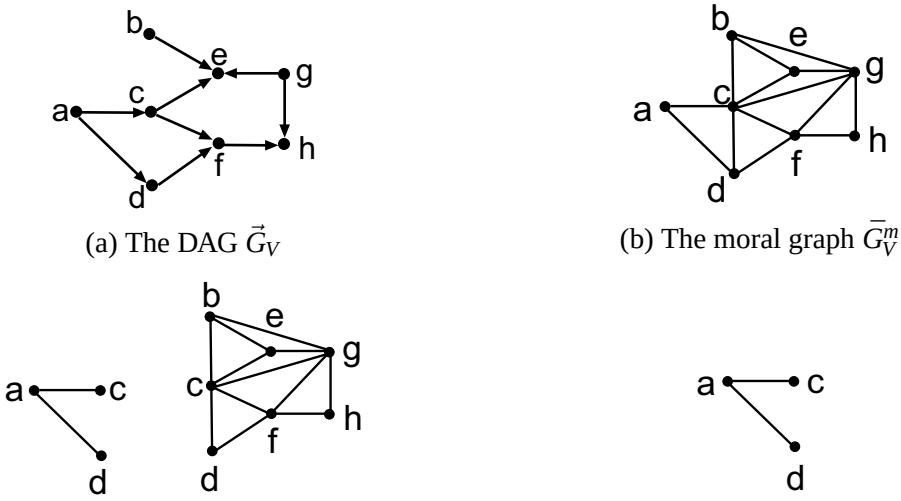
(1) $A \cup B \cup C = V$, and

(2) C separates A and B in $\bar{G}_V$.

Note that the above decomposition does not require that the separator C is complete, which is required for weak decomposition defined by Lauritzen (1996).

For a set $K \subseteq V$, we say that an undirected graph $\bar{G}_K$ is an undirected independence graph for a DAG $\vec{G}_V$ if that a set Z separates X and Y in $\bar{G}_K$ implies that Z d-separates X and Y in $\vec{G}_V$. An undirected independence graph is minimal if the proper subgraph obtained by deleting any edge is no longer an undirected independence graph. The moral graph $\bar{G}^m_V$ is the minimal undirected independence graph for $\vec{G}_V$ with $K = V$ (Lauritzen, 1996). It can also be obtained by connecting each vertex u with all vertices in its Markov blanket $Mb(u)$, which is the minimal set by which u are d-separated from the remaining set in V (that is, $V \setminus [Mb(u) \cup \{u\}]$). For a subset $K \subseteq V$, the Markov blanket for a vertex $u \in K$ can be defined similarly, that is, it is the minimum set that is contained in K and d-separates u from the remaining set in K. When $K = V$, it is easy to verify $Mb(u) = pa(u) \cup ch(u) \cup pa(ch(u))$. Define the local skeleton for a variable set $K \subseteq V$ with respect to $\vec{G}_V$ as an undirected graph $\bar{L}_K(K,E)$ where K is the vertex set and $E = \{(u,v) : \text{ no subset } S \text{ of } K \text{ } d\text{-separates } u \text{ and } v \text{ in } \vec{G}_V\}$ is the edge set. Note that though both minimal undirected independence graphs and local skeletons are undirected graphs and defined on the same vertex subset, they may be different. According to the definition of a minimal undirected independence graph, the absence or presence of an edge between u and v in the minimal undirected independence graph over $K \subseteq V$ depends on whether its two vertices are d-separated by the remaining set $K \setminus \{u,v\}$ in $\vec{G}_V$, while an edge between u and v in the local skeleton is determined by whether there exists a subset of K that can d-separate u and v in $\vec{G}_V$. Thus the edge set of the minimal undirected independence graph contains the edge set of the local skeleton.

The global skeleton is an undirected graph obtained by dropping the directions of the edges in a DAG, which coincides the local skeleton for $K = V$. Two DAGs over the same variable set



(a) The DAG $\vec{G}_V$

(b) The moral graph $\bar{G}_V^m$

(c) One decomposition based on $\bar{G}_V^m$

(d) A local skeleton

Figure 1: A directed graph, a moral graph, a decomposition and a local skeleton.

are called Markov equivalent if they induce the same conditional independence restrictions. Two DAGs are Markov equivalent if and only if they have the same global skeleton and the same set of *v*-structures (Verma and Pearl, 1990). An equivalence class of DAGs consists of all DAGs which are Markov equivalent, and it is represented as a partially directed graph (PDAG) where the directed edges represent arrows that are common to every DAG in the Markov equivalence class, while an undirected edge represents that the edge is oriented one way in some member of the Markov equivalence class, and is oriented the other way in some other member. Therefore the goal of structural learning is to construct a PDAG to represent the equivalence class.

Example 1. Consider the DAG in Figure 1 (a). $b \to e \leftarrow c$, $b \to e \leftarrow g$, $c \to f \leftarrow d$, $c \to e \leftarrow g$ and $f \to h \leftarrow g$ are *v*-structures. A path $l = (c,a,d)$ is d-separated by vertex a, while the path $l' = (c,f,h,g)$ is d-separated by an empty set. We have $an(e) = \{a,b,c,g\}$ and $An(e) = \{a,b,c,g,e\}$. The Markov blanket of c is $Mb(c) = \{a,b,d,e,f,g\}$, which d-separates c and the remaining set $\{h\}$. The moral graph $\bar{G}_V^m$ is given in Figure 1 (b), where edges (b,c), (b,g), (c,g), (c,d) and (f,g) are moral edges. Note that the set $\{c,d\}$ separates $\{a\}$ and $\{b,e,f,g,h\}$ in G_V^m, thus $(\{a\},\{b,e,f,g,h\},\{c,d\})$ forms a decomposition of the undirected graph G_V^m, the decomposed undirected independence subgraphs for $\{a,c,d\}$ and $\{b,c,d,e,f,g,h\}$ are shown in Figure 1 (c). The graph in Figure 1 (d) is the local skeleton $L_K(K,E)$ for $K = \{a,c,d\}$ because we have c and d are d-separated by $\{a\}$ in $\vec{G}_V$. Note that the minimal undirected independence graph for $\{a,c,d\}$ in Figure 1(c) coincides with its local skeleton in Figure 1 (d), which does not hold in general. For example, the local skeleton for $K = \{c,e,g\}$ does not have the edge (c,g), while the corresponding minimal undirected independence graph is complete.

Given a DAG $\vec{G}_V$, a joint distribution or density of variables $X_1,\ldots,X_N$ is

$$P(x_1,\cdots,x_N) = \prod_{i=1}^{N} P(x_i|pa_i),$$

where $P(x_i|pa_i)$ is the conditional probability or density of X_i given $pa(X_i) = pa_i$. The DAG $\vec{G}_V$ and the joint distribution P are said to be compatible (Pearl, 2000) and P obeys the global directed Markov property of $\vec{G}_V$ (Lauritzen, 1996). Let $X \perp\!\!\!\perp Y$ denote the independence of X and Y, and $X \perp\!\!\!\perp Y|Z$ the conditional independence of X and Y given Z. In this paper, we assume that all independencies of a probability distribution of variables in V can be checked by d-separations of $\vec{G}_V$, called the faithfulness assumption (Spirtes et al., 2000), which means that all independencies and conditional independencies among variables can be represented by $\vec{G}_V$. As a consequence, we also use $\perp\!\!\!\perp$ to denote the d-separation in DAGs.

3. A Recursive Method for Structural Learning of a DAG

In this section, we first present theoretical results in this paper and then we apply these results to structural learning of a DAG and show how the problem of searching for d-separators over the full set of all vertices can be recursively split into the problems of searching for d-separators over smaller subsets of vertices. We also discuss how to learn from data the undirected independence graphs which are used to achieve the recursive decomposition at each recursive step.

3.1 Theoretical Results and Recursive Algorithm for Structural Learning

Below we first give two theorems based on which we propose the recursive algorithm for structural learning of DAGs.

Theorem 1. Suppose that $A \perp\!\!\!\perp B|C$ in a DAG $\vec{G}_V$. Let $u \in A$ and $v \in A \cup C$. Then u and v are d-separated by a subset of $A \cup B \cup C$ if and only if they are d-separated by a subset of $A \cup C$.

