Equations defining probability tree models

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Abstract
Coloured probability tree models are statistical models coding conditional independence between events depicted in a tree graph. They are more general than the very important class of context-specific Bayesian networks. In this paper, we study the algebraic properties of their ideal of model invariants. The generators of this ideal can be easily read from the tree graph and have a straightforward interpretation in terms of the underlying model: they are differences of odds ratios coming from conditional probabilities. One of the key findings in this analysis is that the tree is a convenient tool for understanding the exact algebraic way in which the sum-to-1 conditions on the parameter space translate into the sum-to-one conditions on the joint probabilities of the statistical model. This enables us to identify necessary and sufficient graphical conditions for a staged tree model to be a toric variety intersected with a probability simplex.

Keywords: Algebraic Geometry; Algebraic Statistics; Graphical Models; Staged Trees

1. Introduction

Graphical statistical models are of great practical importance and their methodological foundations have now been well developed (Lauritzen 1996; Cowell et al., 2007). The characterisation of decomposable graphical models, and more generally of regular exponential families, as toric varieties has made an important contribution to linking properties of these models to well-known structures in algebraic geometry (Pistone et al., 2001; Geiger et al., 2006). This link can be used for model selection (Geiger et al., 2001).

The term graphical model usually refers to conditional independence models represented by acyclic digraphs. A more recent statistical model which can be represented by coloured probability trees is the staged tree, sometimes called a chain event graph (Collazo et al., 2018). Staged tree models are curved exponential families. They do not rely on pre-specified problem variables but do contain both discrete models represented by acyclic digraphs and context-specific Bayesian networks as a special case.
In contrast to decomposable graphical models, in the algebro-geometric description of staged trees the sum-to-1 conditions on the parameter space cannot be ignored. These hence constitute a wider class of models with new and exciting algebraic properties. In this paper we define a system of polynomial equations and inequalities whose solution set is equal to the set of probability distributions which factorise according to a staged tree. These equations are given by differences of odds ratios and hence allow for a very straightforward interpretation in terms of the underlying model. They can also be easily read from any tree graph representation and are equivalent for any two statistically equivalent staged trees. These results are presented in Section 3. In Section 4 we state a full characterisation of staged tree models using the language of commutative algebra, and we investigate the geometric behaviour of these models. These results pave the way for the analysis conducted in Section 5 leading to the main result of this paper in Theorem 10 where we give necessary and sufficient graphical conditions for a staged tree to represent a toric model. These conditions are formally stated in terms of the algebraic and combinatorial properties of the staged tree. However, centrally, they have a straightforward interpretation in terms of the statistical properties of the staged tree, as seen in Theorem 11. We illustrate these results in a long example developed over Section 6, stressing how they advance the current literature on algebraic characterisations of standard graphical models such as Bayesian networks.

2. Staged tree models

Following the formalism developed by Görgen and Smith (2017), we always let \( T = (V, E) \) denote a directed rooted tree graph where every vertex has either no or at least two emanating edges. The set of these emanating edges is then denoted \( E(v) \subseteq E \) for every vertex \( v \in V \). To every edge \( e \in E \) we assign a positive probability \( \theta(e) \in (0, 1) \) such that the labels of all edges emanating from the same vertex sum to one, \( \sum_{e \in E(v)} \theta(e) = 1 \). We call such a labelled tree graph a probability tree. Probability trees have been shown to provide a powerful framework to transform a problem description given in natural language into a valid statistical model (Collazo et al., 2018) and as representational tools in causal inference (Shafer, 1996). The positivity assumption in probability trees precludes issues related to validity assumptions as present for instance in Bayesian networks. The local sum-to-1 conditions ensure that the multiplication rule of edge labels along root-to-leaf paths in a probability tree induces a well-defined probability distribution over the graph. We denote this distribution as \( p_\theta(\lambda) = \prod_{e \in E(\lambda)} \theta(e) \) where \( E(\lambda) \subseteq E \) denotes the edge set of a root-to-leaf path \( \lambda \) in the tree, and the index \( \theta = (\theta(e) \mid e \in E) \) denotes the vector of all edge labels. A probability tree model is the set of all probability distributions \( p_\theta \) which can be written in this form, for varying values of edge labels:

\[
M_T = \{p_\theta \mid \theta \in \Theta_T\}. \tag{1}
\]

The parameter space \( \Theta_T \) of a probability tree model \( M_T \) is simply a product of probability simplices \( \Theta_T = \times_{v \in V} \Delta^\circ_{\#E(v) - 1} \), one for each vertex, where

\[
\Delta^\circ_{r-1} = \{x \in \mathbb{R}^r \mid \sum_{i=1}^r x_i = 1 \text{ and } 0 < x_i < 1 \text{ for all } i = 1, \ldots, r\}
\]

always denotes the \( r - 1 \)-dimensional probability simplex, for some positive integer \( r \). The probability tree model (1) is itself a subset of the probability simplex \( \Delta^\circ_{n-1} \) where \( n \) denotes the
nume of root-to-leaf paths, or atomic events. In particular, it is the image of a parametrisation

\[ \psi_T : \Theta_T \to \Delta_{n-1}, \quad \theta \mapsto \left( \prod_{e \in E(A)} \theta(e) \right) \]

where \( \psi_T(\Theta_T) = M_T \).

We henceforth denote the vector of all probabilities attached to a vertex \( v \in V \) in a probability tree by the bold character \( \theta_v = (\theta(e) \mid e \in E(v)) \). A staged tree is then a probability tree together with an equivalence relation on the vertex set such that two vertices are in the same stage if and only if their emanating edges have the same attached probabilities: in symbols, \( v \sim w \) if and only if \( \theta_v = \theta_w \), possibly up to a permutation of the components of these vectors. See Fig. 1 for an illustration. A staged tree model is therefore simply a probability tree model where some probability simplices in the parameter space have been identified with each other. Staged trees can be thought of as probability trees together with conditional independence information on the depicted events. Given that a unit in the population modelled by the tree arrives at a vertex then its immediate future unfoldings are independent of whether the unit arrived at that particular vertex or any other vertex in the same stage. In this sense, stages identify historical developments across a tree. In particular, if a tree depicts the product state space of a discrete vector of random variables, then every vertex corresponds to a random variable conditional on specific values taken by its ancestors, and an identification of emanating probabilities amounts to identifying rows of conditional probability tables. As a consequence, staged tree models include discrete and context-specific Bayesian networks as a special case (Smith and Anderson, 2008; Collazo et al., 2018).

Because staged trees often encode a lot of symmetry, we will in Section 5.2 introduce the concept of positions which are stages with identical future developments. Remarkably, we find in Theorem 10 and Theorem 11 in that section that if all stages are positions then the parametrisation (2) behaves like a monomial parametrisation. As a consequence, sum-to-1 conditions on the parameter space can be ignored and the resulting model is a toric variety inside a probability simplex: see also Theorem 3 in the next section.

Staged trees have now been successfully employed over a whole range of applications (Freeman and Smith, 2011; Barclay et al., 2013, 2015; Collazo and Smith, 2015). Their mathematical properties have only recently been analysed for the first time, by Görgen and Smith (2017). In that article, the authors characterise all different staged tree parametrisations of the same discrete model using symbolic nested representations of a polynomial generating function. This provides a framework to define two graphical operations which traverse the whole class of statistically equivalent staged trees, so all representations of the same model. An alternative approach to the question of statistical equivalence—or, in Bayesian networks, to characterise Markov equivalence—is to provide an implicit rather than a parametric description of the model itself. All graphical representations whose corresponding distributions fulfil these implicit constraints are then statistically equivalent. We present such an algebraic characterisation and analyse its properties in this paper.

