Derivation DAGs for Inferring Interaction Models

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Abstract. *A good strategy to save computational time in a model-search problem consists in endowing the search procedure with a mechanism of logical inference, which sometimes allows an interaction model to be accepted or rejected without resorting to the numeric test. In principle, the best inferential mechanism should based on a sound and complete axiomatization of interaction models. We present a sound (and, probably incomplete) axiomatization which can be translated into a graphical inference procedure working with directed acyclic graphs.*

1. Introduction

Interaction models are widely employed in analysis of categorical data [1, 8] and in design of probabilistic expert systems [13]. The model-search problem consists in discovering what interaction models fit a given probability distribution that describes a certain phenomenon of interest. Now, the evaluation of a single interaction model requires the execution of a time-consuming numeric routine (*test*) and, since all possible interaction models are in number exponential in the number of variables (for example, the number of conditional independences involving n variables is itself equal to $(3^n-2^{n+1}+1)/2$), their evaluation is very expensive even for a moderate number of variables.

A strategy to save computational time consists in divising an *informed* search procedure that includes an inferential mechanism which at each step, on the basis of the knowledge of decisions taken on previously examined models, tries to infer on logical grounds the acceptance or the rejection of models that are still to be examined. The *efficiency* of an informed search procedure for a given probability distribution may be measured by the quantity

$$1 - (\text{no. of tests executed})/(\text{size of the search space}) .$$

Examples of informed procedures can be found in [2, 3, 6, 7, 9]. Of course, the efficiency of an informed search procedure depends on the extent that the procedure is informed of the logical properties possessed by the class of interaction models the search space is composed of. In the best case, the inferential routine of an informed search procedure manages to decide the acceptance or the rejection of the model under examination if and only if that decision is a logical consequence of the decisions taken on models that have been previously examined. Unfortunately, an arbitrary class of interaction models need not be such that *all* the consequences of a given set of (accepted) models from the class are derivable by using inference rules or, in equivalent terms, an arbitrary class of interaction models need not admit a sound and complete axiomatization; for example, it is not likely that the whole class of interaction models be (completely) axiomatizable. However, binary models (i.e., of indepenences and conditional independences) admit a sound and complete axiomatization [4, 5, 9].

In this paper, we present a sound set of axioms for arbitrary interaction models from which an informed search procedure can be easily obtained. In spite of its (probable) incompleteness, our axiom set turns out to be complete if it works with decomposable models only, which proves that our axiomatization is quite powerful. Moreover, we provide a graphical translation of the axiomatization proposed: each axiom is translated into a graphical rule on directed acyclic graphs, here called *derivation DAGs,* and a model that has not yet been examined, will be accepted without being tested if one manages to construct a derivation DAG whose leaves represent the generators of the model.

The paper is organized as follows. Section 2 contains basic definitions. In Section 3 we present a sound axiomatization of interaction models, which in Section 4 is translated in a graphical inference mechanism. In Section 5 we state some results which show the power of the axiomatization proposed. Section 6 closes with some open problems.

2. Terminology

Let the universe of discourse be defined by a finite set V of variables with associated finite (variation) domains; a V-tuple, denoted by v, is an element of the Cartesian product of the domains associated with the variables in V. Let p be a probability distribution of V and $\mathbf{S} = \{V_1, \ldots, V_n\}$ $(n \geq 1)$ a set covering of V; if there exist real functions $\psi_1, \ldots, \psi_n$ respectively of $V_1, \ldots, V_n$ such that, for all v

$$p(v) = \psi_1(v_1) \times \ldots \times \psi_n(v_n)\,,$$

then we say that p satisfies the (n-ary) *interaction model* (*model,* for short) *generated* by $\mathbf{S}$, denoted by $[\{V_1, \ldots, V_n\}]$ or by $[\mathbf{S}]$, and we call the sets $V_1, \ldots, V_n$ the *generators* of the model. The set of all probability distributions satisfying a model α will be denoted by $\mathbf{P}(\alpha)$; if Σ is a set of models, by $\mathbf{P}(\Sigma)$ we denote the set of all probability distributions satisfying all models in Σ, that is, $\mathbf{P}(\Sigma) = \bigcap_{\alpha \in \Sigma} \mathbf{P}(\alpha)$.