According to Theorem 1, we can see that all edges falling in A or crossing A and C in the local skeleton $\overline{L}(K,E)$ with $K = A \cup C \cup B$ can be validly recovered from the marginal distribution of variables in $A \cup C$. Note that such a local skeleton over K can be used to recover the entire DAG over V even if there may not exist a marginalized DAG over K (Richardson and Spirtes, 2002).

Theorem 2. Suppose that $A \perp\!\!\!\perp B|C$ in a DAG $\vec{G}_V$. Let u and v be two vertices both of which are contained in the separator C. Then u and v are d-separated by a subset of $A \cup B \cup C$ if and only if they are d-separated by a subset of $A \cup C$ or by a subset of $B \cup C$.

According to Theorem 2, the existence of an edge falling into the separator C in the local skeleton $\overline{L}(K,E)$ with $K = A \cup C \cup B$ can be determined from the marginal distribution of $A \cup C$ or the marginal distribution of $B \cup C$.

Note that the union set $K = A \cup B \cup C$ in Theorems 1 and 2 may be a subset of the full set V (that is, $K \subseteq V$), and they are more general results than Theorem 1 presented in Xie et al. (2006), which requires that the union set K equals V (that is, $K = A \cup B \cup C = V$). These two theorems can guarantee that, for any partition (A,B,C) of a vertex set $K \subseteq V$ that satisfies $A \perp\!\!\!\perp B|C$, two non-adjacent vertices u and v in K are d-separated by a subset S of K in $\vec{G}_V$ if and only if they are d-separated by a subset S' of either $A \cup C$ or $B \cup C$ in $\vec{G}_V$. Therefore, we have the following result.

Theorem 3. Suppose that $A \perp\!\!\!\perp B|C$ in a DAG $\vec{G}_V$. Then the local skeleton $\overline{L}_K = (K, E_K)$ can be constructed by combining local skeletons $\overline{L}_{A\cup C} = (A \cup C, E_{A\cup C})$ and $\overline{L}_{B\cup C} = (B \cup C, E_{B\cup C})$ as follows:

(1) the vertex set $K = A \cup C \cup B$ and

(2) the edge set $E_K = (E_{A\cup C} \cup E_{B\cup C}) \setminus \{(u,v) : u,v \in C \text{ and } (u,v) \notin E_{A\cup C} \cap E_{B\cup C}\}$.

Based on these theorems, we propose a recursive algorithm for learning the structure of a DAG. Our algorithm has a series of operations on a binary tree. The top node of the tree is the full set of all variables, the leaves of the tree are subsets of variables which cannot be decomposed, and the variable set of each parent node in the binary tree is decomposed into two variable sets of its two children. Our algorithm consists of two steps: the top-down step for decomposing the full set of all variables into subsets as small as possible, and the bottom-up step for combining local skeletons into the global skeleton. At the top-down step, a variable set is decomposed into two subsets whenever a conditional independence $A \perp\!\!\!\perp B|C$ is found, and this decomposition is repeated until no new decomposition can be found. The decomposition at each step is done by learning an undirected independence graph over the vertex subset at the tree node, which will be discussed in Subsection 3.3. At the bottom-up step, two small skeletons are combined together to construct a larger skeleton, and the combination is repeated until the global skeleton is obtained. The entire process is formally described in the following algorithm.

Main Algorithm (*The recursive decomposition for structural learning of DAGs*)

1. Input: a target variable set V; observed data D.
2. Call DecompRecovery (V, $\bar{L}_V$) to get the global skeleton $\bar{L}_V$ and a separator list $\mathcal{S}$.
3. For each d-separator S_{uv} in the separator list $\mathcal{S}$, orient the local skeleton $u - w - v$ as a v-structure $u \rightarrow w \leftarrow v$ if $u - w - v$ (Note no edge between u and v) appears in the global skeleton and w is not contained in the separator S_{uv}.
4. Apply Meek's rule (Meek, 1995) to obtain a DAG in the Markov equivalence class: we orient other edges if each opposite of them creates either a directed cycle or a new v-structure. The Markov equivalence class can be obtained by collecting all possible DAGs.
5. Output: the equivalence class of DAGs.

PROCEDURE DecompRecovery (K, $\bar{L}_K$)

1. Construct an undirected independence graph $\bar{G}_K$;
2. If $\bar{G}_K$ has a decomposition (A, B, C)

   Then

   - For each pair (u, v) of $u \in A$ and $v \in B$, save $(u, v, S_{uv} = C)$ to the d-separator list $\mathcal{S}$;
   - DecompRecovery ($A \cup C$, $\bar{L}_{A\cup C}$);
   - DecompRecovery ($B \cup C$, $\bar{L}_{B\cup C}$);
   - Set $\bar{L}_K$ = CombineSubgraphs ($\bar{L}_{A\cup C}$, $\bar{L}_{B\cup C}$)

   Else

   - Construct the local skeleton $\bar{L}_K$ directly (such as using the IC algorithm):
     Start with a complete undirected graph over K.
     For any vertex pair (u, v) in the set K, if there exists a subset S_{uv} of $K \setminus \{u, v\}$ such that $u \perp\!\!\!\perp v|S_{uv}$, then delete the edge (u, v) and save (u, v, S_{uv}) to the d-separator list $\mathcal{S}$.

3. RETURN ($\bar{L}_K$).

FUNCTION CombineSubgraphs ($\bar{L}_U$, $\bar{L}_V$)

1. Combine $\bar{L}_U = (U, E_U)$ and $\bar{L}_V = (V, E_V)$ into an undirected graph $\bar{L}_{U\cup V} = (U \cup V, E_{U\cup V})$ where
$$E_{U\cup V} = (E_U \cup E_V) \setminus \{(u,v) : u,v \in U \cap V \text{ and } (u,v) \notin E_U \cap E_V\};$$
2. Return ($\bar{L}_{U\cup V}$).

As shown in the main algorithm, the equivalence class of $\vec{G}_V$ can be constructed by first calling DecompRecovery (V, $\bar{L}_V$) to get the skeleton, then recover all v-structures using the d-separator list $\mathcal{S}$ to orient the edges in $\bar{L}_V$, and finally orient other edges as much as possible using the rule in Meek (1995). Since a decomposition (A,B,C) of the undirected independence graph $\bar{G}_K$ implies $A \perp\!\!\!\perp B|C$, it is obvious by Theorems 1 and 2 that our algorithm is correct.

A binary decomposition tree is used in DecompRecovery to describe our algorithm simply and clearly. In our implementation, we use a junction tree to decompose a graph into several subgraphs simultaneously and to find the corresponding separators. It is known that the junction tree may not be unique, and thus we may have multiple decompositions. In theory, we prefer to use the junction tree with the minimum tree width. However, this is known to be an NP hard problem (Arnborg et al., 1987); therefore, we may use some sub-optimal method to consruct a junction tree for an undirected graph (Jensen and Jensen, 1994; Becker and Geiger, 2001). For example, two most well-known algorithms are the lexicographic search (Rose et al., 1976) and the maximum cardinality search (Tarjan and Yannakakis, 1984), whose computational expenses are $O(ne)$ and $O(n+e)$ respectively, where e is the number of edges in the graph. Especially, the latter method is used in our implementation. According to our experiences, the junction tree obtained by either method usually leads to very efficient decompositions.

In the recursive algorithm, statistical tests are used only at the top-down step but not at the bottom-up step. Thus the data sets used for statistical tests can be reduced into marginal data sets with decomposition of graphs. In this way, we only need to pass through small marginal data sets for statistical tests of subgraphs and need not pass through the full data set for every statistical test. Other algorithms (such as the PC algorithm) can be used to replace the IC algorithm to improve the performance of constructing the local skeleton $\bar{L}_K$ in DecompRecovery.

3.2 Tests of Conditional Independence

Conditional independence test of two variables u and v given a set C of variables is required at Step 1 and the 'Else' part of Step 2 of Procedure DecompRecovery to construct an undirected independence graph and a local skeleton respectively. Null hypothesis H_0 is $u \perp\!\!\!\perp v|C$ and alternative H_1 is that H_0 may not hold. Generally we can use the likelihood ratio test statistic

$$G^2 = -2\log \frac{\sup\{L(\theta|D) \text{ under } H_0\}}{\sup\{L(\theta|D) \text{ under } H_1\}},$$

where $L(\theta|D)$ is the likelihood function of parameter θ with observed data D. Under H_0, the statistic G^2 asymptotically follows the χ^2 distribution with df degrees of freedom being equal to the difference of the dimensions of parameters for the alternative and null hypothesis (Wilks, 1938).