3. An implicit characterisation of staged trees

In this section, we employ our understanding of the statistical model represented by a staged tree to derive equations which define this model as the solution set of a system of polynomial equations, without explicitly referring to a parametrisation.
over root-to-leaf paths $\lambda$ to a ternary random variable. For $T$, colour . All three of these represent the same statistical model: a discrete independence model on a binary and a

Figure 1: Three staged probability trees where those vertices which are in the same staged are also assigned the same colour. All three of these represent the same statistical model: a discrete independence model on a binary and a

3.1. Conditional probabilities and odds ratios

In Bayesian networks when a probability distribution factorises according to an acyclic directed graph we have an expression of the atomic probabilities as a product of conditional probabilities depending on ancestor configurations, $p(x) = \prod_{i=1}^{k} p_i(x_i|x_{pai(i)})$ for all atoms $x$ in an underlying discrete space. In the same fashion, we can read the distribution $p_\theta(\lambda) = \prod_{e \in E(\lambda)} \theta(e)$ over root-to-leaf paths $\lambda$ in a probability tree as a product of conditional probabilities where every label $\theta(e)$ of an edge $e = (v, v')$ denotes the transition probability of moving on to $v'$ given arrival at $v$. We show below why this is so and how this interpretation gives rise to a nice interpretation of stage identifications.

For clarity, we henceforth denote atomic probabilities as $p_i = p_\theta(\lambda_i)$ for root-to-leaf paths $\lambda_i$ numbered as $i = 1, \ldots, n$. We write $[v] \subseteq \{1, \ldots, n\}$ for the indices of those root-to-leaf paths which pass through a fixed vertex $v \in V$ and we abbreviate the sum of their corresponding atomic probabilities to $p_{[v]} = \sum_{i \in [v]} p_i$. Thus, $p_{[v]}$ is simply the probability of the event ‘passing through $v’$. Whenever a staged tree is used as an equivalent representation of a Bayesian network, this type of vertex-centred event corresponds to a margin of the bigger model (Collazo et al., 2018). Paths in a tree graph which are not root-to-leaf paths are throughout denoted by their head and tail, for instance $v \rightarrow w$ for a path from $v$ to $w$. Note that in a tree graph every such path between two vertices is unique and that for our purposes we can usually ignore its directionality. The set of edges a path $v \rightarrow w$ passes through can then be denoted as $E(v \rightarrow w) \subseteq E$. The root vertex of $T$ is always denoted by $v_0 \in V$.

Two useful properties of $p_{[v]}$ will be employed over the following sections, for $v \in V$. First, because of the additivity of the underlying probability measure, we can split each such probability into the sum of probabilities measured at the children of $v$:

$$p_{[v]} = \sum_{(v, v') \in E(v)} p_{[v']}.$$  

This naturally follows the branching of the tree graph at each vertex and can be translated into graphical-model language as ‘the probability of a margin equals the sum of the probabilities of its margins’. Second, we can either recursively employ this first observation or we can directly write each atomic probability in terms of its parametrisation to find that every probability $p_{[v]}$ can be written in terms of a polynomial associated to a subtree of the bigger probability tree. To state this fact let thus $T(v)$ denote the induced subtree of $T$ which is rooted at $v$ and whose root-to-leaf
paths correspond to v-to-leaf paths in T. Let $w_1, \ldots, w_k$ denote the leaves of $T(v)$, for $k \leq n$. Because $T(v)$ is itself a probability tree, it has an associated probability distribution which for now we write as $q$. Throughout this text, we denote by $t(v) = \sum_{j=1}^{k} q_{[w]} = \sum_{j=1}^{k} \prod_{e \in E(v \rightarrow w_j)} \theta(e)$ the sum of all atomic probabilities in $T(v)$. When imposing sum-to-one conditions, by construction we have that $t(v) = 1$ for all $v \in V$. This notation enables us to elegantly write

$$p_{[v]} = \prod_{e \in E(v \rightarrow v)} \theta(e) \cdot t(v) = \prod_{e \in E(v \rightarrow v)} \theta(e)$$

which implies that each $p_{[v]}$ simply equals the probability arriving at the vertex $v \in V$. For completeness, we also observe that plugging (3) into (4) gives the following recursive relation

$$t(v) = \sum_{(v, v') \in E(v)} \theta(v, v') \cdot t(v')$$

which will enable us to simplify proofs in the following sections.

We can now easily derive the following fact.

**Lemma 1.** The probability label of every edge $(v, v') \in E$ is a fraction of sums of atomic probabilities

$$\theta(v, v') = \frac{p_{[v']}}{p_{[v]}}$$

and is the conditional probability of transitioning from $v$ to $v'$.

**Proof.** We simply observe that by (4), the fraction (6) is equal to

$$\frac{\sum_{j \neq [v']} p_j}{\sum_{i \in [v]} p_i} = \frac{\prod_{e \in E(v \rightarrow v')} \theta(e') \cdot \theta(v, v') \cdot t(v')}{\prod_{e \in E(v \rightarrow v)} \theta(e) \cdot t(v)}$$

where $t(v)$ and $t(v')$ are equal to one. □

A straightforward implication of the above lemma is the following new result, translating a stage identification of conditional probabilities into a collection of odds-ratio equations.

**Lemma 2.** Two vertices $v, w \in V$ are in the same stage, $v \sim w$, if and only if the equation of atomic probabilities

$$p_{[v']}p_{[w]} = p_{[w']}p_{[v]}$$

is true for any two edges $(v, v') \in E(v)$ and $(w, w') \in E(w)$ which share the same label.

**Proof.** Validity of the statement can simply be seen by noting that two vertices are in the same stage $v \sim w$ if and only if their edge labels are identified $\theta(v, v') = \theta(w, w')$ for all emanating edges $(v, v') \in E(v)$ and $(w, w') \in E(w)$. Plugging these equations into (6) yields the claim. □

An equivalent statement has been proven by Sullivant (2018, Proposition 4.1.6) for acyclic digraphs but not for more general discrete statistical models, so in particular not for discrete context-specific conditional independence models and staged trees. We will fill this gap below. We also dedicate a large part of the analysis in Section 4 to the study of the exact role played by the sum-to-one conditions inherent to both the parametrisation and the associated distribution of a probability tree. These conditions are often neglected, not only by Sullivant (2018) but also for instance by Geiger et al. (2006) who make no reference to these subtleties.
Following [Drton and Sullivant 2007], we henceforth call the ideal associated to a staged tree via the polynomials in Theorem 2 its ideal of model invariants, denoted

\[ I_T = \langle p[v|w'] - p[v'|w] \mid \text{for all } v \sim w \text{ and all } (v, v'), (w, w') \in E \text{ with the same label} \rangle. \]

In analogy, we call the variety \( V(I_T) = \{ x \mid f(x) = 0 \text{ for all } f \in I_T \} \) its model variety.

A direct consequence of Lemmata 1 and 2 is the following implicit characterisation of a staged tree model as its model variety intersected with the probability simplex.

**Theorem 3.** Let \( M_T \) be a staged tree model represented by a tree \( T = (V, E) \) with \( n \) root-to-leaf paths and with associated ideal of model invariants \( I_T \). Then \( M_T = V(I_T) \cap \Delta_{n-1}^\circ \).

Thus staged tree models can either be directly specified using a staged tree representation—and hence an explicit parametrisation—or implicitly using a collection of polynomial equations as above. We discuss the implications of this result for statistical inference below and will then in the subsequent section move on to analysing its geometric properties.

We make two key observations.