The unary model $[\{V\}]$ will be also called the *trivial* model. As tobinary models, observe that the assumption that p satisfies the binary model $[\{V_1, V_2\}]$ can be paraphrased by saying that in p the two sets $V_1 \setminus V_2$ and $V_2 \setminus V_1$

are independent given $V_1 \cap V_2$ (if $V_1 \cap V_2 = \emptyset$, then V_1 and V_2 are independent).

Unary and binary models are special cases of decomposable models.

A model is *decomposable* if there is an ordering of its generators, say $<V_1, \ldots, V_n>$, such that if $n > 1$ then for each i, $2 \leq i \leq n$, there exists a $j_i < i$ for which

$$(V_1 \cup \ldots \cup V_{i-1}) \cap V_i = V_{j_i} \cap V_i .$$

Such an ordering of generators of [**S**], to be called a *running-intersection ordering,* allows us to graphically represent [**S**] by a forest whose vertices represent the generators of [**S**] and whose edges link the pairs of vertices representing the pairs of sets (V_i, V_{j_i}).

Example 1. Consider the decomposable model [**S**] with **S** = {*ABC, ABD, ACE, BCF*}. By making use of any running-intersection ordering we can represent [**S**] by the tree shown in Figure 1.

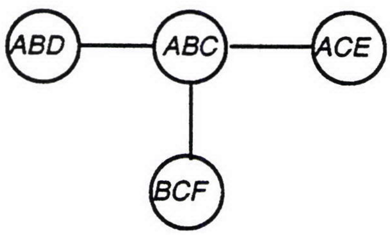

Figure 1. *A tree representing a decomposable model*

Let **S** be a set covering of a nonempty subset of the universe of discourse, which we may denote by $V(\mathbf{S})$. A *path* in **S** is a sequence $<V_1, \ldots, V_k>$ $(k \geq 1)$ of generators of [**S**] such that, if $k > 1$, then $V_i \cap V_{i+1} \neq \emptyset$ for $i = 1, \ldots, k-1$. Let X be a subset of V. A path $<V_1, \ldots, V_k>$ *passes through* X if $k > 1$ and there exists an i $(1 \leq i \leq k-1)$ such that $V_i \cap V_{i+1} \subseteq X$; moreover, two generators Y and Z of [**S**] are *separated* by X if $Y \neq Z$ and every path $<V_1, \ldots, V_k>$ from Y to Z (that is, with $V_1 = Y$ and $V_k = Z$) passes through X. Two generators of [**S**] are *X-nonseparable* if they are not separated by X. The relation of X-nonseparability is an equivalence relation on **S** and the equivalence classes are called the *X-components* of **S**. The *boundary* of an X-component **C** of **S** is the set $V(\mathbf{C}) \cap X$; the set class formed by the boundaries of the X-components of **S** is denoted by $\partial_X \mathbf{S}$ and called the *derivative* of **S** with respect to X.

Example 2. Let **S** = {*ADF, BCE, DE*} and $X = ABCDG$. The X-components of **S** are $\mathbf{C}_1$ = {*ADF*} and $\mathbf{C}_2$ = {*BCE, DE*} and the derivative of **S** with respect to X is $\partial_X \mathbf{S}$ = {*AD, BCD*}.

Remark 1. Let [**S**] be a decomposable model and F a forest that represents [**S**] according to some running-intersection ordering. If X and X' are two generators of [**S**] that are adjacent in F, and **C** is the X-component of **S** containing X', then $X \cap V(\mathbf{C}) = X \cap X'$. It follows that each set in $\partial_X(\mathbf{S})\setminus\{X\}$ is a subset of some generator of [**S**] (distinct from X).

Models can be thought of logical sentences so that the relations of implication and equivalence between models can be stated. Given a (possibly empty) set Σ of models and a single model α, we say that Σ (*logically*) *implies* α or, equivalently, α is a (*logical*) *consequence* of Σ, denoted by $\Sigma \Rightarrow \alpha$, if $\mathbf{P}(\Sigma)$ is a subset of $\mathbf{P}(\alpha)$. Note that a trivial model is a consequence of any (possibly empty) set of models. Moreover, Σ and α are (*logically*) *equivalent* if $\mathbf{P}(\Sigma) = \mathbf{P}(\alpha)$. Finally, the (*logical*) *closure* of Σ is the set

$$\Sigma^+ = \{\alpha: \Sigma \Rightarrow \alpha\} ;$$

of course, Σ is a subset of Σ^+ and we say that Σ is (*logically*) *closed* if $\Sigma = \Sigma^+$.

