Reading Dependencies from the Minimal Undirected Independence Map of a Graphoid that Satisfies Weak Transitivity

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Abstract

We present a sound and complete graphical criterion for reading dependencies from the minimal undirected independence map of a graphoid that satisfies weak transitivity. We argue that assuming weak transitivity is not too restrictive.

1 Introduction

A minimal undirected independence map G of an independence model p is used to read independencies that hold in p. Sometimes, however, G can also be used to read dependencies holding in p. For instance, if p is a graphoid that is faithful to G then, by definition, vertex separation is a sound and complete graphical criterion for reading dependencies from G. If p is simply a graphoid, then there also exists a sound and complete graphical criterion for reading dependencies from G (Bouckaert, 1995).

In this paper, we introduce a sound and complete graphical criterion for reading dependencies from G under the assumption that p is a graphoid that satisfies weak transitivity. Our criterion allows reading more dependencies than the criterion in (Bouckaert, 1995) at the cost of assuming weak transitivity. We argue that this assumption is not too restrictive. Specifically, we show that there exist important families of probability distributions that are graphoids and satisfy weak transitivity.

The rest of the paper is organized as follows. In Section 5, we present our criterion for reading dependencies from G. As will become clear later, it is important to first prove that vertex separation is sound and complete for reading independencies from G. We do so in Section 4. Equally important is to show that assuming that p satisfies weak transitivity is not too restrictive. We do so in Section 3. We start by reviewing some key concepts in Section 2 and close with some discussion in Section 6.

2 Preliminaries

The following definitions and results can be found in most books on probabilistic graphical models, e.g. (Pearl, 1988; Studený, 2005). Let U denote a set of random variables. Unless otherwise stated, all the independence models and graphs in this paper are defined over U. Let X, Y, Z and W denote four mutually disjoint subsets of U. An independence model p is a set of independencies of the form \mathbf{X} is independent of \mathbf{Y} given \mathbf{Z} . We represent that an independency is in p by $\mathbf{X} \perp \mathbf{Y} | \mathbf{Z}$ and that an independency is not in p by $\mathbf{X} \not\perp \mathbf{Y} | \mathbf{Z}$. An independence model is a graphoid when it satisfies the following five properties: Symmetry $\mathbf{X} \perp \mathbf{Y} | \mathbf{Z} \Rightarrow \mathbf{Y} \perp \mathbf{X} | \mathbf{Z}$, decomposition $\mathbf{X} \perp \mathbf{Y} \mathbf{W} | \mathbf{Z} \Rightarrow \mathbf{X} \perp \mathbf{Y} | \mathbf{Z}$, weak union $\mathbf{X} \perp \mathbf{Y} \mathbf{W} | \mathbf{Z} \Rightarrow \mathbf{X} \perp \mathbf{Y} | \mathbf{Z} \mathbf{W}$, contraction $\mathbf{X} \perp \mathbf{X}$ $\mathbf{Y}|\mathbf{Z}\mathbf{W}\wedge\mathbf{X}\perp\mathbf{W}|\mathbf{Z}\Rightarrow\mathbf{X}\perp\mathbf{Y}\mathbf{W}|\mathbf{Z},$ and intersection $\mathbf{X} \perp \mathbf{Y} | \mathbf{Z} \mathbf{W} \land \mathbf{X} \perp \mathbf{W} | \mathbf{Z} \mathbf{Y} \Rightarrow \mathbf{X} \perp \mathbf{Y} \mathbf{W} | \mathbf{Z}$. Any strictly positive probability distribution is a graphoid.

Let $sep(\mathbf{X}, \mathbf{Y}|\mathbf{Z})$ denote that \mathbf{X} is separated from \mathbf{Y} given \mathbf{Z} in a graph G. Specifically, $sep(\mathbf{X}, \mathbf{Y}|\mathbf{Z})$ holds when every path in G between \mathbf{X} and \mathbf{Y} is blocked by \mathbf{Z} . If G is an undirected graph (UG), then a path in G between \mathbf{X} and \mathbf{Y} is blocked by \mathbf{Z} when there exists some $Z \in \mathbf{Z}$ in the path. If G is a directed and acyclic graph (DAG), then a path in G between \mathbf{X} and \mathbf{Y} is blocked by \mathbf{Z} when there exists a node Z in the path such that either (i) Z does not have two parents in the path and $Z \in \mathbf{Z}$, or (ii) Z has two parents in the path and neither Z nor any of its descendants in G is in **Z**. An independence model p is faithful to an UG or DAG G when $\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}$ iff $sep(\mathbf{X}, \mathbf{Y} \mid \mathbf{Z})$. Any independence model that is faithful to some UG or DAG is a graphoid. An UG G is an undirected independence map of an independence model p when $\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}$ if $sep(\mathbf{X}, \mathbf{Y} \mid \mathbf{Z})$. Moreover, G is a minimal undirected independence (MUI) map of pwhen removing any edge from G makes it cease to be an independence map of p. A Markov boundary of $X \in \mathbf{U}$ in an independence model p is any subset MB(X) of $\mathbf{U} \setminus X$ such that (i) $X \perp \mathbf{U} \setminus X \setminus MB(X) \mid MB(X)$, and (ii) no proper subset of MB(X) satisfies (i). If p is a graphoid, then (i) MB(X) is unique for all X, (ii) the MUI map G of p is unique, and (iii) two nodes X and Y are adjacent in G iff $X \in MB(Y)$ iff $Y \in MB(X)$ iff $X \not\perp Y | \mathbf{U} \setminus (XY)$.