First, in statistical inference the system of polynomial equations specified in Theorem 3 is well known. A ratio of probabilities is often called an odds ratio and identifications of odds ratios are frequently used tools in Bayesian inference and gambling [Smith 2010]. Under certain conditions it can be favourable to elicit odds ratios rather than probability distributions in order to specify a model using domain expertise [Garthwaite et al. 2005]. Odds ratios naturally appear when analysing conditional independences in contingency tables [Altham 1969, 1970a,b] and models determined by this type of constraints are now well studied. Because of the correspondence of odds-ratio equations to vanishing 2 \( \times \) 2 minors of contingency tables, these results have also been of interest to the community of algebraic statistics [Drton et al., 2009].

Second, in contrast to other implicit model characterisations—such as those obtained by [Geiger et al. 2006] which are reviewed and extended in the following section—the odds-ratio equations which fully characterise a staged tree model can simply be read from any staged tree graph. See Fig. 1 for an example. Thus there is a simple (visual) algorithm for passing from a parametric to an implicit specification of a staged tree model, making it unnecessary to invert a given parametrisation or to employ implicitisation methods such as Gröbner bases from computational algebra geometry. When checking whether any set of atomic probabilities factorises according to a given tree, we then only need to substitute the given values into the equation specified in Theorem 3 and check whether these evaluate to zero. An extensive discussion of this procedure can be found in Görgen (2017, Section 2.3).

### 3.2. The ideal of model invariants

The polynomial odds-ratio characterisation provided by Theorem 3 enables us employ the language of algebraic geometry to characterise staged tree models. Decomposable graphical statistical models have in the same fashion already been successfully characterised as toric varieties [Pistone et al. 2001; Geiger et al. 2009]. Because staged tree models contain decomposable models as a special case, we can now easily extend these results and verify our advancement in a well-studied context. This section provides the foundation to do so in Section 4.

Before proceeding into a study of their geometry, we note two properties which make staged tree models special from an algebraic viewpoint.
First, by Theorem 3 and because of the ‘if and only if’ in Lemma 2, in an implicit characterisation of staged tree models there are no inequality constraints other than those coming from the probability simplex. As a consequence, staged tree models really are algebraic varieties inside the probability simplex. This makes them pleasingly easy to handle with algebraic tools without diverting into the domain of real semi-algebraic geometry where the notion of closure might force us to handle algebraic approximations of a model rather than the model itself. The presence of hard-to-characterise inequality constraints has been a big challenge in many of the recent attempts to tackle statistical problems using algebra tools. In a similar fashion, in the current algebraic statistics literature, the constraints imposed by the probability simplex have been largely neglected.

Second, by (2), every staged tree model is the image of a parametrisation whose domain is by definition given by a product of probability simplices. If we extend this to the full space $\Theta_T = \mathbb{R}^d$—retaining stage identifications but ignoring sum-to-1 conditions and positivity—then this map becomes monomial and its image a toric variety. However, for staged tree models in general this is not the case. By Theorem 3, staged tree models are only toric in the probabilities of vertex-centred events (or margins of the original model) rather than in the probabilities of atomic events. In Section 4 we will investigate conditions under which staged tree models are toric and provide a more general characterisation of their properties in case they are not. Figure 2 gives examples of a staged tree which neither toric nor decomposable but a Bayesian network, one which is toric but not decomposable and one which is neither toric nor a Bayesian network.

In order to be able to distinguish the toric and non-toric cases, we introduce the following notation for model parametrisations. We henceforth denote by $\mathbb{R}[p] = \mathbb{R}[p_1, \ldots, p_n]$ the polynomial ring whose indeterminates are given by atomic probabilities $p_1, \ldots, p_n$. We denote by $\mathbb{R}[\theta] = \mathbb{R}[\theta(e) | e \in E]$ the polynomial ring whose indeterminates are given by the edge labels of a given staged tree $T = (V, E)$. Then the algebraic analogue of the map (2) is simply the ring map

$$\varphi : \mathbb{R}[p_1, \ldots, p_n] \rightarrow \mathbb{R}[\theta]/(\theta - 1)$$

$$p_i \mapsto \prod_{e \in E_{(i)}} \theta(e) \quad \text{for all } i = 1, \ldots, n$$

(7)

where we use the shorthand $(\theta - 1) = \langle \sum_{v \in V} \theta(e) - 1 | v \in V \rangle$ to denote the ideal coding the local vertex sum-to-1 conditions of the probability tree. These conditions imply two properties of this map. First, $\varphi$ is not a monomial map and hence $\ker \varphi$ is in general not an affine toric variety. Second, the polynomial $p_1 + \ldots + p_n - 1$ is in the kernel of $\varphi$. Thus, following common practice in algebraic statistics, we always consider $\ker \varphi$ as a homogeneous ideal in projective space. For a longer discussion of this subtle point we refer the reader to Sullivant (2018, Section 3.6).

The ring map given by a probability tree parametrisation (2) which ignores the local sum-to-1 conditions is indeed a monomial parameterization and can simply be written as

$$\varphi_{\text{toric}} : \mathbb{R}[p_1, \ldots, p_n] \rightarrow \mathbb{R}[\theta]$$

$$p_i \mapsto \prod_{e \in E_{(i)}} \theta(e) \quad \text{for all } i = 1, \ldots, n.$$  

(8)

The kernel of $\varphi_{\text{toric}}$ is a toric ideal. We will analyse the relation between the kernels of the two maps (7) and (8) in the following section, with a strong focus on the role played by the local
sum-to-1 conditions. In particular, Theorem 10 will give necessary and sufficient graphical and algebraic conditions for the equality \( \ker \varphi = \ker \varphi_{\text{toric}} \) to be true.

Throughout the remainder of this text, we call a staged tree model toric if and only if the kernel of the associated algebraic parametrisation (7) is a toric ideal. In this case, we automatically have that \( \ker \varphi = \ker \varphi_{\text{toric}} \).

**Example 4.** To illustrate the notions above consider the model in Fig. 1. All of the staged trees \( \mathcal{T}_1, \mathcal{T}_2, \mathcal{T}_3 \) in this figure represent the same statistical model which we denote by \( \mathcal{M}_T \). This means that the closed images of all of the parametrisations \( \psi_{\mathcal{T}_i} \) inside the probability simplex \( \Delta_{6-1} \) are the same even though the parametrisation of \( \psi_{\mathcal{T}_i} \) is different from \( \psi_{\mathcal{T}_1} = \psi_{\mathcal{T}_2} \). The different staged tree representations of \( \mathcal{M}_T \) give three ideals of model invariants with different set of generators, namely

\[
\begin{align*}
I_{\mathcal{T}_1} &= \langle p_1 p_5 - p_2 p_4, p_1 p_6 - p_3 p_4, p_2 p_6 - p_3 p_5 \rangle, \\
I_{\mathcal{T}_2} &= \langle p_1 (p_5 + p_6) - p_3 (p_2 + p_3), p_2 (p_4 + p_6) - p_5 (p_1 + p_3), p_3 (p_4 + p_5) - p_6 (p_2 + p_1) \rangle, \\
I_{\mathcal{T}_3} &= \langle p_1 p_5 - p_4 p_6, p_1 (p_4 + p_5) - p_6 (p_2 + p_1) \rangle.
\end{align*}
\]

However, Theorem 3 states that we can implicitly define \( \mathcal{M}_T \) as the vanishing of any of the above ideals \( I_{\mathcal{T}_i} \) intersected with the probability simplex. We will see in Theorem 3 that the closed image of \( \psi_{\mathcal{T}_i} \) in \( \mathbb{R}^6 \) is an irreducible component of all the varieties \( \psi(I_{\mathcal{T}_i}) \). In algebraic language, this simply means that \( \ker \varphi \) is an associated prime of \( I_{\mathcal{T}_i} \) for \( i = 1, 2, 3 \). Let us thus denote \( Q = \ker \varphi \), then the three ideals of model invariants in this example have the following decomposition

\[
I_{\mathcal{T}_1} = Q, \quad I_{\mathcal{T}_2} = Q \cap \langle p_4 + p_5 + p_6, p_1 + p_2 + p_3 \rangle, \quad I_{\mathcal{T}_3} = Q \cap \langle p_1 + p_2, p_4 + p_5 \rangle.
\]
4. Properties of staged tree models

In this section, we explore algebraic properties such as dimension of the model variety of a general staged tree. We state these precisely in the language of commutative algebra. In particular, we find that the ideal of model invariants easily links to the kernel of the associated algebraic parametrisation (7) via saturation.