3. An Axiomatization of Interaction Models

Given a class of models (e.g., the class of binary models), there may exist inference rules that describe the structure of any closed set of models from the class. A typical inference rule is one that asserts that if certain models hold, then so must others. Such rules are called the *axioms* for that class of models.

Let Σ be a set of models, and let α be a model. Given a set of axioms, we say that α is *derivable* from Σ, denoted by $\Sigma \rightarrow \alpha$, if it is possible to use the axioms on the models in Σ to generate α. A set of axioms is *sound* if $\Sigma \Rightarrow \alpha$ whenever $\Sigma \rightarrow \alpha$, and is *complete* if $\Sigma \rightarrow \alpha$ whenever $\Sigma \Rightarrow \alpha$. Since the purpose of axioms is to describe the logical structure of a class of models and to correctly infer other models implied by a given set, it is assumed that any axiom set at least should be sound; furthermore, if it is also complete, then we are able to infer *every* model implied by a given set. In this paper, we are interested in sound axioms for the whole class of interaction models since it is not very likely that they have a sound and complete axiomatization.

Now, consider the following set of axioms **A**:

A1:	$[\mathbf{S}] \Rightarrow [\mathbf{S} \cup \{X\}]$,	for $X \subseteq V(\mathbf{S})$.
A2:	$[\mathbf{S} \cup \{X, Y\}] \Rightarrow [\mathbf{S} \cup \{XY\}]$.	
A3:	$\{[\mathbf{S} \cup \{X\}], [\mathbf{R}]\} \Rightarrow [\mathbf{S} \cup \mathbf{R}_X \cup \partial_X \mathbf{S}]$	if each variable that belongs to two or more generators of [**R**] also belongs to X,

where $\mathbf{R}_X$ denotes the class formed by the intersections of X with the generators of [**R**].

Remark 2. In [10] it is proved that [**S**] ⇒ [**R**] if and only if each generator of [**S**] is a subset of some generator of [**R**]. It follows that the set composed of axioms A1 and A2 is sound and complete for determining the closure of a set Σ that is a singleton, that is, $\Sigma = \{\alpha\}$, as well for determining the set of models that imply α.

On the basis of the axiomatization **A**, it is not difficult in principle to work out an inferential routine.
Suppose that we are given a probability distribution p and we want to determine the set of all interaction models satisfied by p. We make use of two set variables $\mathbb{Y}$ and $\mathbb{N}$ that will contain the sets of models evaluated as they are accepted and rejected, respectively. Initially, both of them are empty and the test is executed on a model; so, after the first test either $\mathbb{Y}$ or $\mathbb{N}$ is nonempty. During the execution of the search procedure, $\mathbb{Y}$ and $\mathbb{N}$ will change their contents on consequence of the results of test or of the inferential routine. After each run of the test, we will execute the inferential routine according to the following procedure scheme.

Case 1: *the test resulted in the acceptance of model* α.
STEP 1. By applying axioms A1 and A2, determine $\{\alpha\}^+$ (Remark 2).

STEP 2. Determine the set Σ of models that can be inferred by applying axiom A3 to α and to some model in $\mathbb{Y}$ (if any), that is,

$$\Sigma := \{\sigma : \exists\, \beta \in \mathbb{Y}\ A3(\alpha, \beta\} = \sigma\}.$$

STEP 3. Set $\mathbb{Y} := \cup_{\sigma\in\Sigma} \{\sigma\}^+ \cup \{\alpha\}^+ \cup \mathbb{Y}$.

Case 2: *the numeric routine resulted in the rejection of model* α.
STEP 1. By applying axioms A1 and A2, determine the set Σ of models that imply α.

STEP 2. Set $\mathbb{N} := \Sigma \cup \mathbb{N}$.