Let $\mathbf{X}_k$ be a vector of variables and N be the sample size. For the case of a Gaussian distribution, the test statistic for testing $X_i \perp\!\!\!\perp X_j | \mathbf{X}_k$ can be simplified to

$$\begin{aligned} G^2 &= -N \times \log(1 - \text{corr}^2(X_i, X_j | \mathbf{X}_k)) \\ &= N \times \log \frac{\det(\hat{\Sigma}_{\{i,k\}\{i,k\}}) \det(\hat{\Sigma}_{\{j,k\}\{j,k\}})}{\det(\hat{\Sigma}_{\{i,j,k\}\{i,j,k\}}) \det(\hat{\Sigma}_{k,k})}, \end{aligned}$$

which has an asymptotic χ^2 distribution with $df = 1$. Actually, the exact null distribution or a better approximate distribution of G^2 can be obtained based on Bartlett decomposition, see Whittaker (1990) for more detailed discussion on this.

For the discrete case, let N_s^m be the observed frequency in a cell of $X_s = m$ where s is an index set of variables and m is a category of variables X_s. For example, N_{ijk}^{abc} denotes the frequency of $X_i = a$, $X_j = b$ and $\mathbf{X}_k = c$. The G^2 statistic for testing $X_i \perp\!\!\!\perp X_j | \mathbf{X}_k$ is then given by

$$G^2 = 2 \sum_{a,b,c} N_{ijk}^{abc} \log \frac{N_{ijk}^{abc} N_k^c}{N_{ik}^{ac} N_{jk}^{bc}},$$

which is asymptotically distributed as a χ^2 distribution under H_0 with degree of freedom

$$\text{df} = (\#(X_i) - 1)(\#(X_j) - 1) \prod_{X_l \in \mathbf{X}_k} \#(X_l),$$

where $\#(X)$ is the number of categories of variable X.

For discrete data, the size of conditional variable sets cannot be so large that independence tests become inefficient. Thus the algorithm restricts the cardinality of conditioning sets. There are many methods that can be used to find a small conditioning set, such as a forward selection of variables. With the recursive decomposition, independence tests are localized to smaller and smaller subsets of variables, and thus the recursive algorithm has higher power for statistical tests.

3.3 Constructing Undirected Independence Graphs

In this subsection, we discuss how to construct undirected independence graphs at Step 1 of Procedure DecompRecovery. At first we call DecompRecovery with the full set V as the input argument, and construct an undirected independence graph $\bar{G}_V$ at Step 1. Then at each recursive calling, to construct a local undirected independence graph $\bar{G}_K$ with a subset K (say $K = A \cup C$) as the input argument, we shall present a theoretical result based on which we only need to check edges over the separator C without need of testing conditional independencies between any pair of variables in A and between any pair of variables crossing A and C.

To construct an undirected independence graph $\bar{G}_V$, we start with a complete undirected graph, and then we check an edge between each pair of vertices u and v. The edge (u,v) is removed if u and v are independent conditionally on the set of all other variables. For linear Gaussian models, the undirected graph can be constructed by removing an edge (u,v) if and only if the corresponding entry in the inverse covariance matrix is zero (Dempster, 1972; Whittaker, 1990). After decomposing a graph $\bar{G}_{A \cup B \cup C}$ into two subsets $A \cup C$ and $B \cup C$, we need to construct a local undirected independence graph $\bar{G}_K$ (say $\bar{G}_{A \cup C}$) at Step 1 of Procedure DecompRecovery. We show in the following theoretical result that an initial $\bar{G}_{A \cup C}$ can be constructed by using all undirected edges contained

by $A \cup C$ in the previous graph $\bar{G}_{A \cup B \cup C}$ and then only pairs of vertices contained in C need to be checked via conditional independence tests.

Theorem 4. Suppose that the distribution of $V = A \cup B \cup C$ is positive and has the conditional independence $A \perp\!\!\!\perp B | C$. Then for any u in A and any v in $A \cup C$, we have that $u \perp\!\!\!\perp v | [(A \cup C) \setminus \{u, v\}]$ if and only if $u \perp\!\!\!\perp v | [(A \cup B \cup C) \setminus \{u, v\}]$.

Note that Theorems 1 and 4 are different. The former is used to determine an edge in a DAG, and the latter is used to determine an edge in an undirected independence graph. According to this theorem, there exists an edge (u, v) in the minimal undirected independence graph $\bar{G}_{A \cup C}$ for u in A and v in $A \cup C$ if and only if there exists an edge (u, v) in the minimal undirected independence graph $\bar{G}_{A \cup B \cup C}$. Thus given an undirected independence graph $\bar{G}_{A \cup B \cup C}$ obtained in the preceding step, an undirected independence graph $\bar{G}_{A \cup C}$ has the same set of edges as $\bar{G}_{A \cup B \cup C}$ each of which has at least one vertex in A, but all of possible edges within the separator C need to be checked for $\bar{G}_{A \cup C}$.

When there is a large number of variables and a small sample size, it is infeasible or statistically unstable to test an independence between two variables conditionally on all other variables, and this problem is more serious when variables are discrete. Many current methods for learning undirected graphical models can also be used in our algorithm. For example, procedures based on *limited-order partial correlations* (Wille and Bühlmann, 2004; Castelo and Roverato, 2006) are rather suitable and can be even used in the case where the number of variables is larger than the number of samples. Another way of learning undirected independence graphs is to apply current available Markov blanket learning algorithms. By connecting each vertex with those in its Markov blanket, an independence graph is then obtained. Indeed, it is neither new nor uncommon to learn the Markov blanket as either an initial step for learning a DAG or as a special problem of interest. Koller and Sahami (1996) developed a method for feature selection which employs the concept of Markov blanket. Margaritis and Thrun (1999) proposed a two-phase algorithm to first identify a Markov blanket for each variable and then obtain a DAG by connecting vertices in a maximally consistent way. Tsamardinos et al. (2003) proposed a method that can soundly identify all Markov blankets and scale-up to a graph with thousands of variables.

Another particular method for learning the undirected independence graph may use Lasso-type estimators (Tibshirani, 1996; Meinshausen and Bühlmann, 2006; Zhao and Yu, 2006; Wainwright et al., 2006). We can apply Lasso method to select a neighborhood set of a vertex which contains the Markov blanket of the vertex. Schmidt et al. (2007) developed a new method of learning structure of a DAG. Note that it is not necessary to learn neighborhoods exactly in our algorithm, and there may be extra edges in our undirected independence graph.

4. Illustration and Evaluation of the Recursive Algorithm

In this section, we first illustrate the recursive algorithm step by step via a concrete example and then show simulation results to evaluate its performance.

4.1 Illustration of the Recursive Algorithm

In this subsection, we illustrate our recursive algorithm using a concrete example. We suppose in the following example that conditional independencies can be implemented correctly, that is, each conditional independence is checked by using the underlying DAG. Therefore the purpose of the example is simply to illustrate the overall scheme of the recursive algorithm presented in Section 3.1. The performance of conditional independence tests is discussed in the next subsection. We

compare the recursive algorithm with the decomposition algorithm proposed in Xie et al. (2006), in which an entire undirected independence graph is first constructed and then it is decomposed into many small subgraphs at one step instead of recursive steps. We show that, in our algorithm, search for separators is localized to smaller vertex subsets than those obtained by using the decomposition algorithm.

Example 1. (Continued) Consider again the DAG $\vec{G}_V = (V, \vec{E}_V)$ in Figure 1 (a). We call Procedure DecompRecovery to construct the global skeleton over V. At the top-down step (that is, at the 'Then' part of Step 2 in DecompRecovery), we construct the binary tree shown in Figure 2. At the top of the binary tree, the first decomposition is done by splitting the full vertex set V in G_1 (that is, the moral graph) into two subsets $\{a,c,d\}$ and $\{b,c,\ldots,h\}$ with the separator $\{c,d\}$. Next we learn the undirected independence graphs G_2 and G_3 for the two subsets separately. To construct the subgraphs G_2 and G_3, by Theorem 5, we only need to check the edge (c,d) in the separator $\{c,d\}$, and other edges in G_2 and G_3 can be obtained directly from G_1. Repeat this procedure until no further decomposition is possible. Finally we get the entire binary tree T as shown in Figure 2, where each leaf node is a complete graph and cannot be decomposed further.