4.1. Dimension of \( \mathcal{M}_T \)

The dimension of the variety \( V(I_T) \) specified in Theorem 3 can simply be inferred from the tree graph \( T \). This is because the parametrisation (2) between the product parameter space \( \Theta_T \) and the corresponding model \( \mathcal{M}_T \) is birational onto its image: see Theorem 1 and compare Theorem 4 in the subsequent section. As a consequence, the dimension of \( V(I_T) \) is equal to the dimension of \( \Theta_T \), so equal to the number of free parameters in the statistical model.

In particular, assuming that the vertices of a tree graph \( T = (V,E) \) are partitioned into \( r \) equivalence classes, each class corresponding to one stage (or one assignment of a colour), letting \( m_i \) denote the number of vertices which are assigned the \( i \)th colour and letting \( k_i \) be their number of edges, \( i = 1, \ldots, r \), we can write the parameter space \( \Theta_T \) as the product of probability simplices \( \times_{i=1}^r \Delta_{k_i}^E \subseteq \mathbb{R}^{\# E} \). This space is of dimension \( \sum_{i=1}^r (k_i - 1) \). Equivalently, it can easily be seen that the total number of free parameters is equal to the number of parameters labelling the edges of the tree, minus sum-to-1 conditions and stage assignments:

\[
d = \# E - \# V' - \sum_{i=1}^r (m_i - 1)(k_i - 1)
\]

where \( V' \subseteq V \) denotes the set of non-leaf vertices of the tree. The equation \( d = \sum_{i=1}^r (k_i - 1) \) is true because \( \# V' = \sum_{i=1}^r m_i \) and \( \# E = \sum_{i=1}^r m_i k_i \).

**Example 5.** The model represented by the staged tree \( T_2 \) in Fig. 2 is not toric. It is of dimension six (and codimension one) and \( I_{T_2} = \ker \varphi = \langle (p_1 + p_2)(p_5 + p_6) \rangle \). In this case, the kernel of the map \( \varphi_{\text{toric}} \) is empty because the atomic probabilities of this model do not satisfy any relations unless local sum-to-1 conditions are imposed on the parameters.

However, if in \( T_2 \) we colour the vertices \( v_3, v_5 \) blue and \( v_4, v_6 \) green, we obtain \( T_1 \) and thus \( \ker \varphi = \ker \varphi_{\text{toric}} = \langle p_1 p_3 - p_5 p_7, p_7 p_8 - p_5 p_4, p_2 p_5 - p_6 p_3, p_2 p_8 - p_6 p_4, p_1 p_6 - p_5 p_2, p_5 p_8 - p_7 p_4 \rangle \) which is a toric ideal whose corresponding variety is of dimension four.

In the above example, we observe that if we add extra colour to a staged tree, we lower the dimension of the corresponding model and we can end up with a toric variety even when the original model was not toric. This is systematic. In fact, whenever we identify new edge labels we constrain the parameter space by projecting it onto a lower dimensional product of simplices. This corresponds to creating a submodel of the original model. If in this way we superpose two staged trees with the same tree graphs but different colourings, we merge more vertices into common stages and thus add extra odds-ratio equations. This corresponds to intersecting the corresponding model varieties.

We abstain from introducing cumbersome extra notation to formalise the point made above but note that this can be done by characterising a staged trees’ model variety as the sum of its stage ideals defined in (9) below.
4.2. Local properties of \( I_T \)

In Theorem 6, the main result of this section, we state Theorem 3 in the language of commutative algebra. This result is then used to clarify the close relation between \( I_T \) and \( \ker \varphi \) in terms of local rings.

In general, we always have that the ideal of model invariants \( I_T \subset \ker \varphi \) is contained in the kernel of its algebraic parametrisation \( \mathcal{V}(I_T) \), or equivalently, that the model variety \( \mathcal{V}(I_T) \) contains the closed image of \( \varphi \). However, as was illustrated in Theorem 4, equality does not always hold. Compare also the long discussion given in Section 6.

Let henceforth \( p \in \mathbb{R}[p_1, \ldots, p_n] \) denote the product of all the denominators which appear in the identified conditional probabilities (6) in a staged tree.

**Theorem 6.** For any staged tree \( T \), the localized map

\[
\varphi_p : (\mathbb{R}[p_1, \ldots, p_n]/I_T)_p \to (\mathbb{R}[\Theta]/(\theta - 1))_{\varphi(p)}
\]

is an isomorphism of \( \mathbb{R} \)-algebras. Hence \( (\ker \varphi)_p = (I_T)_p \).

**Proof.** To prove that \( \varphi_p \) is an isomorphism we define the map

\[
\psi : (\mathbb{R}[\Theta]/(\theta - 1))_{\varphi(p)} \to (\mathbb{R}[p_1, \ldots, p_n]/I_T)_p
\]

\[
\theta(v, v') \mapsto \frac{p[v]}{p[v]}
\]

and check that this is an inverse for \( \varphi_p \). Let thus \( \lambda = (e_1, \ldots, e_k) \) denote the ordered sequence of edges of the root-to-leaf path which is assigned atomic probability \( p_i \). Then

\[
\psi(\varphi_p(p_i)) = \psi(\prod_{i=1}^{k} \theta(e_i)) = \prod_{i=1}^{k} \psi(\theta(e_i)).
\]

Writing the edges \( e_i \) in terms of pairs of vertices, so \( e_1 = (v_0, v_1), e_2 = (v_1, v_2), \ldots, e_k = (v_{k-1}, v_k) \), we see that the above can be further simplified to:

\[
\prod_{i=1}^{k} \psi(\theta(e_i)) = \prod_{i=1}^{k} \frac{p[v_i]}{p[v_{i-1}]},
\]

for any \( i = 1, \ldots, n \).

For the other direction, we see that

\[
\varphi_p(\psi(\theta(v, v'))) = \varphi_p \left( \frac{p[v]}{p[v]} \right) = \theta(v, v')
\]

where the last equality follows from the Lemma [1]. This proves the claim.

The next two corollaries follow immediately from properties of ideals after localising at an element of the ring. Theorem 7 provides a way to compute \( \ker \varphi \) without the use of elimination theory.

**Corollary 7.** The kernel of \( \varphi \) is the saturation of \( I_T \) with respect to \( p \), so

\[
\ker \varphi = I_T : (p)^\infty.
\]
Proof. For any ideal $I$ in a polynomial ring $R$ and any non-nilpotent element $x$, we have $I \cap R = I : (x)^\infty$ where $I_x$ denotes the extension of the ideal $I$ to the local ring $R_x$. Then from Theorem 6 it follows that
\[
\ker \varphi = (\ker \varphi)_p \cap R = (I_T)_p \cap R = I_T : (p)^\infty.
\]

In Theorem 3 we saw that the ideal of model invariants $I_T$ defines the model $M_T$ as a variety $V(I_T)$ inside the probability simplex. Theorem 8 states that the closed image of the parametrisation $\psi_T$ is an irreducible component of $I_T$.