Now, to prove that this inference procedure works well, we have to show the soundnesss of the axiom set **A**. Indeed, **A** can be derived from another (more general) axiom set which involves both models and "partial" models. A partial model differs from a model in involving a subset of the universe of discourse.

Consider the following set of axioms **A'**:

A0:	$\varnothing \Rightarrow [\{X\}]$,	for $X \subseteq V$.
A1:	$[\mathbf{S}] \Rightarrow [\mathbf{S} \cup \{X\}]$,	for $X \subseteq V(\mathbf{S})$.
A2:	$[\mathbf{S} \cup \{X, Y\}] \Rightarrow [\mathbf{S} \cup \{XY\}]$.	
A3':	$[\mathbf{S} \cup \{XA\}] \Rightarrow [\mathbf{S} \cup \{X\}]$	if $A \notin V(\mathbf{S})$.
A4':	$\{[\mathbf{S} \cup \{X\}], [\mathbf{R}]\} \Rightarrow [\mathbf{S} \cup \mathbf{R} \cup \partial_X \mathbf{S}]$	if $X = V(\mathbf{R})$.

Notice that axiom A3 of **A** is easily derivable from A3' and A4'. Since **A'** has been proved to be sound [11], also the axiom set **A** is sound.
After checking the soundness of **A**, we have to ascertain the pratical usefulness of **A**, which takes much more than soundness since, for example, an axiom set capable of inferring trivial models only, is certainly sound but useless. As noted above (see Remark 2), the axioms A1 and A2 of **A** are sound and complete for inferring all the models that are implied by a single interaction model (an informed search procedure essentially based on A1 and A2, which may attain an efficiency also greater than 99.0 %, appeared in [2, 3]). In Section 5, we shall prove that the axiom set **A** is complete if its use is restricted to decomposable models.

4. Derivation DAGs

In the previous section we introduced the axiom set **A'**. The graphical structure we make use of to infer new models is a directed acyclic graph, called *derivation DAG*, and show that for a given set Σ of (possibly partial) models, $\Sigma \rightarrow \alpha$ via **A'** if and only if there exists a derivation DAG such that the leaves of the DAG are exactly the generators of α; thus, the task of inferring a model reduces to that of finding a suitable DAG with leaves the generators of the model.
Let Σ be a set of models. Assume without loss of generality that for each subset X of V, the trivial model $[\{X\}] \in \Sigma$. Then the *derivation DAGs for* Σ are defined as follows.

(0) If $[\mathbf{S}] \in \Sigma$ and $\mathbf{S} = \{V_1, \ldots, V_n\}$, then the DAG root $V(\mathbf{S})$ and children $V_1, \ldots, V_n$, is a derivation DAG for Σ.

(1) If a derivation DAG for Σ has leaves $V_1, \ldots, V_n$ and X is a subset of the variable set $\cup_i V_i$, then the DAG formed by making X the child of any non-leaf vertex, is a derivation DAG for Σ.

(2) If X and Y are leaves of a derivation DAG for Σ, then the DAG formed by adding XY as a child of both X and Y is a derivation DAG for Σ.

(3) If a derivation DAG for Σ has leaves $V_1, \ldots, V_n, XA$, and $A \notin V_i$ for $i = 1, \ldots, n$, then the DAG formed by adding a vertex X as a child of XA is a derivation DAG for Σ.

(4) If G, G' and G'' are derivation DAGs for Σ such that

> the leaves of G are $V_1, \ldots, V_n, X$,
> the leaves of G' are the boundaries of the X-components of the set class $\{V_1, \ldots, V_n, X\}$, and
> the leaves of G'' form a set covering of X,

then the DAG formed by putting each leaf of G' distinct from X and each leaf of G'' as a child of both the leaves of G and G' representative of X, is a derivation DAG for Σ.

Example 3. Let $\mathbf{S} = \{CE, DE\}$, $X = ABCD$, $\mathbf{R} = \{AC, BD\}$, $\Sigma = \{\mathbf{S} \cup \{X\}, \mathbf{R}\}$ and $\mathbf{Q} = \{AC, BD, CD, CE, DE\}$. We prove that $\Sigma \Rightarrow [\mathbf{Q}]$ by constructing a derivation DAG for Σ whose leaves are the generators of $[\mathbf{Q}]$, that is, AC, BD, CD, CE and DE.