A Bayesian network (BN) is a pair (G, θ) where G is a DAG and θ are parameters specifying a probability distribution for each $X \in$ **U** given its parents in G, p(X|Pa(X)). The BN represents the probability distribution p = $\prod_{X \in \mathbf{U}} p(X|Pa(X))$. Then, G is an independence map of a probability distribution p iff p can be represented by a BN with DAG G.

3 WT Graphoids

Let **X**, **Y** and **Z** denote three mutually disjoint subsets of **U**. We call WT graphoid to any graphoid that satisfies weak transitivity $\mathbf{X} \perp$ $\mathbf{Y}|\mathbf{Z} \wedge \mathbf{X} \perp \mathbf{Y}|\mathbf{Z}V \Rightarrow \mathbf{X} \perp V|\mathbf{Z} \vee V \perp \mathbf{Y}|\mathbf{Z}$ with $V \in \mathbf{U} \setminus (\mathbf{XYZ})$. We now argue that there exist important families of probability distributions that are WT graphoids and, thus, that WT graphoids are worth studying. For instance, any probability distribution that is Gaussian or faithful to some UG or DAG is a WT graphoid (Pearl, 1988; Studený, 2005). There also exist probability distributions that are WT graphoids although they are neither Gaussian nor faithful to any UG or DAG. For instance, it follows from the theorem below that the probability distribution that results from marginalizing some nodes out and instantiating some others in a probability distribution that is faithful to some DAG is a WT graphoid, although it may be neither Gaussian nor faithful to any UG or DAG.

Theorem 1. Let *p* be a probability distribution that is a WT graphoid and let $\mathbf{W} \subset \mathbf{U}$. Then, $p(\mathbf{U} \setminus \mathbf{W})$ is a WT graphoid. If $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} =$ \mathbf{w}) has the same independencies for all \mathbf{w} , then $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} = \mathbf{w})$ for any \mathbf{w} is a WT graphoid. *Proof.* Let \mathbf{X} , \mathbf{Y} and \mathbf{Z} denote three mutually disjoint subsets of $\mathbf{U} \setminus \mathbf{W}$. Then, $\mathbf{X} \perp \mathbf{Y} | \mathbf{Z}$ in $p(\mathbf{U} \setminus \mathbf{W})$ iff $\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}$ in p and, thus, $p(\mathbf{U} \setminus \mathbf{W})$ satisfies the WT graphoid properties because psatisfies them. If $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} = \mathbf{w})$ has the same independencies for all \mathbf{w} then, for any \mathbf{w} , $\mathbf{X} \perp \mathbf{Y} | \mathbf{Z}$ in $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} = \mathbf{w})$ iff $\mathbf{X} \perp \mathbf{Y} | \mathbf{Z} \mathbf{W}$ in p. Then, $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} = \mathbf{w})$ for any **w** satisfies the WT graphoid properties because p satisfies them.

We now show that it is not too restrictive to assume in the theorem above that $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} =$ \mathbf{w}) has the same independencies for all \mathbf{w} , because there exist important families of probability distributions whose all or almost all the members satisfy such an assumption. For instance, if p is a Gaussian probability distribution, then $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} = \mathbf{w})$ has the same independencies for all \mathbf{w} , because the independencies in $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} = \mathbf{w})$ only depend on the variancecovariance matrix of p (Anderson, 1984). Let us now consider all the multinomial probability distributions for which a DAG G is an independence map and denote them by M(G). The following theorem, which is inspired by (Meek, 1995), proves that the probability of randomly drawing from M(G) a probability distribution p such that $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} = \mathbf{w})$ does not have the same independencies for all \mathbf{w} is zero.

Theorem 2. The probability distributions p in M(G) for which there exists some $\mathbf{W} \subseteq \mathbf{U}$ such that $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} = \mathbf{w})$ does not have the same independencies for all \mathbf{w} have Lebesgue measure zero wrt M(G).

Proof. The proof basically proceeds in the same way as that of Theorem 7 in (Meek, 1995), so we refer the reader to that paper for more details.