Corollary 8. The ideal $I_T$ decomposes as
\[
I_T = \ker \varphi \cap Q
\]
where $Q$ is an intersection of primary components containing $p$.

Proof. This follows by localizing the primary decomposition for $I_T$.

We remark that a result similar to Theorem 7 has been proven by Garcia Puente et al. (2005b) for Bayesian networks. In that paper, the authors obtain their results without explicitly referring to a parametrisation of the models they study. The big advantage of our result in Theorem 6 is that the explicit probability-tree parametrisation admits simple interpretations of the algebraic notions in terms of the underlying model. In particular, whilst for the authors above the element $p$ is the product of certain marginals of the random variables in a Bayesian network, for us it is simply the product of all normalising constants we need to keep track of when identifying conditional probabilities, so ratios of sums of atomic probabilities, across a staged tree. Thus, the odds-ratio equations tell us precisely what an algebraic characterisation of the model looks like. In addition, because Bayesian networks are simple special cases of staged trees, our Theorem 6 holds for a much more general class of models.

5. Toric staged tree models

These sections form the core of our algebraic analysis of staged tree models. In particular, we are now ready to provide conditions under which the kernel of the ring map $\varphi$ is a toric ideal. In order to study these conditions, we introduce an ideal $I_{\text{paths}}$ whose generators can be read from a staged tree in a way slightly different to the odds ratios. This ideal captures in a finer way the implicit equations that define $M_T$ and is a key ingredient to understand the case when $\ker \varphi = \ker \varphi_{\text{toric}}$. Surprisingly, we will find in Theorem 10 that these kernels are equal if and only if the local sum-to-1 conditions imposed on the domain of a probability tree parametrisation can be ignored.

5.1. Definition and properties of $I_{\text{paths}}$

Let $v, w \in V$ and suppose the two vertices are in the same stage, so their attached labels are identified $\theta_v = \theta_w$. For simplicity of notation, let $\theta_v = (s_1, \ldots, s_k)$ be this vector of labels. Write the sets $E(v)$ and $E(w)$ of edges emanating from $v$ and $w$ as $E(v) = \{(v, v_1), \ldots, (v, v_k)\}$ and $E(w) = \{(w, w_1), \ldots, (w, w_k)\}$, respectively. Without loss of generality assume that $s_i = \theta(v, v_i) = \theta(w, w_i)$. We define the ideal associated to this stage as
\[
I_{v \sim w} = (p_{[v_i]}p_{[w_j]} - p_{[w_i]}p_{[v_j]} \mid i, j = 1, \ldots, k)
\]
and denote the sum of all of these ideals as

$$I_{\text{paths}} = \sum_{v \sim w \in \mathcal{T}} I_{v \sim w}. \tag{10}$$

The generators of $I_{\text{paths}}$ are quadratic polynomials that vanish on the closed image of $\psi_{\mathcal{T}}$. They are both algebraically and graphically closely related to the generators of $I_{\mathcal{T}}$ and provide an excellent tool to study the kernel of the corresponding parametrisation $\phi$: we investigate the details of this connection in this section.

The reason we denote the ideal in (10) as $I_{\text{paths}}$ is because each generator $p_{[v]} p_{[w]} - p_{[w]} p_{[v]}$ can be read off the staged tree by following two paths starting and ending at the identified vertices: this is shown in Fig. 3. We thus call these generators path differences. For simplicity, we henceforth denote the two paths coding such a path difference as the pair $(v_i \rightarrow w_j, w_j \rightarrow v_j)$.

Using the identity $p_{[v]} = \sum_{(v,e) \in \mathcal{E}(v)} p_{[v]}$ derived in (3), we immediately see that if $\mathcal{T}$ is a binary staged tree then any odds-ratio equation $p_{[v]} p_{[w]} - p_{[w]} p_{[v]} = 0$ from Theorem 2 which identifies two edges $(v, v_i)$ and $(w, w_j)$ is a path difference, $i = 1, 2$. These reduce to the unique generator of $I_{v \sim w}$. Indeed, we can explicitly calculate that $p_{[v]} = p_{[v_1]} + p_{[v_2]}$ and $p_{[w]} = p_{[w_1]} + p_{[w_2]}$ so that

$$p_{[v]} p_{[w]} - p_{[w]} p_{[v]} = (p_{[v_1]} + p_{[v_2]})p_{[w]} - p_{[v]}(p_{[w_1]} + p_{[w_2]}) = p_{[v_2]}p_{[w_1]} - p_{[v_1]}p_{[w_2]}.$$

This equality between odds-ratio differences and path differences does not hold in case $\mathcal{T}$ is not a binary tree: see tree $\mathcal{T}_2$ in Fig. 4 for an illustration. More generally, for non-binary trees each odds-ratio difference can be written as a sum of elements in the ideal $I_{\text{paths}}$. We can see this simply by writing the odds-ratio difference which identifies the labels $\theta(v, v_i) = \theta(w, w_j)$ as

$$p_{[v]} p_{[w]} - p_{[w]} p_{[v]} = p_{[v]} \left( \sum_{(w_j, j) \in \mathcal{E}(w)} p_{[w_j]} \right) - p_{[w]} \left( \sum_{(v_i, j) \in \mathcal{E}(v)} p_{[v_j]} \right) = \sum_{j=0}^{k} p_{[v]} p_{[w_j]} - p_{[w]} p_{[v_j]}.$$

The differences $p_{[v]} p_{[w_j]} - p_{[w]} p_{[v_j]}$ for $v \sim w$ and $i, j \in \{1, \ldots, k\}$ are exactly the generators of $I_{v \sim w}$. This discussion proves the first containment in the next lemma.

**Lemma 9.** $I_{\mathcal{T}} \subseteq I_{\text{paths}} \subseteq \ker \phi$.

**Proof.** From the definition of $I_{\text{paths}}$, it is enough to show that for any two vertices $v, w$ in the same stage, the generators of $I_{v \sim w}$ are in $\ker \phi$. Using the relation obtained in (4) from Section 3.1 we have

$$\phi(p_{[v]}) = t(v) \cdot \prod_{e \in \mathcal{E}(v \rightarrow w)} \theta(e) = \prod_{e \in \mathcal{E}(v \rightarrow w)} \theta(e).$$

This implies that

$$\phi(p_{[v]} p_{[w]} - p_{[w]} p_{[v]}) = \left( s_v \cdot \prod_{e \in \mathcal{E}(v \rightarrow w)} \theta(e) \right) \left( s_w \cdot \prod_{e \in \mathcal{E}(w \rightarrow v)} \theta(e) \right) - \left( s_w \cdot \prod_{e \in \mathcal{E}(w \rightarrow v)} \theta(e) \right) \left( s_v \cdot \prod_{e \in \mathcal{E}(v \rightarrow w)} \theta(e) \right) = 0. \tag{11}$$
5.2. Characterization of toric staged tree models

Theorem 10 presented in this section is the key result of this paper. It gives necessary and sufficient algebraic criteria for a staged tree model to be toric. Most pleasantly, we find that such criteria can be formulated in terms of the polynomials \( t(v) \) defined in Section 3 for \( v \in V \), and can be therefore be interpreted in terms of the statistical properties of the staged tree model.