STEP 1. {*A DAG with leaves the generators of* $[\mathbf{S} \cup \{X\}]$ *is constructed*}
By applying rule (0) to $[\mathbf{S} \cup \{X\}]$, we construct the DAG G (see Figure 2) with root $ABCDE$ and children ABC, CE and DE.

STEP 2. {*A DAG with leaves the sets composing* $\partial_X(\mathbf{S} \cup \{X\})$ *is constructed*}
Starting from a copy of G, we construct the DAG G' (see Figure 2) with root $ABCDE$ and children $ABCD$ and CD, obtained by applying rule (2) to the children CE and DE of $ABCDE$ and, hence, rule (3) to the resulting vertex CDE.

STEP 3. {*A DAG with leaves the generators of* $[\mathbf{R}]$ *is constructed*}
By applying rule (0) to $[\mathbf{R}]$, construct the DAG G'' (see Figure 2) with root $ABCD$ and children AC and BD.

STEP 4. {*A DAG with leaves the generators of* $[\mathbf{Q}]$ *is constructed*}
The DAGs G, G' and G'' are merged into one DAG (see Figure 3) by applying rule (4). The resulting DAG has leaves AC, BD, CD, CE and DE, that is, the generators of $\mathbf{Q}$.

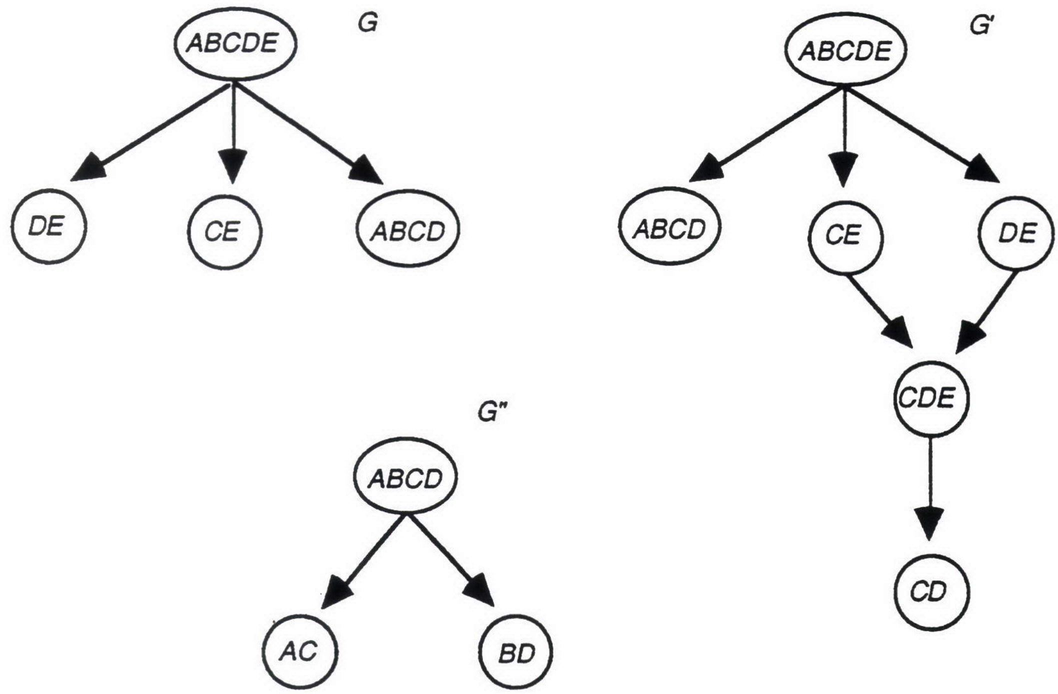

Figure 2. *Three derivation DAGs*

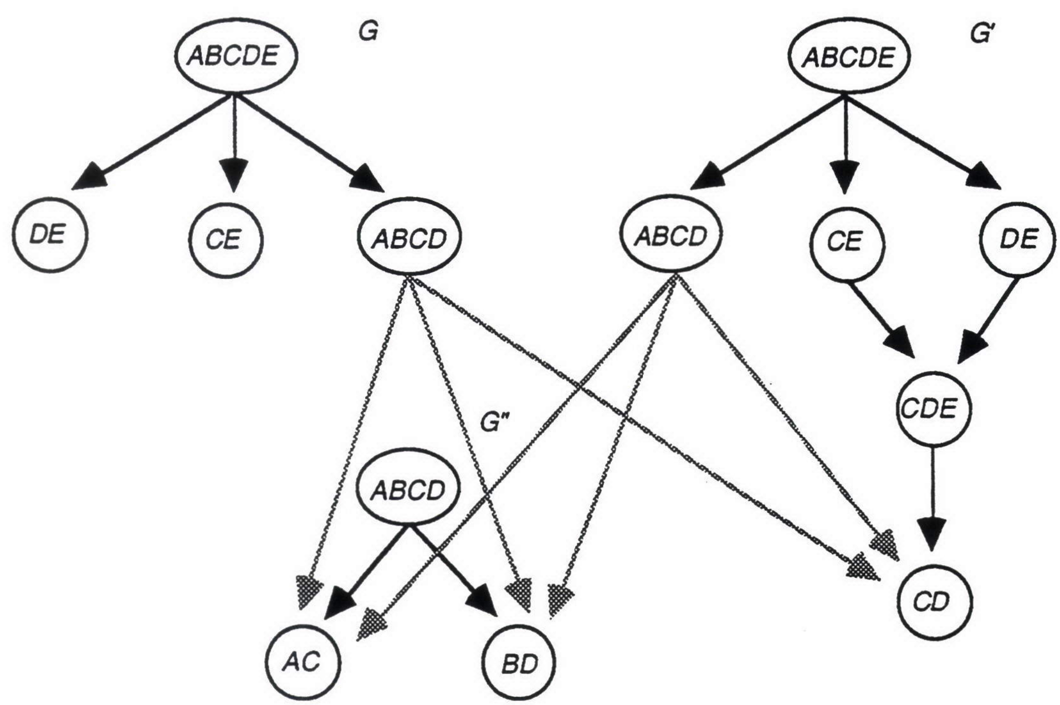

Figure 3. *The derivation DAG obtained by merging the derivation DAGs of Figure 2*

It is important to note that parts (0)-(4) of the above definition correspond exactly to the axioms of **A'**. In fact, derivation DAGs and the axioms are equivalent, which can be proved by structural induction by distinguishing five cases, corresponding to the five parts of the definition.