Let $\mathbf{W} \subseteq \mathbf{U}$ and let \mathbf{X} , \mathbf{Y} and \mathbf{Z} denote three disjoint subsets of $\mathbf{U} \setminus \mathbf{W}$. For a constraint such as $\mathbf{X} \perp \mathbf{Y} | \mathbf{Z}$ to be true in $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} = \mathbf{w})$ but false in $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} = \mathbf{w}')$, two conditions must be met. First, $sep(\mathbf{X}, \mathbf{Y} | \mathbf{Z} \mathbf{W})$ must not hold in G and, second, the following equations must be satisfied: $p(\mathbf{X} = \mathbf{x}, \mathbf{Y} = \mathbf{y}, \mathbf{Z} =$ $\mathbf{z}, \mathbf{W} = \mathbf{w})p(\mathbf{Z} = \mathbf{z}, \mathbf{W} = \mathbf{w}) - p(\mathbf{X} = \mathbf{x}, \mathbf{Z} = \mathbf{z})$ $\mathbf{z}, \mathbf{W} = \mathbf{w})p(\mathbf{Y} = \mathbf{y}, \mathbf{Z} = \mathbf{z}, \mathbf{W} = \mathbf{w}) = 0$ for all \mathbf{x} , \mathbf{y} and \mathbf{z} . Each equation is a polynomial in the BN parameters corresponding to G, because each term $p(\mathbf{V} = \mathbf{v})$ in the equations is the summation of products of BN parameters (Meek, 1995). Furthermore, each polynomial is non-trivial, i.e. not all the values of the BN parameters corresponding to G are solutions to the polynomial. To see it, note that there exists a probability distribution q in M(G)that is faithful to G (Meek, 1995) and, thus, that $\mathbf{X} \not\perp \mathbf{Y} | \mathbf{Z} \mathbf{W}$ in q because $sep(\mathbf{X}, \mathbf{Y} | \mathbf{Z} \mathbf{W})$ does not hold in G. Then, by permuting the states of the random variables, we can transform the BN parameter values corresponding to q into BN parameter values for p so that the polynomial does not hold. Let $sol(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{w})$ denote the set of solutions to the polynomial for \mathbf{x}, \mathbf{y} and \mathbf{z} . Then, $sol(\mathbf{x}, \mathbf{y}, \mathbf{z}, \mathbf{w})$ has Lebesgue measure zero wrt \mathbb{R}^n , where *n* is the number of linearly independent BN parameters corresponding to G, because it consists of the solutions to a non-trivial polynomial (Okamoto, 1973). Let sol = $\bigcup_{\mathbf{X},\mathbf{Y},\mathbf{Z},\mathbf{W}} \bigcup_{\mathbf{w}} \bigcap_{\mathbf{x},\mathbf{y},\mathbf{z}} sol(\mathbf{x},\mathbf{y},\mathbf{z},\mathbf{w})$ and recall from above that the outer-most union only involves those cases for which $sep(\mathbf{X}, \mathbf{Y} | \mathbf{Z} \mathbf{W})$ does not hold in G. Then, sol has Lebesgue measure zero wrt \mathbb{R}^n , because the finite union and intersection of sets of Lebesgue measure zero has Lebesgue measure zero too. Consequently, the probability distributions p in M(G) such that $p(\mathbf{U} \setminus \mathbf{W} | \mathbf{W} = \mathbf{w})$ does not have the same independencies for all \mathbf{w} have Lebesgue measure zero wrt \mathbb{R}^n because they are contained in *sol*. These probability distributions also have Lebesgue measure zero wrt M(G), because M(G) has positive Lebesgue measure wrt \mathbb{R}^n (Meek, 1995).

Finally, we argue in Section 6 that it is not

unrealistic to assume that the probability distribution underlying the learning data in most projects on gene expression data analysis, one of the hottest areas of research nowadays, is a WT graphoid.

4 Reading Independencies

By definition, *sep* is sound for reading independencies from the MUI map G of a WT graphoid p, i.e. it only identifies independencies in p. Now, we prove that sep in G is also complete in the sense that it identifies all the independencies in p that can be identified by studying G alone. Specifically, we prove that there exist multinomial and Gaussian probability distributions that are faithful to G. Such probability distributions have all and only the independencies that sep identifies from G. Moreover, such probability distributions must be WT graphoids because *sep* satisfies the WT graphoid properties (Pearl, 1988). The fact that sep in G is complete, in addition to being an important result in itself, is important for reading as many dependencies as possible from G (see Section 5).

Theorem 3. Let G be an UG. There exist multinomial and Gaussian probability distributions that are faithful to G.

Proof. We first prove the theorem for multinomial probability distributions. Create a copy Hof G and, then, replace every edge X - Y in H by $X \to W_{XY} \leftarrow Y$ where $W_{XY} \notin \mathbf{U}$ is an auxiliary node. Let \mathbf{W} denote all the auxiliary nodes created. Then, H is a DAG over \mathbf{UW} . Moreover, for any three mutually disjoint subsets \mathbf{X} , \mathbf{Y} and \mathbf{Z} of \mathbf{U} , $sep(\mathbf{X}, \mathbf{Y} | \mathbf{ZW})$ in H iff $sep(\mathbf{X}, \mathbf{Y} | \mathbf{Z})$ in G.

The probability distributions $p(\mathbf{U}, \mathbf{W})$ in M(H) that are faithful to H and satisfy that $p(\mathbf{U}|\mathbf{W} = \mathbf{w})$ has the same independencies for all \mathbf{w} have positive Lebesgue measure wrt M(H) because (i) M(H) has positive Lebesgue measure wrt \mathbb{R}^n (Meek, 1995), (ii) the probability distributions in M(H) that are not faithful to H have Lebesgue measure zero wrt M(H) (Meek, 1995), (iii) the probability distributions $p(\mathbf{U}, \mathbf{W})$ in M(H) such that $p(\mathbf{U}|\mathbf{W} = \mathbf{w})$ does not have the same independencies for all \mathbf{w} have

Lebesgue measure zero wrt M(H) by Theorem 2, and (iv) the union of the probability distributions in (ii) and (iii) has Lebesgue measure zero wrt M(H) because the finite union of sets of Lebesgue measure zero has Lebesgue measure zero.