To formulate this connection precisely, we briefly recall a definition from Smith and Anderson (2008). Two vertices \( v \) and \( w \) in a staged tree \( T = (V,E) \) are said to be in the same position if they are in the same stage \( v \sim w \) and their induced subtrees \( T(v) \) and \( T(w) \) have the same parameterisation \( \psi_{T(v)} = \psi_{T(w)} \). The notion of positions is of practical importance in staged tree models because it both provides a vocabulary to address vertices which have identical future unfoldings (independent of their different histories) and it provides a tool to classify subtrees representing the same statistical (sub-)model. We refer the reader to Collazo et al. (2018) for a detailed discussion of the subtle relations between stages and positions. Görren and Smith (2017) show that two vertices \( v \) and \( w \) are in the same position if and only if the symbolic polynomials \( t(v) \) and \( t(w) \) as defined in (4) are identical: this notion is also known as polynomial equivalence.

Consider now a path difference \( p_{[v]} | p_{[w]} - p_{[w]} | p_{[v]} \in I_{v \sim w} \). We showed in Lemma 9 that \( \varphi( p_{[v]} | p_{[w]} - p_{[w]} | p_{[v]} ) = 0 \). In the proof of this lemma, the equation in (11) can equivalently be written as

\[
\varphi( p_{[v]} | p_{[w]} - p_{[w]} | p_{[v]} ) = s_is_j \left( \prod_{e \in E(v \rightarrow i)} \theta(e) \cdot \prod_{e \in E(v \rightarrow w)} \theta(e) \right) \cdot (t(v) | t(w) - t(w) | t(v)).
\]

Now the expression (12) is equal to zero either if we use the property \( t(v) = t(w) = t(w) = t(v) = 1 \) or if the polynomial equation \( t(v) | t(w) = t(w) | t(v) \) is true in \( \mathbb{R}[I] \) where we are not taking the quotient by the ideal of sum-to-1 conditions. This observation implies that if...
t(v_i)t(w_j) = t(w_i)t(v_j) is true then the path difference \( p_{[v_i]p_{[w_i]} - p_{[v_j]p_{[w_j]}} \in \ker \varphi\text{toric} \) lies in the kernel of the monomial parametrisation associated to the tree.

In other words, if we assume that in the ring \( \mathbb{R}[\Theta] \) spanned by the edge labels the equation

\[
i(v_i)t(w_j) = t(w_i)t(v_j) \quad \text{for all } i, j = 1, \ldots, k
\]

is true then the stage ideal \( I_{v \sim w} \subset \ker \varphi\text{toric} \) lies in the kernel of the toric map. This leads us to the main result of this paper.

**Theorem 10.** Let \( \mathcal{T} \) be a staged tree. Then

\[
\ker \varphi\text{toric} = \ker \varphi
\]

if and only if condition (⋆) holds for all vertices \( v, w \) of \( \mathcal{T} \) which are in the same stage.

**Proof.** If condition (⋆) holds for all vertices \( v, w \) in the same stage, it follows that \( I_{\text{paths}} \subset \ker \varphi\text{toric} \) by the definition of \( I_{\text{paths}} \) and the discussion before the theorem. Hence, using Theorem 9 we deduce that \( I_{\mathcal{T}} \subset \ker \varphi\text{toric} \). It is also straightforward to see that \( \ker \varphi\text{toric} \subset \ker \varphi \). We thus arrive at the chain of containments

\[
I_{\mathcal{T}} \subset \ker \varphi\text{toric} \subset \ker \varphi.
\]

Using Theorem 6 and localizing at \( \mathfrak{p} \), we see that

\[
(I_{\mathcal{T}})_\mathfrak{p} = (\ker \varphi\text{toric})_\mathfrak{p} = (\ker \varphi)_\mathfrak{p}.
\]

Since both \( \ker \varphi\text{toric} \) and \( \ker \varphi \) are prime, we obtain \( \ker \varphi\text{toric} = \ker \varphi \). \( \square \)

Theorem 10 has two main implications for our algebraic characterisation of staged tree models.

First, whenever condition (⋆) holds, the algebraic parametrisation (7) behaves exactly like the monomial parametrisation (6). As a consequence, (⋆) is true if and only if the sum-to-1 conditions on the parameter space of the staged can be ignored.

Second, we can simply read from the tree graph a sufficient condition for (⋆) to hold. In fact, if two vertices \( v \sim w \) with children \( v_1, v_2 \) and \( w_1, w_2 \), respectively, are in the same stage then \( t(v_1)t(w_2) = t(w_1)t(v_2) \) is satisfied whenever \( t(v_1) = t(w_1) \) and \( t(w_2) = t(v_2) \). In this case, the vertices \( v_1 \) and \( w_1 \), and \( v_1 \) and \( w_2 \), are in the same position, respectively. This implies the following:

**Corollary 11.** If in a staged tree all vertices which are in the same stage are also in the same position then the corresponding staged tree model is toric.

In the language of Collazo et al. (2018), simple chain event graphs are toric.

Intuitively, coloured probability trees for which all stages are also positions have many symmetries. For example, the tree \( \mathcal{T}_2 \) from Fig. 2 satisfies condition (⋆) for all staged vertices whereas the tree \( \mathcal{T}_3 \) in the same figure does not. Indeed, the kernel of the monomial parametrisation belonging to \( \mathcal{T}_3 \) is empty. This straightforward visual property of staged trees and the fact that the polynomials \( t(\cdot) \) can be easily read from a staged tree without any knowledge about either the underlying statistical model or the algebraic characterisation, is precisely what makes our models so appealing and Theorem 10 so powerful.

We illustrate in the next example that the result in Corollary 11 is sufficient but not necessary: even if none of the vertices \( v_i, v_j \) from condition (⋆) are in the same position it could still be the case that \( t(v_i)t(w_j) = t(w_i)t(v_j) \).
Example 12. Consider a staged tree $T$ where the vertices $v, w$ are the only children of the root $v_0$ and $v \sim w$. Suppose $v, w$ only have two emanating edges and denote $E(v) = \{(v, v_1), (v, v_2)\}$ and $E(w) = \{(w, w_1), (w, w_2)\}$. If $t(v_1) = (a_0 + a_1)(b_0 + b_1 + b_2), r(w_2) = c_0 + c_1$ and $t(w_1) = (a_0 + a_1)(c_0 + c_1), r(v_2) = b_0 + b_1 + b_2$ then the equation $t(v_1)t(w_2) = t(w_1)t(v_2)$ is satisfied but none of the vertices $v_1, v_2, w_1, w_2$ are in the same position.

5.3. Extension of paths and binomial generators of $\ker \varphi_{\text{toric}}$

We proved in Lemma 9 that $I_{\text{paths}}$ is contained in $\ker \varphi$. In addition, each generator of $I_{\text{paths}}$ can be read from $T$ as in Figure 3. In this section we describe a way to extend pairs of paths associated to generators of $I_{\text{paths}}$ in such a way that when we write down the path difference of an extended pair, we automatically get an element in $\ker \varphi$.

If we extend each path $(v_1 \rightarrow w_2, w_1 \rightarrow v_2)$ by one edge in such a way that the two added edges have the same parameter label, we see that from the extended paths we can write a new path difference in $\mathbb{R}[p_1, \ldots, p_e]$ that is also in $\ker \varphi$. More precisely, a pair of paths $(v_h \rightarrow w_1, w_h \rightarrow v_1)$ is said to be an extension of $(v_1 \rightarrow w_2, w_1 \rightarrow v_2)$ by $l$ edges if the next two conditions hold.