5. Decomposable models

To show the power of the axiom set **A** introduced in Section 3, we prove that **A** is complete for decomposable models.

We begin by showing that **A** can be simplified when only decomposable models are involved. Let us consider axiom A3. Since $[\mathbf{S} \cup \{X\}]$ is a decomposable model, by Remark 1 each set in $\partial_X\mathbf{S}$ is a subset of some set in **S**; therefore, axiom A3 reduces to:

A3*: $\{[\mathbf{S} \cup \{X\}], [\mathbf{R}]\} \Rightarrow [\mathbf{S} \cup \mathbf{R}_X]$ if each variable that belongs to two or more generators of $[\mathbf{R}]$ also belongs to X.

We shall prove that the set of axioms $\mathbf{A}^* = \{A1, A2, A3^*\}$ is complete for decomposable models.

First of all, we show that $\mathbf{A}^*$ is complete for binary models. These models have a sound and complete axiomatization [9] which consists of axioms A1, A2 and the following axiom:

(*branching axiom*) $\{[\{U, X\}], [\{Y, Z\}]\} \Rightarrow [\{U, X \cap Y\}]$ if $U \cap X = Z$.

Now, we prove that the branching axiom is derivable from A3*. The set $Y \cap Z$ is a subset of Z and, since $U \cap X = Z$, it is also a subset of X. Therefore, we can apply axiom A3* with $\mathbf{R} = \{Y, Z\}$, and infer the model with generators U, $X \cap Y$ and $X \cap Z$. Finally, the set $X \cap Z$ is a subset of Z and, since $U \cap X = Z$, it is also a subset of U; hence, the generator $X \cap Z$ is redundant and can be eliminated.