Let $p(\mathbf{U}, \mathbf{W})$ denote any probability distribution in M(H) that is faithful to H and satisfies that $p(\mathbf{U}|\mathbf{W} = \mathbf{w})$ has the same independencies for all \mathbf{w} . As proven in the paragraph above, such a probability distribution exists. Fix any \mathbf{w} and let \mathbf{X} , \mathbf{Y} and \mathbf{Z} denote three mutually disjoint subsets of \mathbf{U} . Then, $\mathbf{X} \perp \mathbf{Y} | \mathbf{Z}$ in $p(\mathbf{U}|\mathbf{W} = \mathbf{w})$ iff $\mathbf{X} \perp \mathbf{Y} | \mathbf{Z} \mathbf{W}$ in $p(\mathbf{U}, \mathbf{W})$ iff $sep(\mathbf{X}, \mathbf{Y} | \mathbf{Z} \mathbf{W})$ in H iff $sep(\mathbf{X}, \mathbf{Y} | \mathbf{Z})$ in G. Then, $p(\mathbf{U}|\mathbf{W} = \mathbf{w})$ is faithful to G.

The proof for Gaussian probability distributions is analogous. In this case, $p(\mathbf{U}, \mathbf{W})$ is a Gaussian probability distribution and thus, for any \mathbf{w} , $p(\mathbf{U}|\mathbf{W} = \mathbf{w})$ is Gaussian too (Anderson, 1984). Theorem 2 is not needed in the proof because, as discussed in Section 3, any Gaussian probability distribution $p(\mathbf{U}, \mathbf{W})$ satisfies that $p(\mathbf{U}|\mathbf{W} = \mathbf{w})$ has the same independencies for all \mathbf{w} .

The theorem above has previously been proven for multinomial probability distributions in (Geiger and Pearl, 1993), but the proof constrains the cardinality of **U**. Our proof does not constraint the cardinality of \mathbf{U} and applies not only to multinomial but also to Gaussian probability distributions. It has been proven in (Frydenberg, 1990) that sep in an UG G is complete in the sense that it identifies all the independencies holding in every Gaussian probability distribution for which G is an independence map. Our result is stronger because it proves the existence of a Gaussian probability distribution with exactly these independencies. We learned from one of the reviewers, whom we thank for it, that a rather different proof of the theorem above for Gaussian probability distributions is reported in (Lněnička, 2005).

The theorem above proves that sep in the MUI map G of a WT graphoid p is complete in the sense that it identifies all the independencies in p that can be identified by studying

G alone. However, sep in G is not complete if being complete is understood as being able to identify all the independencies in p. Actually, no sound criterion for reading independencies from G alone is complete in the latter sense. An example follows.

Example 1. Let p be a multinomial (Gaussian) probability distribution that is faithful to the DAG $X \to Z \leftarrow Y$. Such a probability distribution exists (Meek, 1995). Let G denote the MUI map of p, namely the complete UG. Note that p is not faithful to G. However, by Theorem 3, there exists a multinomial (Gaussian) probability distribution q that is faithful to G. As discussed in Section 3, p and q are WT graphoids. Let us assume that we are dealing with p. Then, no sound criterion can conclude $X \perp Y | \emptyset$ by just studying G because this independency does not hold in q, and it is impossible to know whether we are dealing with p or q on the sole basis of G.

5 Reading Dependencies

In this section, we propose a sound and complete criterion for reading dependencies from the MUI map of a WT graphoid. We define the dependence base of an independence model p as the set of all the dependencies $X \not\perp Y | \mathbf{U} \setminus (XY)$ with $X, Y \in \mathbf{U}$. If p is a WT graphoid, then additional dependencies in p can be derived from its dependence base via the WT graphoid properties. For this purpose, we rephrase the WT graphoid properties as follows. Let X, Y, Z and \mathbf{W} denote four mutually disjoint subsets of U. Symmetry $\mathbf{Y} \not\perp \mathbf{X} | \mathbf{Z} \Rightarrow \mathbf{X} \not\perp \mathbf{Y} | \mathbf{Z}$. Decomposition $\mathbf{X} \not\perp \mathbf{Y} | \mathbf{Z} \Rightarrow \mathbf{X} \not\perp \mathbf{Y} \mathbf{W} | \mathbf{Z}$. Weak union $\mathbf{X} \not\perp \mathbf{Y} | \mathbf{Z} \mathbf{W} \Rightarrow \mathbf{X} \not\perp \mathbf{Y} \mathbf{W} | \mathbf{Z}$. Contraction $\mathbf{X} \not\perp \mathbf{Y} \mathbf{W} | \mathbf{Z} \Rightarrow \mathbf{X} \not\perp \mathbf{Y} | \mathbf{Z} \mathbf{W} \lor \mathbf{X} \not\perp \mathbf{W} | \mathbf{Z}$ is problematic for deriving new dependencies because it contains a disjunction in the right-hand side and, thus, it should be split into two properties: Contraction 1 $\mathbf{X} \not\perp \mathbf{YW} | \mathbf{Z} \land \mathbf{X} \perp \mathbf{Y} | \mathbf{ZW} \Rightarrow \mathbf{X}$ $\bot \mathbb{U} | \mathbb{Z} \Rightarrow \mathbb{X} \not\!\!\!\! \perp \mathbb{Y} | \mathbb{Z} \mathbb{W}$. Likewise, intersection $\mathbf{X} \not\perp \mathbf{Y} \mathbf{W} | \mathbf{Z} \Rightarrow \mathbf{X} \not\perp \mathbf{Y} | \mathbf{Z} \mathbf{W} \lor \mathbf{X} \not\perp \mathbf{W} | \mathbf{Z} \mathbf{Y}$ gives rise to intersection 1 X $\not\perp$ YW |Z \wedge X $\bot \mathbf{Y} | \mathbf{Z} \mathbf{W} \Rightarrow \mathbf{X} \not\perp \mathbf{W} | \mathbf{Z} \mathbf{Y}$, and intersection 2