1. The path $v_h \rightarrow w$ is obtained from $v_1 \rightarrow w_2$ by adding $l$ edges either at the head or tail of $v_1 \rightarrow w_2$ and likewise for $w_h \rightarrow v$ and $w_1 \rightarrow v_2$.
2. Let $\{e_1, \ldots, e_l\} = E(v_h \rightarrow w) \setminus E(v_1 \rightarrow w_2)$ and $\{e'_1, \ldots, e'_l\} = E(w_h \rightarrow v) \setminus E(w_1 \rightarrow v_2)$ then

$$\prod_{i=1}^l \theta(e_i) = \prod_{i=1}^l \theta(e'_i).$$

We associate the path difference $p_{v_h}(v_1)p_{w_1}(w_2) - p_{w_1}(v_1)p_{v_h}(w_2)$ to the extended pair $(v_h \rightarrow w_1, w_h \rightarrow v_1)$ and note that the second condition implies that $p_{v_h}(v_1)p_{w_1}(w_2) - p_{w_1}(v_1)p_{v_h}(w_2) \in \ker \varphi$.

Example 13. We consider the staged tree $T_1$ in Figure 2. We label the leaves of $T_2$ from top to bottom by $l_1, \ldots, l_8$ and in the same fashion for the atomic probabilities $p_1, \ldots, p_8$. Consider the pair $(v_3 \rightarrow v_6, v_5 \rightarrow v_4)$ and its associated path difference

$$p_{v_3}(v_1)p_{v_5}(v_4) - p_{v_1}(v_3)p_{v_4}(v_5) = (p_1 + p_3)(p_2 + p_4) - (p_2 + p_3)(p_1 + p_3).$$

Notice that a possible extension of $(v_3 \rightarrow v_6, v_5 \rightarrow v_4)$ by one edge is given by $(l_1 \rightarrow v_6, l_5 \rightarrow v_4)$ because $\theta(v_3, l_1) = \theta(v_5, l_5) = \alpha_0$. The path difference associated to this extension is

$$p_{l_1}(v_6)p_{v_4}(v_5) - p_{v_4}(v_5)p_{l_1}(v_6) = p_1(p_3 + p_5) - p_3(p_1 + p_3).$$

We can further extend this path by using an edge with label $p_0$ or $\eta_1$. For instance the extension $(l_1 \rightarrow l_7, l_5 \rightarrow l_3)$ with associated path difference $p_1p_7 - ps_3p_3$.

From the above example, we see that each path difference in $I_{\sim w}$ can have several extensions to paths in $T$. We call an extension $(v_h \rightarrow w, w_h \rightarrow v_i)$ of $(v_1 \rightarrow w_2, w_1 \rightarrow v_2)$ a maximal extension if it is not possible to add edges to the pair $(v_h \rightarrow w, w_h \rightarrow v_i)$ in such a way that condition (2) is satisfied. For example, the extension $(l_1 \rightarrow l_7, l_5 \rightarrow l_3)$ in Theorem 15 is maximal but $(l_1 \rightarrow v_6, l_5 \rightarrow v_4)$ is not.

We define the ideal $I_{\text{paths}}$ generated by all maximal path differences in an analogous way to $I_{\text{paths}}$. Explicitly, given $v \sim w$, we denote by $I_{\text{paths}}(v \sim w)$ the ideal generated by all path differences associated to all maximal paths extending a pair $(v_i \rightarrow w_j, w_i \rightarrow v_j)$ for all $i, j \in \{1, \ldots, k\}$. Then

$$I_{\text{paths}} = \sum_{v \sim w \in T} I_{\text{paths}}(v \sim w).$$
We say that a pair of paths \((v_1 \rightarrow w_2, w_1 \rightarrow v_2)\) fully extends if for each maximal extension \((v_h \rightarrow v_i, w_h \rightarrow v_j)\), all of the vertices \(v_h, w_i, w_h, v_j\) are leaves of \(T\). When this is the case, we see that all path differences associated to extensions are actually binomials. For instance, it is easy to see that all paths in \(T_1\) from Theorem \(13\) fully extend and

\[
I_{\text{mpaths}} = \langle p_1 p_7 - p_5 p_3, p_1 p_8 - p_5 p_4, p_2 p_7 - p_6 p_3, p_2 p_8 - p_6 p_4, p_1 p_6 - p_5 p_2, p_3 p_8 - p_7 p_4 \rangle
\]

is binomial. For this ideal the first four generators correspond to extended paths and the other two are the path differences of the blue and green stages. Furthermore \(M_{T_1}\) is toric and \(\ker \varphi = I_{\text{mpaths}}\).

Following the strategy from the previous section, we now first characterise staged trees in terms of (maximal) path differences and then use these results to understand the ideal of model invariants.

Below, we thus start by giving a necessary condition for a path difference to fully extend. Interestingly, this condition is the same that comes up in Theorem \(10\) to decide whether \(\ker \varphi\) is toric. In the discussion at the end of this paper, we conjecture that this is the case because for toric staged trees, the ideal \(I_{\text{mpaths}}\) is equal to the kernel of \(\varphi\).

**Lemma 14.** Suppose that \(v \sim w\) and \(t(v_i)t(w_j) - t(w_i)t(v_j) = 0\) for all \(i, j \in \{1, \ldots, k\}\). Then every path \((v_i \rightarrow w_j, w_i \rightarrow v_j)\) fully extends.

**Proof.** For convenience, assume \(i = 1, j = 2\). Suppose that \(t(v_1)t(w_2) - t(w_1)t(v_2) = 0\). For \(v \in V\), each \(t(v)\) is a sum of atomic probabilities of the subtree \(T(v)\). The expansion of \(t(v_1)t(w_2)\) is a sum of products of atomic probabilities in \(T(v_1), T(w_2)\). Therefore each term in \(t(v_1)t(w_2)\) cancels with a term in \(t(w_1)t(v_2)\). We may write this cancelation as \(m_{v_1}m_{w_2} - m_{w_1}m_{v_2} = 0\) where

\[
m_{v_1} = \prod_{e \in E(v_1 \rightarrow i_1)} \theta(e), \quad m_{w_2} = \prod_{e \in E(w_2 \rightarrow i_2)} \theta(e), \quad m_{w_1} = \prod_{e \in E(w_1 \rightarrow i_2)} \theta(e), \quad m_{v_1} = \prod_{e \in E(v_1 \rightarrow l_3)} \theta(e)
\]

are atomic probabilities of the subtrees \(T(v_1), T(w_2), T(w_1), T(v_2)\), respectively. Thus the pair \((l_1 \rightarrow l_2, l_3 \rightarrow l_4)\) is an extension of \((v_1 \rightarrow w_2, w_1 \rightarrow v_2)\), namely

\[
l_1 \rightarrow l_2 = l_1 \rightarrow v_1 \rightarrow w_2 \rightarrow l_2
\]

\[
l_3 \rightarrow l_4 = l_3 \rightarrow v_2 \rightarrow w_1 \rightarrow l_4
\]

and \(m_{v_1}m_{w_2} = m_{w_1}m_{v_2}\). The path \((l_1 \rightarrow l_2, l_3 \rightarrow l_4)\) is a full maximal extension because \(l_1, l_2, l_3, l_4\) are leaves of \(T\). Conversely, every maximal extension is a cancellation of terms in \(t(v_1)t(w_2) - t(w_1)t(v_2)\).

We can now directly derive the following result, providing a sufficient condition for \(I_{\text{mpaths}}\) to be binomial.

**Theorem 15.** Let \(T\) be a staged tree and suppose that condition \(\Box\) holds for all \(v, w \in T\) in the same stage. Then \(I_{\text{mpaths}}\) is a binomial ideal.

**Proof.** Using Lemma \(14\), we see that the path differences in \(I_{\sim w}\) fully extend for all vertices of \(T\) in the same stage. By the definition of full extension of paths this implies that the generators of \(I_{\text{mpaths}}\) are binomials.
6. An example and connections to graphical models

In this section we illustrate the concepts introduced over the course of this paper in a simple real system: see Collazo et al. (2018) Examples 3.4 and 3.6) for details. The discrete statistical models represented by the graphs in Fig. 4 were built to explain the unfoldings of events in a cell culture. Within this culture the environment might be hostile or benign and the activity between cells might be high or low, independent of the state of the environment. If the environment is hostile then cells suffer damage and either die or survive with the same respective probabilities. Surviving cells make either a full or partial recovery, independent of their history.