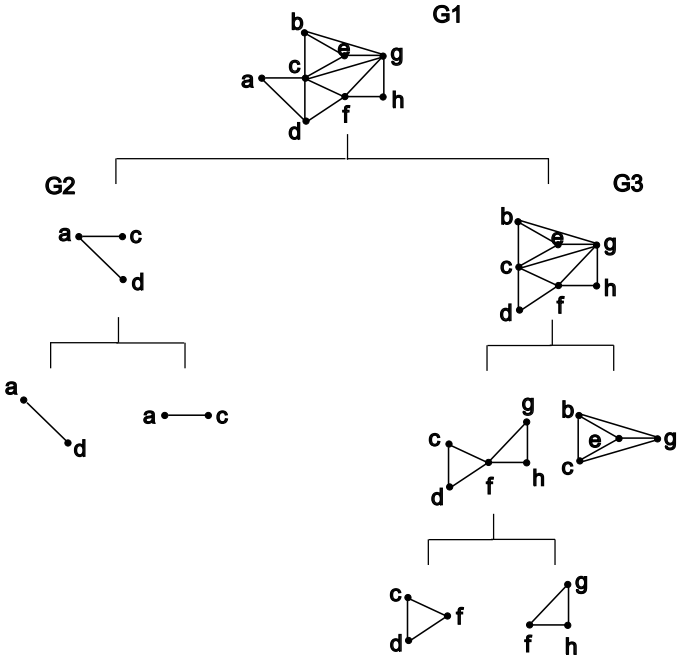


Figure 2: The binary tree T obtained at the top-down step (at 'Then' of Step 2).

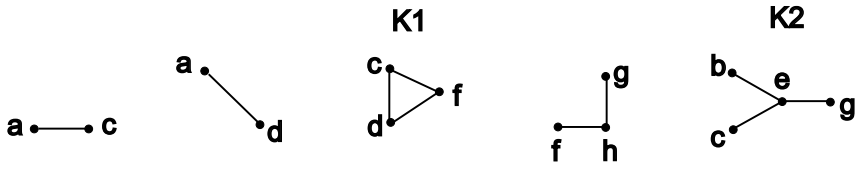


Figure 3: The local skeletons obtained at 'Else' of Step 2.

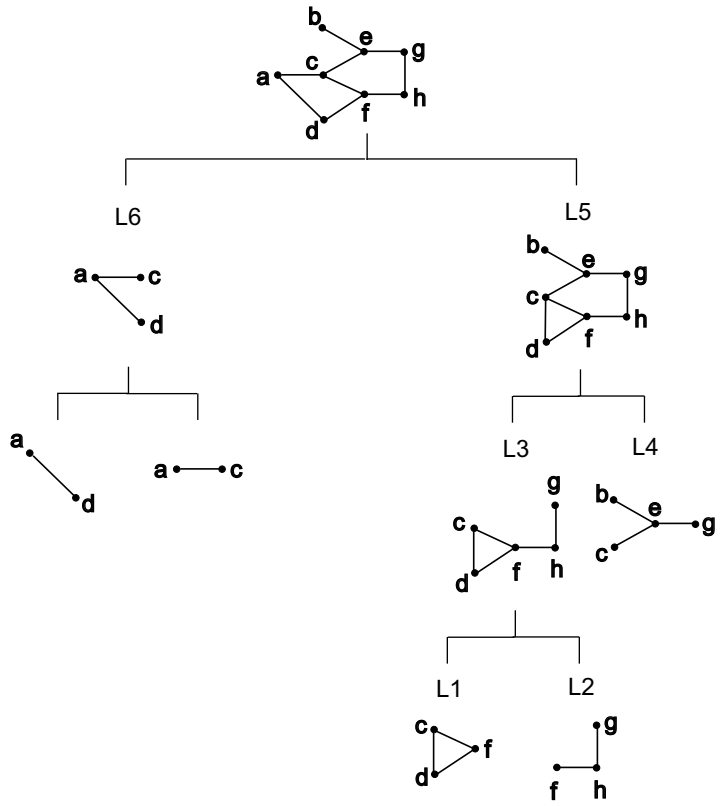


Figure 4: Combinations of local skeletons in Procedure CombineSubgraphs.

Before the bottom-up step (that is, the 'Else' part of Step 2 in Procedure DecompRecovery), for each leaf node K, we construct a local skeleton over K. For each vertex pair (u,v) in K, we search a separator set S_{uv} in all possible subsets of $K \setminus \{u,v\}$ to construct the local skeleton. All local skeletons of leaf nodes are shown in Figure 3. For example, the vertices c and d are adjacent in the local skeleton K_1 since no vertex set in K_1 d-separates them, whereas b and g are non-adjacent in the local skeleton K_2 since an empty set d-separates them in $\vec{G}_V$. At the bottom-up step, calling Function CombineSubgraphs, we combine the local skeletons from the leaf nodes to the root node to form the global skeleton, as shown in Figure 4. For example, local skeletons L_1 and L_2 are combined to L_3, and then L_3 and L_4 are combined to L_5, as shown in Figure 4. Similarly, we get the local skeleton L_6. At the last step, we combine L_5 and L_6 into the global skeleton. Note that the edge (c,d) in L_5 is deleted at Step 1 of Function CombineSubgraphs since the edge is not contained in L_6. After all the combinations are done, we get the global skeleton in Figure 5. We can see that the undirected independence graphs and the local skeletons are different as shown in Figure 2 and Figure 4 respectively and that the former has more edges than the latter.

At Step 2 of Procedure DecompRecovery, we save all separators to the d-separator list $\mathcal{S}$. At Step 3 of the main Algorithm, we use separators in the list $\mathcal{S}$ to recover all v-structures of the DAG. For example, there is a d-separator $\{a\}$ in $\mathcal{S}$ which d-separates c and d, and there is a structure $c - f - d$ in the global skeleton $\bar{L}_V$ where f is not contained in the separator $\{a\}$. Thus we can orient the structure $c - f - d$ as a v-structure $c \to f \leftarrow d$. Similarly, since an empty set d-separates

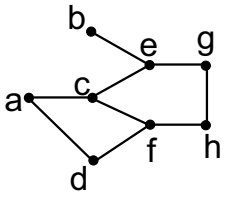


Figure 5: The global skeleton $\bar{L}_V$.

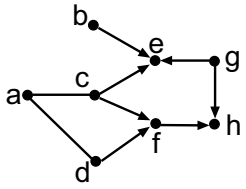


Figure 6: The recovered equivalence class.

b and g in $\vec{G}_V$, we can orient $b-e-g$ as $b \to e \leftarrow g$. After recovering all *v*-structures, we apply the orientation rule in Meek (1995) and get the desired equivalence class of $\vec{G}_V$ in Figure 6. In this equivalence class, the undirected edge (a,c) cannot be oriented uniquely because any of its orientation leads to a Markov equivalent DAG.

Below we compare the recursive algorithm with the decomposition algorithm proposed in Xie et al. (2006). We show that theoretically the recursive algorithm can decompose the entire graph into smaller subgraphs than the decomposition algorithm does because the decomposition in the decomposition algorithm is done only once, whereas the recursive algorithm tries to re-decompose undirected independence subgraphs at each recursive step. When there are a lot of *v*-structures in a DAG, many moral edges can be deleted in construction of a subgraph, and thus the recursive algorithm is more efficient than the decomposition algorithm. The following example illustrates the difference of decompositions obtained by these two algorithms.

Example 2. Consider the DAG in Figure 7. By using the decomposition algorithm proposed in Xie et al. (2006), a '*d*-separation tree' is built from an undirected independence graph (that is, the moral graph in this example), and the full variable set is decomposed into three subsets of variables at one time, see Figure 8 (a). By using the recursive algorithm proposed in this paper, we can decompose the graph into four subgraphs in Figure 8 (b), which have smaller subsets of variables. This is because the undirected independence graph over $\{a,b,c\}$ in Figure 8 (b) is re-constructed and the edge (b,c) is deleted for $b \perp\!\!\!\perp c|a$.