 $\mathbf{X} \not\perp \mathbf{YW} | \mathbf{Z} \land \mathbf{X} \perp \mathbf{W} | \mathbf{ZY} \Rightarrow \mathbf{X} \not\perp \mathbf{Y} | \mathbf{ZW}.$ Note that intersection1 and intersection2 are equivalent and, thus, we refer to them simply as intersection. Finally, weak transitivity X *I* $V|\mathbf{Z} \wedge V \not\perp \mathbf{Y}|\mathbf{Z} \Rightarrow \mathbf{X} \not\perp \mathbf{Y}|\mathbf{Z} \vee \mathbf{X} \not\perp \mathbf{Y}|\mathbf{Z}V$ with $V \in \mathbf{U} \setminus (\mathbf{XYZ})$ gives rise to weak transitivity1 $\mathbf{X} \not\perp V | \mathbf{Z} \land V \not\perp \mathbf{Y} | \mathbf{Z} \land \mathbf{X} \perp \mathbf{Y} | \mathbf{Z} \Rightarrow \mathbf{X} \not\perp \mathbf{Y} | \mathbf{Z} V,$ and weak transitivity $2 \mathbf{X} \not\perp V | \mathbf{Z} \wedge V \not\perp \mathbf{Y} | \mathbf{Z} \wedge \mathbf{X}$ $\bot \mathbf{Y} | \mathbf{Z} V \Rightarrow \mathbf{X} \not\perp \mathbf{Y} | \mathbf{Z}$. The independency in the left-hand side of any of the properties above holds if the corresponding *sep* statement holds in the MUI map G of p. This is the best solution we can hope for because, as discussed in Section 4, sep in G is sound and complete. Moreover, this solution does not require more information about p than what it is available, because G can be constructed from the dependence base of p. We call the WT graphoid closure of the dependence base of p to the set of all the dependencies that are in the dependence base of p plus those that can be derived from it by applying the WT graphoid properties.

We now introduce our criterion for reading dependencies from the MUI map of a WT graphoid. Let \mathbf{X} , \mathbf{Y} and \mathbf{Z} denote three mutually disjoint subsets of U. Then, $con(\mathbf{X}, \mathbf{Y}|\mathbf{Z})$ denotes that \mathbf{X} is connected to \mathbf{Y} given \mathbf{Z} in an UG G. Specifically, $con(\mathbf{X}, \mathbf{Y} | \mathbf{Z})$ holds when there exist some $X_1 \in \mathbf{X}$ and $X_n \in \mathbf{Y}$ such that there exists exactly one path in G between X_1 and X_n that is not blocked by $(\mathbf{X} \setminus X_1)(\mathbf{Y} \setminus$ X_n **Z**. Note that there may exist several unblocked paths in G between **X** and **Y** but only one between X_1 and X_n . We now prove that *con* is sound for reading dependencies from the MUI map of a WT graphoid, i.e. it only identifies dependencies in the WT graphoid. Actually, it only identifies dependencies in the WT graphoid closure of the dependence base of p. Hereinafter, $X_{1:n}$ denotes a path X_1, \ldots, X_n in an UG.

Theorem 4. Let p be a WT graphoid and G its MUI map. Then, con in G only identifies dependencies in the WT graphoid closure of the dependence base of p.

Proof. We first prove that if $X_{1:n}$ is the only path in G between X_1 and X_n that is not blocked by $\mathbf{Y} \subseteq \mathbf{U} \setminus X_{1:n}$, then $X_1 \not\perp X_n | \mathbf{Y}$. We

prove it by induction over n. We first prove it for n = 2. Let **W** denote all the nodes in $\mathbf{U} \setminus X_{1:2} \setminus \mathbf{Y}$ that are not separated from X_1 given X_2 **Y** in G. Since X_1 and X_2 are adjacent in $G, X_1 \not\perp X_2 | \mathbf{U} \setminus X_{1:2}$ and, thus, $X_1 \mathbf{W} \not\perp X_2 (\mathbf{U} \setminus X_{1:2} \setminus \mathbf{Y} \setminus \mathbf{W}) | \mathbf{Y}$ due to weak union. This together with $sep(X_1\mathbf{W}, \mathbf{U} \setminus X_{1:2} \setminus$ $\mathbf{Y} \setminus \mathbf{W}|X_2\mathbf{Y})$, which follows from the definition of W, implies $X_1 \mathbf{W} \not\perp X_2 | \mathbf{Y}$ due to contraction 1. Note that if $\mathbf{U} \setminus X_{1:2} \setminus \mathbf{Y} \setminus \mathbf{W} = \emptyset$, then $X_1 \mathbf{W} \not\perp X_2(\mathbf{U} \setminus X_{1:2} \setminus \mathbf{Y} \setminus \mathbf{W}) | \mathbf{Y}$ directly implies $X_1 \mathbf{W} \not\perp X_2 | \mathbf{Y}$. In any case, this independency together with $sep(\mathbf{W}, X_2|X_1\mathbf{Y})$, because otherwise there exist several unblocked paths in G between X_1 and X_2 which contradicts the definition of **Y**, implies $X_1 \not\perp X_2 | \mathbf{Y}$ due to contraction 1. Note that if $\mathbf{W} = \emptyset$, then $X_1 \mathbf{W} \not\perp X_2 | \mathbf{Y}$ directly implies $X_1 \not\perp X_2 | \mathbf{Y}$. Let us assume as induction hypothesis that the statement that we are proving holds for all n < m. We now prove it for n = m. Since the paths $X_{1:2}$ and $X_{2:m}$ contain less than m nodes and **Y** blocks all the other paths in G between X_1 and X_2 and between X_2 and X_m , because otherwise there exist several unblocked paths in Gbetween X_1 and X_m which contradicts the definition of **Y**, then $X_1 \not\perp X_2 | \mathbf{Y}$ and $X_2 \not\perp X_m | \mathbf{Y}$ due to the induction hypothesis. This together with $sep(X_1, X_m | \mathbf{Y} X_2)$, which follows from the definition of $X_{1:m}$ and \mathbf{Y} , implies $X_1 \not\perp X_m | \mathbf{Y}$ due to weak transitivity2.