The next step consists in finding an expression of a decomposable model in terms of binary models in the sense that the decomposable model be equivalent to the set binary models appearing in the expression. At this end, we resort to the graphical representation of decomposable models introduced in Section 2. Without loss of generality, we limit our considerations to decomposable models that can be represented by a tree. Given a tree T for a decomposable model α, for each edge e of T, consider the two subtrees T' and T'' of T resulting from the deletion of the edge e from T; let V' and V'' be the sets of variables appearing in T' and T'' (that is, V' is the union of the generators represented in T' and analogously for

V''). Denote by β_e the binary model $[\{V', V''\}]$, which will be referred to as the binary model *associated* to edge e of T. The set $B(\alpha) = \{\beta_e : e \in E(T)\}$ turns out to be equivalent to α (see, for example, [12]). Notice that, by Remark 2, each binary model in $B(\alpha)$ is inferable from α using the axiomatization **A** and, hence, **A***; furthermore, by recursively applying the axiom A3* we can infer α from $B(\alpha)$, as specified by the following procedure.

Input: $B(\alpha)$ and a tree T representing α

Initialization. Set ALPHA := $[\{V\}]$.

Procedure. If T contains exactly one vertex, then exit; otherwise, choose a leaf v of T, set ALPHA := A3*(ALPHA, β_e), where e is the edge incident to v, and delete v and e from T. Repeat.

Output: ALPHA

Example 4. Consider the decomposable model α of Example 1 with generators ABC, ABD, ACE and BCF, and the tree T shown in Figure 1. The set $B(\alpha)$ consists of the following three binary models

$$[\{ABD, ABCEF\}] \quad [\{ACE, ABCDF\}] \quad [\{ACE, ABCDF\}].$$

Now, we prove that the equivalence of $B(\alpha)$ and α can be proved by using axioms of **A***. By Remark 2, A1 and A2 are sufficient to prove that α implies each binary model in $B(\alpha)$; to prove that $B(\alpha)$ implies α we run the procedure above.

INITIALIZATION. Set ALPHA := $[\{ABCDEF\}]$.

STEP 1. Choose the leaf ABD of T; its incident edge is $e = (ABD, ABC)$ and $\beta_e = [\{ABD, ABCEF\}]$. Set ALPHA := A3*(ALPHA, β_e) = $[\{ABD, ABCEF\}]$. Delete the vertex ABD and the edge (ABD, ABC) from T.

STEP 2. Choose the leaf ACE of T; its incident edge is $e = (ABC, ACE)$ and $\beta_e = [\{ACE, ABCDF\}]$. Set ALPHA := A3*(ALPHA, β_e) = $[\{ABD, ACE, ABCF\}]$. Delete the vertex ACE and the edge (ABC, ACE) from T.

STEP 3. Choose the leaf BCF of T; its incident edge is $e = (ABC, BCF)$ and $\beta_e = [\{ABCDE, BCF\}]]$. Set ALPHA := A3*(ALPHA, β_e) = $[\{ABD, ACE, ABC, BCF\}]$.
Delete the vertex BCF and the edge (ABC, BCF) from T.

At this point T contains one vertex, that is, ABC; the procedure terminates and the final value of the variable ALPHA coincides with α.

Finally, we are able to prove that the axiom set **A*** is complete for decomposable models.
Let $\Sigma \cup \{\alpha\}$ be a set of decomposable models. Let us assume that $\Sigma \Rightarrow \alpha$; we shall prove that α is inferable from Σ using the axioms A1-A3*. Consider the set of binary models $B = \cup_{\sigma \in \Sigma} B(\sigma)$. Since Σ is equivalent to B and α is equivalent to $B(\alpha)$, from $\Sigma \Rightarrow \alpha$ it follows that B implies each binary model in $B(\alpha)$. Now, by Remark 2, B is inferable from Σ using axioms A1 and A2; furthermore, since **A*** is complete for binary models, each binary model in $B(\alpha)$ is inferable from B via **A***. Finally, since α is inferable from $B(\alpha)$ using axiom A3*, we can conclude that α is inferable from Σ using the axioms A1-A3*.

6. Open Problems

After closing, we wish to mention some open questions.

— Is **A*** sound for interaction models?

— Is there an algorithm that, given a set $\Sigma \cup \{\alpha\}$ of interaction models, allows us to decide whether α is or is not implied by Σ?

— Is the axiom set **A** sound for statistical hypotheses (with a given measure of the goodness of fit)?

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