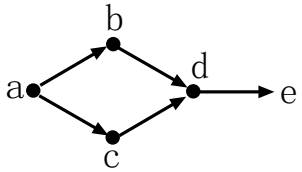
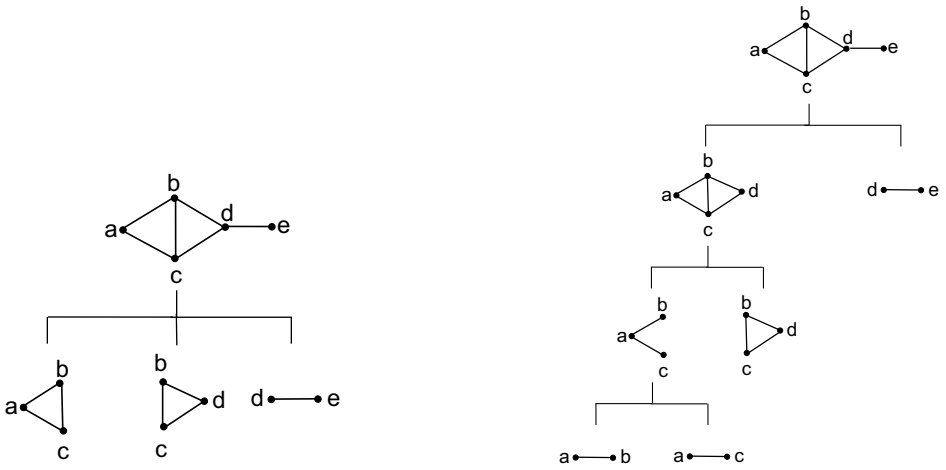


Figure 7: A DAG.



(a) The decomposition algorithm.

(b) The recursive algorithm.

Figure 8: Comparison of two different algorithms for structural learning.

4.2 Simulation Studies

Below we give numerical examples to evaluate the performance of the recursive algorithm. We first present simulation results for the ALARM network, which is a medical diagnostic network and is shown in Figure 9 (Beinlich et al., 1989; Heckerman, 1998). It is a DAG with 37 vertices and 46 edges and it is often used to evaluate performance of learning algorithms. In the following two subsections, we use the ALARM network to do simulation for the Gaussian case and the discrete case separately. Next we show simulation results for several other networks in the final subsection.

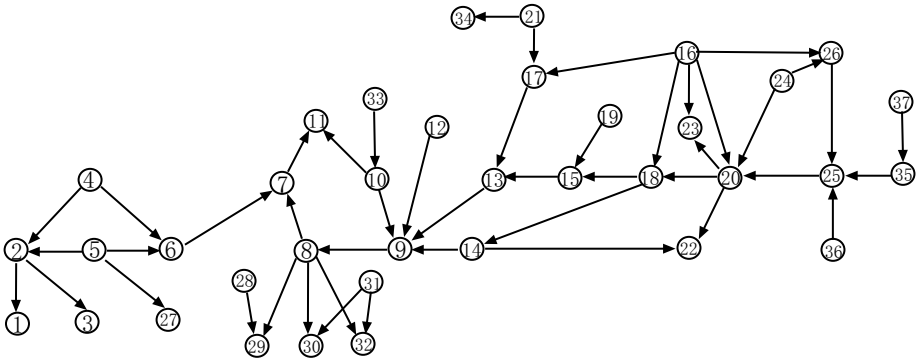


Figure 9: The ALARM network.

4.2.1 THE GAUSSIAN CASE

In this subsection, for the underlying DAG of the ALARM network, we generate a sample from a joint Gaussian distribution using a structural equation model of recursive linear regressions, whose coefficients are randomly generated from the uniform distribution in the interval $(-1.5,-0.5)\cup(0.5,1.5)$ and the residual variance is 1 for each linear regression. We apply the recursive algorithm to the generated sample to construct a DAG, and then we compare the underlying DAG with the

constructed DAG and record the number of extra edges, the number of missing edges and the structural hamming distance (SHD), where SHD is defined as the total number of operations to verify the constructed PDAG to the Markov equivalence class of the underlying DAG, and where the operations may be: add or delete an undirected edge, and add, remove or reverse an orientation of an edge (Tsamardinos et al., 2006). The likelihood ratio test introduced in Subsection 3.2 is used to test the partial correlation coefficient at the significance level $\alpha = 0.01$. We repeatedly draw $n = 1000$ sets of samples and obtain the average numbers of extra edges, missing edges and SHD from $n = 1000$ simulations. The first 3 simulation results are shown in Table 1 for different sample sizes 1000, 2000, 5000 and 10000. In Table 1, three values in a bracket denote the number of extra edges, the number of missing edges and SHD respectively. The column 'Ave' in Table 1 shows the averages of $n = 1000$ simulations. It can be seen that the algorithm performs better as the sample size increases. From the simulations, we found that most decompositions at the top-down step are correct, and we also found that when coefficients make the faithfulness assumption close to fail (that is, some of the edges only reflect weak or nearly zero associations), the learned PDAG from simulation may not be exactly the same as the underlying PDAG, and most of edge mistakes appear for these edges that represent rather weak associations.

Sample Size	1	2	3	Ave
1000	(2, 2, 13)	(0, 1, 6)	(2, 4, 10)	(1.20, 2.70, 12.8)
2000	(0, 1, 5)	(1, 0, 5)	(0, 1, 8)	(0.96, 1.77, 9.12)
5000	(1, 2, 5)	(0, 0, 2)	(1, 2, 4)	(0.85, 1.07, 6.18)
10000	(0, 1, 2)	(0, 0, 0)	(0, 2, 4)	(0.75, 0.77, 4.99)

Table 1: Extra edges, missing edges, and SHD for the first 3 simulations and averages from 1000 simulations.

Our implementation is based on the Bayesian network toolbox written by Murphy (2001) and the simulations run particularly fast. For a single simulation for all sample sizes $N = 1000$, 2000, 5000, 10000, when conditional independence tests are used to check edges, it costs only around 3 seconds in Matlab 7 on a laptop Intel 1.80GHz Pentium(R)M with 512 MByte RAM running Windows XP.

We also compare our methods with the PC algorithm (Spirtes and Glymour, 1991) and the Three Phaze Dependency Analysis (TPDA) algorithm (Cheng et al., 2002), which are readily available in the Causal Explorer System developed by Aliferis et al. (2003). The simulation is repeated 100 times for each of different network parameters and sample sizes. For each generated data set, the structure learned from each method is then compared with the true underlying structure. For each algorithm, we choose two different significance levels, that is, $\alpha = 0.01$ and 0.05. In the second row of Table 2, the underlined values in a bracket denote the number of extra edges, the number of missing edges and SHD respectively, and other rows give values relative to the second row,

Alg (Level α)	N = 1000	N = 2000	N = 5000	N = 10000	Ave Time
	(1.2, 2.4, 12)	(1.0, 1.5, 8.2)	(0.9, 0.9, 5.8)	(0.7, 0.6, 4.6)	2.55 sec
Rec(0.01)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	(1.0 ,1.0, 1.0)	1.0
Rec(0.05)	(3.1, 1.0, 1.5)	(3.5, 1.1, 1.7)	(4.2, 1.1, 2.2)	(4.7, 1.2, 2.3)	1.5
PC(0.01)	(1.8, 4.5, 3.5)	(2.6, 6.3, 4.7)	(2.8, 8.0, 6.0)	(4.0, 9.7, 7.2)	21.2
PC(0.05)	(2.9, 4.0, 3.5)	(4.3, 3.5, 4.7)	(6.0, 4.0, 6.2)	(8.6, 5.1, 7.3)	24.8
TPDA(0.01)	(3.9, 4.1, 3.5)	(4.3, 5.7, 4.8)	(3.9, 7.5, 6.1)	(3.7, 8.5, 6.8)	73.6
TPDA(0.05)	(4.4, 3.7, 3.5)	(4.7, 5.1, 4.7)	(5.7, 4.3, 6.0)	(8.5, 4.8, 7.1)	88.3

Table 2: Results relative to the recursive algorithm with $\alpha = 0.01$ and $\alpha = 0.05$: extra edges, missing edges, and SHD

which are obtained by dividing their real values by the underlined values in the second row. A relative value larger than 1 denotes that its real value is larger than the corresponding value in the second row. For example, the third row labeled *Rec*(0.01) with all values equal to 1 shows that our algorithm with $\alpha = 0.01$ has the same results as the second row; the seventh row labeled PC(0.01) shows the relative results for the PC algorithm with $\alpha = 0.01$, where $(1.8, 4.5, 3.5)$ means the real values as $(1.8 \times 1.2, 4.5 \times 2.4, 3.5 \times 12)$. The last column labeled 'Ave Time' denotes average time cost for one simulation of all 4 sample sizes. In Table 2, all values are larger than 1, which means our algorithm Rec(0.01) has the least number of extra edges, the least number of missing edges and the least SHD, and further it costs the least times.