Let \mathbf{X} , \mathbf{Y} and \mathbf{Z} denote three mutually disjoint subsets of \mathbf{U} . If $con(\mathbf{X}, \mathbf{Y}|\mathbf{Z})$ holds in G, then there exist some $X_1 \in \mathbf{X}$ and $X_n \in \mathbf{Y}$ such that $X_1 \not\perp X_n | (\mathbf{X} \setminus X_1) (\mathbf{Y} \setminus X_n) \mathbf{Z}$ due to the paragraph above and, thus, $\mathbf{X} \not\perp \mathbf{Y} | \mathbf{Z}$ due to weak union. Then, every *con* statement in G corresponds to a dependency in p. Moreover, this dependency must be in the WT graphoid closure of the dependence base of p, because we have only used in the proof the dependence base of p and the WT graphoid properties. \Box

We now prove that con is complete for reading dependencies from the MUI map of a WT graphoid p, in the sense that it identifies all the dependencies in p that follow from the information about p that is available, namely the dependence base of p and the fact that p is a WT graphoid.

Theorem 5. Let p be a WT graphoid and G its MUI map. Then, con in G identifies all the dependencies in the WT graphoid closure of the dependence base of p.

Proof. It suffices to prove (i) that all the dependencies in the dependence base of p are identified by *con* in G, and (ii) that *con* satisfies the WT graphoid properties. Since the first point is trivial, we only prove the second point. Let **X**, **Y**, **Z** and **W** denote four mutually disjoint subsets of **U**.

- Symmetry $con(\mathbf{Y}, \mathbf{X} | \mathbf{Z}) \Rightarrow con(\mathbf{X}, \mathbf{Y} | \mathbf{Z})$. Trivial.
- $con(\mathbf{X}, \mathbf{Y}|\mathbf{Z})$ • Decomposition \Rightarrow $con(\mathbf{X}, \mathbf{YW}|\mathbf{Z})$. Trivial if **W** contains no node in the path $X_{1:n}$ in the left-hand side. If **W** contains some node in $X_{1:n}$, then let X_m denote the closest node to X_1 such that $X_m \in X_{1:n} \cap \mathbf{W}$. Then, the path $X_{1:m}$ satisfies the right-hand side because $(\mathbf{X} \setminus X_1)(\mathbf{Y}\mathbf{W} \setminus X_m)\mathbf{Z}$ blocks all the other paths in G between X_1 and X_m , since $(\mathbf{X} \setminus X_1)(\mathbf{Y} \setminus X_n)\mathbf{Z}$ blocks all the paths in G between X_1 and X_m except $X_{1:m}$, because otherwise there exist several unblocked paths in G between X_1 and X_n , which contradicts the left-hand side.
- Weak union $con(\mathbf{X}, \mathbf{Y}|\mathbf{Z}\mathbf{W}) \Rightarrow$ $con(\mathbf{X}, \mathbf{Y}\mathbf{W}|\mathbf{Z})$. Trivial because \mathbf{W} contains no node in the path $X_{1:n}$ in the left-hand side.
- Contraction1 $con(\mathbf{X}, \mathbf{YW}|\mathbf{Z}) \land$ $sep(\mathbf{X}, \mathbf{Y}|\mathbf{ZW}) \Rightarrow con(\mathbf{X}, \mathbf{W}|\mathbf{Z})$. Since \mathbf{ZW} blocks all the paths in G between \mathbf{X} and \mathbf{Y} , then (i) the path $X_{1:n}$ in the left-hand side must be between \mathbf{X} and \mathbf{W} , and (ii) all the paths in G between X_1 and X_n that are blocked by \mathbf{Y} are also blocked by $(\mathbf{W} \setminus X_n)\mathbf{Z}$ and, thus, \mathbf{Y} is not needed to block all the paths in G between X_1 and X_n except $X_{1:n}$. Then, $X_{1:n}$ satisfies the right-hand side.