4.2.2 THE DISCRETE CASE

Now we show simulations of the ALARM network for the discrete case where these discrete variables have two to four levels. For every simulation, the conditional probability distribution of each variable X_i given its parents pa_i is draw randomly in the following way: for each fixed configuration pa_i of the parents, we first generate a sequence $\{r_1, \ldots, r_L\}$ of random numbers from the uniform distribution $U(0,1)$, where L is the number of levels of X_i; then let $P(X_i = j | pa_i) = r_j / \sum_k r_k$ as the distribution of X_i conditional on the fixed configuration pa_i of X_i's parents. Note that the joint distribution generated in this way may be unfaithful, which together with the problem of discreteness makes the learning task harder than that for the Gaussian case. We run 100 simulations for each sample size $N = 1000$, 2000, 5000 or 10000, and then we compare our method with several other algorithms by averages from 100 simulations. In addition to the PC algorithm and the TPDA algorithm used in the Gaussian case, we also compare our method with the Sparse Candidate (SC) algorithm (Friedman et al., 1999) and the MMHC algorithm (Tsamardinos et al., 2006). For the PC

algorithm, we set the parameter max-fan-in (that is, the maximum in-degree) to its true value so that the PC algorithm can run fast. We use the TPDA and the MMHC algorithms that are implemented in the Causal Explorer System (Aliferis et al., 2003) with the default setting. For all algorithms except the SC algorithm, we use two significance levels ($\alpha = 0.01$, $\alpha = 0.05$) in the simulations. For the SC algorithm, the most important parameter to be specified is the number of candidates (the maximum size of potential parent sets), which are set to 5 and 10 separately.

Alg (Level α)	N = 1000	N = 2000	N = 5000	N = 10000	Ave Time
	(1.3, 10, 33)	(1.2, 6.6, 23)	(0.8, 4.0, 16)	(0.7, 2.6, 11)	27 sec
Rec(0.01)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	1.0
Rec(0.05)	(4.0, 0.8, 1.1)	(3.6, 0.8, 1.2)	(4.8, 0.8, 1.3)	(4.9, 0.8, 1.4)	1.3
PC(0.01)	(0.2, 1.5, 1.9)	(0.1, 1.5, 2.6)	(0.2, 1.6, 3.3)	(0.1, 1.8, 4.5)	1.7
PC(0.05)	(0.8, 1.2, 1.9)	(0.5, 1.3, 2.5)	(0.7, 1.3, 3.2)	(0.7, 1.5, 4.4)	1.9
TPDA(0.01)	(10.2, 1.2, 2.7)	(2.7, 1.6, 3.0)	(1.9, 2.7, 4.1)	(0.9, 4.1, 5.8)	0.9
TPDA(0.05)	(0.0, 2.5, 2.2)	(0.1, 3.9, 3.1)	(0.1, 6.5, 4.5)	(0.1, 9.9, 6.6)	0.2
SC(5)	(2.0, 0.8, 0.8)	(2.4, 0.8, 1.0)	(3.6, 0.9, 1.1)	(4.3, 0.9, 1.4)	4.7
SC(10)	(2.2, 0.8, 0.8)	(2.7, 0.9, 1.0)	(3.8, 0.8, 1.1)	(4.2, 0.7, 1.2)	6.6
MMHC(0.01)	(0.3, 1.3, 1.1)	(0.3, 1.4, 1.1)	(0.4, 1.5, 1.1)	(0.7, 1.5, 1.2)	1.1
MMHC(0.05)	(0.5, 1.2, 1.0)	(0.4, 1.3, 1.0)	(0.5, 1.3, 1.0)	(1.0, 1.3, 1.1)	1.4

Table 3: Results relative to the recursive algorithm with $\alpha = 0.01$ and $\alpha = 0.05$: extra edges, missing edges, and SHD

We summarize the simulation results in Table 3. In terms of SHD, our algorithm, the SC algorithm and the MMHC algorithm perform better than the PC and TPDA algorithms. It can also be seen that the performance difference between our method and the others becomes larger as the sample size increases. Although it can be seen from the last column labeled 'Ave Time' that the average CPU time cost for our algorithm is the second least, the fastest algorithm TPDA has the largest SHD among all algorithms. From the results in Tables 3, we can see that although the recursive algorithm seems to have a better performance in most cases, it is still not quite clear which one of these algorithms is superior in general. Their performance depends on preference of reducing the false positive error (including an edge that is not in the true DAG) or the false negative error

(excluding an edge that is in the true DAG). For example, the PC and MMHC algorithms have a smaller false positive error; the SC algorithm has a smaller false negative error; and the recursive algorithm has smaller SHD. We also found that choosing a good parameter is also important to achieve an optimal performance for each algorithm. The recursive algorithm seems to work better when we choose a significance level $\alpha = 0.01$, while for MMHC it is better to choose $\alpha = 0.05$.

The above comparison is based on results from randomly generated values of parameters of joint distributions. The results may change when different values of these parameters are used. The performance of an algorithm also depends on the structures of a network.

4.2.3 SIMULATIONS OF OTHER NETWORKS

In this subsection we show simulation results for other three networks: Insurance with 27 vertices and 52 edges (Binder et al., 1997), HailFinder with 56 vertices and 66 edges (Abramson et al., 1996) and Carpo with 61 vertices and 74 edges, all of which can be obtained through the online Bayesian network repository (http://www.cs.huji.ac.il/labs/compbio/ Repository). We compare the recursive algorithm with the SC and MMHC algorithms since these two have been extensively compared with many state-of-art algorithms and shown in general outperforming other algorithms by Tsamardinos et al. (2006). In our simulations, the parameter values of the joint distributions are set to the original values from the repository. For each network, 10 data sets are generated, and we give one better result in Table 4 for each algorithm with two criteria ($\alpha = 0.01$ and 0.05 for Rec and MMHC, the number of candidates = 5 and 10 for SC). From the last column 'Ave Time' of Table 4, it can be seen that the recursive algorithm is fastest in average CPU time and it also has a better performance in most cases for these networks.

4.3 Complexity Analysis

Below we discuss the complexity of the recursive algorithm proposed in this paper. We mainly focus on the number of conditional independence tests for constructing the equivalence class since decomposition of graphs is a computationally simple task compared to the conditional independence tests. In the recursive algorithm DecompRecovery, two steps (Step 1 for constructing an undirected independence graph $\bar{G}_K$ and the 'Else' part of Step 2 for constructing a local skeleton $\bar{L}_K$) involve conditional independence tests, where K is the vertex set of the subgraph. At Step 1, an undirected independence graph can be constructed by testing independence between any pair of variables conditionally on other variables, and thus the complexity is $O(|K|^2)$, where $|K|$ denotes the number of vertices in the set K. As discussed in Section 3.3, an undirected independence graph $\bar{G}_{A\cup C}$ can be constructed from the previous graph $\bar{G}_{A\cup B\cup C}$ by checking only all possible edges within the separator C. Thus the complexity for constructing an undirected independence graph can be reduced. At Step 2, we construct a local skeleton over a vertex subset K. Suppose that we use the IC algorithm. Then the complexity for constructing the local skeleton L_K is $O(|K|^2 2^{|K|-2})$. Below we consider the total expenses and suppose that the full vertex set V is recursively decomposed into H subsets $\{K_1,\ldots,K_H\}$, where $H \le n$ and $K_h \le n$ for all h. For each decomposition, we need to construct an undirected independence graph, and thus the total expenses for all decompositions is less than $O(Hn^2)$. The total expenses for constructing all skeletons is $O(\sum_h |K_h| 2^{|K_h|-2})$, which is less than $O(Hk_{max}2^{k_{max}-2})$, where $k_{\max} = \max\{|K_1|,\ldots,|K_H|\}$. The complexity for the IC algorithm is known to be $O(n^2 2^{n-2})$. Since $K_{\max}$ usually is much less than n, the recursive decomposition can greatly reduce the complexity of the IC algorithm. Of course, when no decomposition is available,

Alg (Level α)	N = 1000	N = 2000	N = 5000	N = 10000	Ave Time
			Insurance		
	(2.4, 13, 43)	(1.5, 10, 40)	(1.3, 7.4, 32)	(1.1, 6.7, 27)	16 sec
Rec(0.01)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	1.0
SC(5)	(1.6, 1.0, 1.0)	(2.3, 1.2, 1.2)	(2.5, 1.3, 1.3)	(2.9, 1.4, 1.5)	6.7
MMHC(0.05)	(0.6, 1.3, 1.1)	(1.1, 1.4, 1.2)	(1.2, 1.5, 1.2)	(1.1, 1.4, 1.2)	8.0
			Hailfinder		
	(5.9, 16, 53)	(7.1, 14, 47)	(8.0, 14, 43)	(7.3, 14, 41)	62 sec
Rec(0.01)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	1.0
SC(10)	(2.0, 1.0, 1.1)	(1.8, 1.1, 1.1)	(2.0, 1.1, 1.3)	(2.1, 0.8, 1.2)	5.6
MMHC(0.05)	(1.6, 1.2, 1.1)	(1.6, 1.1, 1.0)	(1.7, 1.1, 1.2)	(1.0, 1.9, 1.2)	17.4
			Carpo		
	(10, 12, 49)	(9.0, 5.0, 36)	(6.5, 2.6, 21)	(6.3, 1.0, 18)	74 sec
Rec(0.01)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	(1.0, 1.0, 1.0)	1.0
SC(10)	(2.3, 0.5, 1.2)	(2.6, 0.5, 1.7)	(2.8, 0.9, 2.2)	(2.3, 1.3, 2.0)	6.6
MMHC(0.05)	(2.5, 2.4, 2.1)	(2.6, 4.5, 2.6)	(3.1, 6.0, 3.4)	(3.0, 12, 3.4)	44

Table 4: Results relative to the recursive algorithm for other networks: extra edges, missing edges, and SHD

the complexity of our algorithm becomes the same as the IC algorithm, which reflects the fact that structural learning of DAGs is an NP-hard problem (Chickering et al., 2004). Similarly, the recursive decomposition can also be used to improve the performance of the PC algorithm and other algorithms.

5. Conclusion

In this paper, we proposed a recursive algorithm for structural learning of DAGs. We first present its theoretical properties, then show its experimental results and compare it with other algorithms. In the recursive algorithm, a structural learning for a large DAG is first split recursively into those for small subgraphs until each subgraph cannot be decomposed further, then we perform local learning for these subgraphs which cannot be decomposed, finally we gradually combine these locally learned subgraphs into the entire DAG. The main problem for structural learning of a DAG is the search for d-separators, which becomes exponentially complicated with the number of vertices increases. In the recursive algorithm, all searches for d-separators are localized into subsets of vertices. Thus the efficiency of structural learning and the power of statistical tests can be improved by decomposition.

There are several works related to our recursive approach. Friedman et al. (1999) discussed how the idea of recursive decomposition can be used in accelerating their Sparse Candidate algorithm, Narasimhan and Bilmes (2005) discussed the application of this idea to find a sub-optimal graphical models by noticing the corresponding decomposition of the Kullback and Leibler divergence (Kullback and Leibler, 1951) with respect to the graph separation. Geng et al. (2005) and Xie et al. (2006) proposed the decomposition algorithms for structural learning of DAGs. However, the method proposed in Geng et al. (2005) requires that each separator has a complete undirected graph. Xie et al. (2006) removed the condition, but their algorithm performs decomposition only based on the entire undirected independence graph $\overline{G}_V$ of the full vertex set V and cannot perform decomposition of undirected independence subgraphs. Theorems 1, 2 and 3 in this paper relax this requirement, and they do not require the union set $K = A \cup B \cup C$ of a decomposition (A,B,C) to be equal to the full vertex set V. Thus the recursive algorithm can delete more edges in undirected independence subgraphs and further decompose them, see Example 2. Theorems 1, 2 and 3 are also useful properties for collapsibility of DAGs.

Now we discuss several potential utilities and further works of the recursive approach. This recursive decomposition approach can also be used to localize a learning problem of interest. Suppose that V is the full set of all observed variables, but we are interested only in a local structure over a variable subset A. Using the recursive approach, we can recursively decompose the variable sets into small sets, only focus on the subtrees that contain variables in A, and ignore other subtrees that are unrelated to A. In such a way, the local structure over A can be obtained without need of learning other structures that are unrelated to A. The recursive approach can also use a prior knowledge of independencies among variables to decompose structural learning.

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Appendix A.

We first give some lemmas which will be used in proofs of theorems.

Lemma 1. A subset S of vertices separates u from v in $[\vec{G}_{An(\{u\}\cup\{v\}\cup S)}]^m$ if and only if $u \perp\!\!\!\perp v|S$.
Proof. The result can be obtained directly from Proposition 3.25 of Lauritzen (1996) and Theorem 1.2.4 of Pearl (2000). □

Lemma 2. Let S be a subset of V. Then two vertices u and v in S are d-separated by a subset of S if and only if they are d-separated by $an(\{u,v\}) \cap S$.
Proof. Define $S' = an(\{u,v\}) \cap S$. The necessity is obvious since $S \supseteq S'$. For sufficiency, suppose that u and v are not d-separated by S'. Since $An(\{u,v\} \cup S') = An(\{u,v\})$, we have from Lemma 1 that there is a path l connecting u and v in $[\vec{G}_{An(\{u,v\})}]^m$ which is not separated by S' in the moral graph, that is, the path l does not contain any vertex in S'. Since l is contained in $[\vec{G}_{An(\{u,v\})}]^m$ and $S' = an(\{u,v\}) \cap S$, we then have that l does not contain any vertex in $S \setminus \{u,v\}$. Now from the condition, suppose that u and v are d-separated by $S_0 \subseteq S$. Then we also have from $an(u,v) \cap S_0 \subseteq S'$ that l does not contain any vertex in $an(u,v) \cap S_0$. Thus we obtain that l is not separated by S_0 in $[\vec{G}_{An(u,v,S)}]^m$, which by Lemma 1 implies that u and v are not d-separated by S_0. However, this contradicts the condition that u and v are d-separated by $S_0 \subseteq S$, which concludes the proof for Lemma 2. □

Lemma 3. If four disjoint sets X, Y, Z and W satisfy $X \perp\!\!\!\perp Y \cup Z|W$, then we have $X \perp\!\!\!\perp Y|Z \cup W$.
Proof. This result is obvious. □

Under the faithfulness assumption, a conditional independence is equivalent to the corresponding d-separation, and thus d-separation also has the above property.

Lemma 4. Suppose that l is a path that connects two nonadjacent vertices u and v. If l is not contained completely in $An(u) \cup An(v)$, then l is d-separated by any subset S of $an(u) \cup an(v)$.
Proof. Since l is not completely contained in $An(u) \cup An(v)$, there exists vertices m and n in $l = (u,\ldots,m,x,\ldots,y,n,\ldots,v)$ such that both m and n are contained in $An(u) \cup An(v)$ and no vertices from x to y are contained in $An(u) \cup An(v)$ where x and y, u and m, n and v may be separately the same vertex. So we have that the arrows must be oriented as $\langle m,x\rangle$ and $\langle n,y\rangle$, and then there must be a collider between m and n on l. Let $s \to w \leftarrow t$ be the collider that is closest to m. Then we have that the sub-path of l from m to w is directed. Notice that $m \in An(u) \cup An(v)$ and $w \notin An(u) \cup An(v)$. Thus we obtain that S and its subset do not contain the middle vertex w or its descendants, which implies that l is d-separated by any subset of S at the collider $s \to w \leftarrow t$. □

Proof of Theorem 1: The necessity is obvious since $(A \cup B \cup C) \supseteq (A \cup C)$. For sufficiency, let a and d be two vertices in A and $A \cup C$ respectively that are d-separated by a subset of $A \cup B \cup C$. Define $W = (an(a) \cup an(d)) \cap (A \cup B \cup C)$. By Lemma 2, a and d must be d-separated by W. Define $S' = (an(a) \cup an(d)) \cap (A \cup C)$. Then we only need to show that S' ($\subseteq A \cup C$) can d-separate every path l connecting a and d in $\vec{G}_V$. We consider the following two cases separately:

(1) a path l is not contained completely in $An(a) \cup An(d)$, and

(2) a path l is contained completely in $An(a) \cup An(d)$.