- Contraction2 $con(\mathbf{X}, \mathbf{YW}|\mathbf{Z}) \land$ $sep(\mathbf{X}, \mathbf{W}|\mathbf{Z}) \Rightarrow con(\mathbf{X}, \mathbf{Y}|\mathbf{ZW})$. Since \mathbf{Z} blocks all the paths in G between \mathbf{X} and \mathbf{W} , the path $X_{1:n}$ in the left-hand side must be between \mathbf{X} and \mathbf{Y} and, thus, it satisfies the right-hand side.
- Intersection $con(\mathbf{X}, \mathbf{YW}|\mathbf{Z}) \land$ $sep(\mathbf{X}, \mathbf{Y}|\mathbf{ZW}) \Rightarrow con(\mathbf{X}, \mathbf{W}|\mathbf{ZY})$. Since \mathbf{ZW} blocks all the paths in *G* between \mathbf{X} and \mathbf{Y} , the path $X_{1:n}$ in the left-hand side must be between \mathbf{X} and \mathbf{W} and, thus, it satisfies the right-hand side.
- $con(\mathbf{X}, X_m | \mathbf{Z})$ • Weak transitivity2 Λ $con(X_m, \mathbf{Y}|\mathbf{Z}) \wedge sep(\mathbf{X}, \mathbf{Y}|\mathbf{Z}X_m)$ \Rightarrow $con(\mathbf{X}, \mathbf{Y} | \mathbf{Z})$ with $X_m \in \mathbf{U} \setminus (\mathbf{X} \mathbf{Y} \mathbf{Z})$. Let $X_{1:m}$ and $X_{m:n}$ denote the paths in the first and second, respectively, con statements in the left-hand side. Let $X_{1:m:n}$ denote the path $X_1, \ldots, X_m, \ldots, X_n$. Then, $X_{1:m:n}$ satisfies the right-hand side because (i) \mathbf{Z} does not block $X_{1:m:n}$, and (ii) **Z** blocks all the other paths in G between X_1 and X_n , because otherwise there exist several unblocked paths in G between X_1 and X_m or between X_m and X_n , which contradicts the left-hand side.
- Weak transitivity1 $con(\mathbf{X}, X_m | \mathbf{Z}) \land con(X_m, \mathbf{Y} | \mathbf{Z}) \land sep(\mathbf{X}, \mathbf{Y} | \mathbf{Z}) \Rightarrow con(\mathbf{X}, \mathbf{Y} | \mathbf{Z} X_m)$ with $X_m \in \mathbf{U} \setminus (\mathbf{X} \mathbf{Y} \mathbf{Z})$. This property never applies because, as seen in weak transitivity2, $sep(\mathbf{X}, \mathbf{Y} | \mathbf{Z})$ never holds since \mathbf{Z} does not block $X_{1:m:n}$.

Note that the meaning of completeness in the theorem above differs from that in Theorem 3. It remains an open question whether con in G identifies all the dependencies in p that can be identified by studying G alone. Note also that con in G is not complete if being complete is understood as being able to identify all the dependencies in p. Actually, no sound criterion for reading dependencies from G alone is complete in this sense. Example 1 illustrates this point. Let us now assume that we are dealing with q instead of with p. Then, no sound criterion can

conclude $X \not\perp Y | \emptyset$ by just studying G because this dependency does not hold in p, and it is impossible to know whether we are dealing with p or q on the sole basis of G.

We have defined the dependence base of a WT graphoid p as the set of all the dependencies $X \not\perp Y | \mathbf{U} \setminus (XY)$ with $X, Y \in \mathbf{U}$. However, Theorems 4 and 5 remain valid if we redefine the dependence base of p as the set of all the dependencies $X \not\perp Y \mid MB(X) \setminus Y$ with $X, Y \in \mathbf{U}$. It suffices to prove that the WT graphoid closure is the same for both dependence bases of p. Specifically, we prove that the first dependence base is in the WT graphoid closure of the second dependence base and vice versa. If $X \not\perp Y | \mathbf{U} \setminus (XY)$, then $X \not\perp Y(\mathbf{U} \setminus (XY) \setminus (MB(X) \setminus Y)) \mid MB(X) \setminus Y$ due to weak union. This together with $sep(X, \mathbf{U} \setminus$ $(XY) \setminus (MB(X) \setminus Y) | Y(MB(X) \setminus Y))$ implies $X \not\perp Y | MB(X) \setminus Y$ due to contraction 1. On the other hand, if $X \not\perp Y | MB(X) \setminus Y$, then $X \not\perp Y(\mathbf{U} \setminus (XY) \setminus (MB(X) \setminus Y)) | MB(X) \setminus$ Y due to decomposition. This together with $sep(X, \mathbf{U} \setminus (XY) \setminus (MB(X) \setminus Y) | Y(MB(X) \setminus Y))$ implies $X \not\perp Y | \mathbf{U} \setminus (XY)$ due to intersection.

In (Bouckaert, 1995), the following sound and complete (in the same sense as con) criterion for reading dependencies from the MUI map of a graphoid is introduced: Let \mathbf{X} , \mathbf{Y} and Z denote three mutually disjoint subsets of U, then $\mathbf{X} \not\perp \mathbf{Y} | \mathbf{Z}$ when there exist some $X_1 \in \mathbf{X}$ and $X_2 \in \mathbf{Y}$ such that $X_1 \in MB(X_2)$ and either $MB(X_1) \setminus X_2 \subseteq (\mathbf{X} \setminus X_1)(\mathbf{Y} \setminus X_2)\mathbf{Z}$ or $MB(X_2) \setminus X_1 \subseteq (\mathbf{X} \setminus X_1)(\mathbf{Y} \setminus X_2)\mathbf{Z}$. Note that $con(\mathbf{X}, \mathbf{Y} | \mathbf{Z})$ coincides with this criterion when n = 2 and either $MB(X_1) \setminus X_2 \subseteq (\mathbf{X} \setminus X_1)(\mathbf{Y} \setminus X_2)$ X_2)**Z** or $MB(X_2) \setminus X_1 \subseteq (\mathbf{X} \setminus X_1)(\mathbf{Y} \setminus X_2)\mathbf{Z}$. Therefore, con allows reading more dependencies than the criterion in (Bouckaert, 1995) at the cost of assuming weak transitivity which, as discussed in Section 3, is not a too restrictive assumption.