For case (1), we get from Lemma 4 that l must be d-separated by S' since S' is a subset of $an(a) \cup an(d)$.

For case (2), we have from condition $A \perp\!\!\!\perp B|C$ that $[\{a\} \cup (S' \cap A)] \perp\!\!\!\perp b|C$ for any $b \in B$, which implies, by Lemma 3, $a \perp\!\!\!\perp b|(S' \cap A) \cup C$. Since $S' \subseteq (A \cup C)$, we get

$$a \perp\!\!\!\perp b|(S' \cup C).$$

By reduction to absurdity, suppose that there is a path l contained in $An(a) \cup An(d)$ connecting a and d which cannot be d-separated by S'. Because W $(\supseteq S')$ d-separates a and d and thus d-separates l but S' does not, there must exist at least one vertex on the path l which is contained in $W \setminus S'$ $(\subseteq B)$. Let b be such a vertex that is closest to a on the path l and define l' to be the sub-path of l from a to b. It is obvious that l' is d-connected by S'; otherwise l will be d-separated by S'. Since b is closest to a on l and $b \in B$, any of other vertices on l' is not in B. From $l' \subseteq l \subseteq (An(a) \cup An(d))$ and $S' = (an(a) \cup an(d)) \cap (A \cup C)$, we have that all vertices of l' except a and b are contained in S'. Since l' is d-connected by S', l' is also d-connected by $S' \cup C$, which contradicts (A.1). Thus we showed that every path in case (2) is also d-separated by S', which concludes our proof for Theorem 1. □

The following lemma, which is non-trivial due to the fact that a sequence can contain the same vertex more than once, indicates that the d-separation for a path can be made equivalent to that for a sequence.

Lemma 5. Two non-adjacent vertices u and v are d-separated by S in $\vec{G}_V$ if and only if for any sequence $l = (u, \ldots, v)$ connecting u and v

1. l contains a "chain" $i \to m \to j$ or a "fork" $i \leftarrow m \to j$ such that the middle vertex m is in S, or

2. l contains a "collider" $i \to m \leftarrow j$ such that the collision vertex m is not in S and no descendant of m is in S.

When a sequence $l = (u, \ldots, v)$ satisfies the above conditions 1 and 2, we also say that the sequence l is d-separated by S.

Proof. The sufficiency is obvious from definition of d-separation. For necessity, suppose there are sequences connecting u and v that satisfy neither condition 1 nor 2. Let $l = (z_0 = u, z_1 \ldots, z_{k-1}, z_k = v)$ be the shortest one of such sequences, it's easy to show that such a sequence is itself a path which contradicts with the condition that u and v are d-separated by S in $\vec{G}_V$. □

Proof of Theorem 2: The necessity is obvious since $(A \cup B \cup C) \supseteq (A \cup C)$. We show the sufficiency in a similar way to proof of Theorem 1. Let c and c' be two vertices in C that are d-separated by a subset of $A \cup B \cup C$. Thus from Lemma 2 they are also d-separated by $S = (an(c) \cup an(c')) \cap (A \cup B \cup C)$. Without loss of generality, suppose that c is not an ancestor of c'. Define $S_1 = (an(c) \cup an(c')) \cap (A \cup C)$ and $S_2 = (an(c) \cup an(c')) \cap (B \cup C)$. To prove that either S_1 $(\subseteq A \cup C)$ or S_2 $(\subseteq B \cup C)$ can d-separate c and c' in $\vec{G}_V$, it is sufficient to show that there will not exist a path l_1 in $A \cup C$ and a path l_2 in $B \cup C$ such that l_1 cannot be d-separated by S_1 and l_2 cannot be d-separated by S_2. To show this, we consider the following two cases separately:

(1) a path l_i is not completely contained in $An(c) \cup An(c')$, and

(2) both paths l_1 and l_2 are contained in $An(c) \cup An(c')$.

For case (1), since both S_1 and S_2 are subsets of $an(c) \cup an(c')$, we know from Lemma 4 that l must be d-separated both by S_1 and by S_2.

For case (2), by reduction to absurdity, we suppose that there are two paths l_1 and l_2 such that l_i cannot be d-separated by S_i for $i = 1$ and 2. Since every path l_i between c and c' is d-separated by S which equals $S_1 \cup S_2$, we have that for path l_i, there is at least one vertex contained in $S \setminus S_i$. Let d_1 and d_2 be such vertices that are closest to c on l_1 and l_2 respectively. We have $d_1 \in (S \setminus S_1)$ and thus $d_1 \in B$, and similarly $d_2 \in (S \setminus S_1)$ and thus $d_2 \in A$. Let l_1' denote the sub-path from c to d_1 of

l_1 and l_2' denote the sub-path from c to d_2 of l_2. Since l_i cannot be d-separated by S_i, we have that l_i' cannot be d-separated by S_i. Connecting l_1' and l_2' at c, we get a sequence l' from d_1 to d_2 through c. Note that l' may have the same vertices and thus it may not be a path. Below we show that l' is not d-separated by C, that is, the middle vertex of each collider or its descendant is in C but any of other vertices on l' is not in C.

For any vertex u which is not the middle vertex of a collider on l_1', since u is in $an(c) \cup an(c')$ and l_1 and l_1' is not d-separated by S_1, we have that $u \notin S_1$ and thus $u \notin C$. Similarly, we can show that C does not contain any vertex u which is not the middle vertex of a collider on l_2'. Thus we have shown that C does not contain any vertex which is not a middle vertex of colliders on l' except that vertex c has not yet been considered. Now we show that vertex c is a middle vertex of a collider on l'. Let v denote the neighbor of c on l_1'. Since v is in $an(c) \cup an(c')$ and it cannot be c', v is an ancestor of c or c'. If the edge between c and v is oriented as $c \to v$, then v must be an ancestor of c'. This contradicts the supposition that c is not an ancestor of c', and thus the edge between c and v must be oriented as $c \leftarrow v$. Similarly for the neighbor w of c on l_2', we can also show that the edge between c and w must be oriented as $c \leftarrow w$, which implies that the sequence (v, c, w) must form a collider on l'. Thus we have shown that C does not contain any vertex which is not a middle vertex of colliders on l'.

For any vertex u which is a middle vertex of a collider on l_i', u or its descendant must be in S_i, otherwise l_i' and so l_i are d-separated by S_i, which contradicts the supposition. Since u is contained in $an(c) \cup an(c')$, we have that c ($\in C$) or c' ($\in C$) is a descendant of u, and thus u or its descendant must be in C. For the collider $u \to c \leftarrow v$ on the sequence l', we also have that c is in C. Thus we have shown that the middle vertex of each collider on l' or its descendant is in C.

By the above result and Lemma 5, we have $d_2 \not\perp\!\!\!\perp d_1 | C$, where $d_2 \in A$ and $d_1 \in B$. This contradicts $A \perp\!\!\!\perp B | C$. Thus either S_1 or S_2 must d-separate c and c' in $\vec{G}_V$. □

Proof of Theorem 3: This is an immediate consequence of Theorems 1 and 2. □

Proof of Theorem 4: For necessity, since $A \perp\!\!\!\perp B | C$, we have from the property of conditional independence that $u \perp\!\!\!\perp B | A \cup C \setminus \{u\}$. This and the condition $u \perp\!\!\!\perp v | A \cup C \setminus \{u, v\}$ imply $u \perp\!\!\!\perp v \cup B | A \cup C \setminus \{u, v\}$. Again, from the property of conditional independence, we have $u \perp\!\!\!\perp v | A \cup B \cup C \setminus \{u, v\}$. For sufficiency, from $A \perp\!\!\!\perp B | C$, we get $u \perp\!\!\!\perp B | A \cup C \setminus \{u\}$. This and the condition $u \perp\!\!\!\perp v | A \cup B \cup C \setminus \{u, v\}$ imply $u \perp\!\!\!\perp B \cup \{v\} | A \cup C \setminus \{u, v\}$. Then we obtain $u \perp\!\!\!\perp v | A \cup C \setminus \{u, v\}$, and this completes our proof for the theorem. □

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