Finally, the soundness of *con* allows us to give an alternative proof to the following theorem, which was originally proven in (Becker et al., 2000).

Theorem 6. Let p be a WT graphoid and G its

MUI map. If G is a forest, then p is faithful to it.

Proof. Any independency in p for which the corresponding separation statement does not hold in G contradicts Theorem 4.

6 Discussion

In this paper, we have introduced a sound and complete criterion for reading dependencies from the MUI map of a WT graphoid. In (Peña et al., 2006), we show how this helps to identify all the nodes that are relevant to compute all the conditional probability distributions for a given set of nodes without having to learn a BN first. We are currently working on a sound and complete criterion for reading dependencies from a minimal directed independence map of a WT graphoid.

Due to lack of time, we have not been able to address some of the questions posed by the reviewers. We plan to do it in an extended version of this paper. These questions were studying the relation between the new criterion and lack of vertex separation, studying the complexity of the new criterion, and studying the uniqueness and consistency of the WT graphoid closure.

Our end-goal is to apply the results in this paper to our project on atherosclerosis gene expression data analysis in order to learn dependencies between genes. We believe that it is not unrealistic to assume that the probability distribution underlying our data satisfies strict positivity and weak transitivity and, thus, it is a WT graphoid. The cell is the functional unit of all the organisms and includes all the information necessary to regulate its function. This information is encoded in the DNA of the cell, which is divided into a set of genes, each coding for one or more proteins. Proteins are required for practically all the functions in the cell. The amount of protein produced depends on the expression level of the coding gene which, in turn, depends on the amount of proteins produced by other genes. Therefore, a dynamic Bayesian network is a rather accurate model of the cell (Murphy and Mian, 1999): The nodes represent the genes and proteins, and the edges and parameters represent the causal relations between the gene expression levels and the protein amounts. It is important that the Bayesian network is dynamic because a gene can regulate some of its regulators and even itself with some time delay. Since the technology for measuring the state of the protein nodes is not widely available yet, the data in most projects on gene expression data analysis are a sample of the probability distribution represented by the dynamic Bayesian network after marginalizing the protein nodes out. The probability distribution with no node marginalized out is almost surely faithful to the dynamic Bayesian network (Meek, 1995) and, thus, it satisfies weak transitivity (see Section 3) and, thus, so does the probability distribution after marginalizing the protein nodes out (see Theorem 1). The assumption that the probability distribution sampled is strictly positive is justified because measuring the state of the gene nodes involves a series of complex wet-lab and computer-assisted steps that introduces noise in the measurements (Sebastiani et al., 2003).

Additional evidence supporting the claim that the results in this paper can be helpful for learning gene dependencies comes from the increasing attention that graphical Gaussian models of gene networks have been receiving from the bioinformatics community (Schäfer and Strimmer, 2005). A graphical Gaussian model of a gene network is not more than the MUI map of the probability distribution underlying the gene network, which is assumed to be Gaussian, hence the name of the model. Then, this underlying probability distribution is a WT graphoid and, thus, the results in this paper apply.

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References

- Theodore W. Anderson. 1984. An Introduction to Multivariate Statistical Analysis. John Wiley & Sons.
- Ann Becker, Dan Geiger and Christopher Meek. 2000. Perfect Tree-Like Markovian Distributions. In 16th Conference on UAI, pages 19–23.
- Remco R. Bouckaert. 1995. Bayesian Belief Networks: From Construction to Inference. PhD Thesis, University of Utrecht.
- Morten Frydenberg. 1990. Marginalization and Collapsability in Graphical Interaction Models. Annals of Statistics, 18:790–805.
- Dan Geiger and Judea Pearl. 1993. Logical and Algorithmic Properties of Conditional Independence and Graphical Models. *The Annals of Statistics*, 21:2001–2021.
- Radim Lněnička. 2005. On Gaussian Conditional Independence Structures. Technical Report 2005/ 14, Academy of Sciences of the Czech Republic.
- Christopher Meek. 1995. Strong Completeness and Faithfulness in Bayesian Networks. In 11th Conference on UAI, pages 411–418.
- Kevin Murphy and Saira Mian. 1999. Modelling Gene Expression Data Using Dynamic Bayesian Networks. Technical Report, University of California.
- Masashi Okamoto. 1973. Distinctness of the Eigenvalues of a Quadratic Form in a Multivariate Sample. *Annals of Statistics*, 1:763–765.
- Judea Pearl. 1988. Probabilistic Reasoning in Intelligent Systems: Networks of Plausible Inference. Morgan Kaufmann.
- Jose M. Peña, Roland Nilsson, Johan Björkegren and Jesper Tegnér. 2006. Identifying the Relevant Nodes Without Learning the Model. In 22nd Conference on UAI, pages 367–374.
- Juliane Schäfer and Korbinian Strimmer. 2005. Learning Large-Scale Graphical Gaussian Models from Genomic Data. In Science of Complex Networks: From Biology to the Internet and WWW.
- Paola Sebastiani, Emanuela Gussoni, Isaac S. Kohane and Marco F. Ramoni. 2003. Statistical Challenges in Functional Genomics (with Discussion). *Statistical Science*, 18:33–60.
- Milan Studený. 2005. Probabilistic Conditional Independence Structures. Springer.