These highly asymmetric stories can be represented by the undirected graph given in Fig. 4b, the directed acyclic graph in Fig. 4c, the staged tree in Fig. 4a, or the staged tree in Fig. 4d. We can now analyse the different statistical and algebraic properties of each of these models, contrasting our results to those obtained by Garcia Puente et al. (2005b); Geiger et al. (2006) for decomposable graphical models and Bayesian networks.

Consider first the decomposable model from Fig. 4b. This graph represents the single conditional independence assumption that recovery of a cell is independent of its activity and of the state of the environment, given survival. In symbols, \( X_3 \perp \perp (X_1, X_2) \mid X_3 \). As a staged tree, this model can be represented by the graph in Fig. 4a with the vertices \( v_7, v_9, v_{11}, v_{13} \) and \( v_8, v_{10}, v_{12}, v_{14} \) in the same stage, respectively. So rather than working on the undirected graph, we can equivalently exclusively consider the red and yellow colouring of this tree, for the moment ignoring the other colours: for simplicity, we denote this staged tree as \( T_{\text{red}} \). The ideal of model invariants of \( T_{\text{dec}} \) is given by

\[
I_{T_{\text{dec}}} = I_{\text{red}} + I_{\text{yellow}}
\]

where the generators of the stage ideals \( I_{\text{red}} = I_{v_7 \rightarrow v_8} + I_{v_9 \rightarrow v_{11}} + I_{v_{11} \rightarrow v_{13}} \) and \( I_{\text{yellow}} = I_{v_8 \rightarrow v_{10}} + I_{v_{10} \rightarrow v_{12}} + I_{v_{12} \rightarrow v_{14}} \) are odds-ratio differences which can be read from the tree as

\[
I_{\text{red}} = (p_{1100} p_{1100} - p_{1000} p_{1101} - p_{0101} p_{1100} - p_{0100} p_{1101} - p_{0001} p_{1101} - p_{0000} p_{1101},
\]

\[
i_{\text{yellow}} = (p_{1101} p_{1110} - p_{1011} p_{1110} - p_{1010} p_{1111} - p_{1010} p_{1111} - p_{0110} p_{1111} - p_{0110} p_{1111} - p_{0101} p_{1111} - p_{0101} p_{1111}).
\]

Because \( T_{\text{dec}} \) is a binary tree, the ideal \( I_{T_{\text{dec}}} = I_{\text{paths}} \) is equal to the ideal generated by path differences. By construction, \( I_{T_{\text{dec}}} \) is also equal to the ideal \( I_{\text{local}(G)} \) generated by cross-product differences coding the local Markov property in the decomposable graph \( G \) in Fig. 4b as defined by Geiger et al. (2006). In particular, the model is thus equal to the variety \( V(I_{T_{\text{dec}}} \cap V(I_{\text{local}(G)})) \) intersected with the probability simplex. To illustrate the direct translation of our methods into their framework, here we use notation used by the authors cited above and denote by \( p_{ijkl} = P(X_1 = i, X_2 = j, X_3 = k, X_4 = l) \) an atomic probability and by \( p_{ij++} = \sum_{k,l} p_{ijkl} \) a marginal probability, for \( i, j, k, l = 0, 1 \). Naturally, the atomic probabilities are attached to leaves of the tree, so \( p_{ijkl} \) is the probability of the root-to-leaf path labelled \( X_1 = i, X_2 = j, X_3 = k, X_4 = l \). The marginal probabilities can equivalently clearly be expressed as probabilities of vertex-centred events in the tree graph: for instance, \( p_{00++} = p_{v_1} = \theta(v_0, v_1) \theta(v_1, v_3) \cdot t(v_3) \) where the labels \( \theta(v_0, v_1) = P(X_1 = 0) \) and \( \theta(v_1, v_3) = P(X_2 = 0 | X_1 = 0) \) are conditional probabilities and \( t(v_3) \) is the sum of atomic probabilities in the induced subtree \( T(v_3) \).

We observe that the ideal \( I_{\text{red}} + I_{\text{yellow}} \) is toric because the path differences coding the red and the yellow stage belong to pairs of paths which extend to the leaves of the tree simply because
Figure 4: Four graphical models for the unfoldings of events in a cell culture. For simplicity, here stages which do not contain more than one vertex have been coloured white.
the children of these stages are leaves. Using any computer algebra software, we can check that the ideal of model invariants of the staged tree is also equal to the kernel of the algebraic parametrisation: \( I_{\text{dec}} = \ker \varphi \).

Equivalently, Geiger et al. (2006) prove in their Theorem 4.3 that \( I_{\text{dec}} = I_{\text{local}(G)} \) is toric because it is the ideal of model invariants of a decomposable graphical model. We can see here that, in contrast to the staged tree, the generators of this ideal cannot be directly read from the decomposable graph but need to be calculated via other methods, for instance using the Macaulay2 package GraphicalModels (Garcia Puente et al., 2005a).

Consider now the Bayesian network given in Fig. 4c which is not decomposable. This graph codes the additional condition that the state of the environment and the activity within a cell culture are independent of each other: so here, \( X_1 \perp X_2 \) as well as \( X_3 \perp (X_1, X_2) \mid X_3 \). This model can alternatively be represented by a staged tree denoted \( T_{\text{BN}} \) which has the same coloured graph as \( T_{\text{dec}} \) but with an additional stage \( v_1 \sim v_2 \), coloured blue. The ideal of model invariants of this tree is again generated by path differences and is equal to \( I_{\text{gen}} = I_{\text{dec}} + I_{\text{blue}} \) where

\[
I_{\text{blue}} = \langle p_{[v_1]}p_{[v_a]} - p_{[v_4]}p_{[v_3]} \rangle = \langle p_{000+}p_{11++} - p_{011+}p_{100+} \rangle.
\]

By construction, \( I_{\text{blue}} \) is toric in the marginal probabilities. However, by Theorem 10, it is not toric in the atomic probabilities. Indeed, the full ideal of model invariants of this tree is not toric because the condition \( \Box \) is not fulfilled: we can easily use the tree graph to check that

\[
t(v_1) = t(v_4) = t(v_5).
\]

Using any computer algebra software, we find that the ideal of model invariants \( I_{\text{dec}} = \ker \varphi \) is still equal to the kernel of the algebraic parametrisation. The theory developed by Geiger et al. (2006) did not supply the means to find this algebraic characterisation. However, here we study a Bayesian network on four binary random variables, so one of the subjects of the thorough analysis provided by Garcia Puente et al. (2005b Table 1, #21). Using prime decomposition of the conditional independence ideal, these authors find that the ideal of model invariants of this Bayesian network is prime, of codimension 7, of degree 32, and has 13 minimal generators.

In a third step, consider the context-specific Bayesian network represented by the graph in Fig. 4a and with the extra condition that \( X_3 \perp X_2 \mid X_1 = 0 \) is true. In words, we now embed the information that the probability of survival of a cell in the culture does not depend on its activity, given that the environment was hostile. Whilst the directed acyclic graph cannot code this condition graphically, we can immediately read it from the green stage in the staged tree \( T \) given in Fig. 4a. The full ideal of model invariants \( I_{\text{F}} = I_{\text{gen}} + I_{\text{green}} \) is now equal to

\[
I_{\text{F}} = I_{\text{red}} + I_{\text{yellow}} + I_{\text{blue}} + I_{\text{green}}
\]

just like discussed in Section 4.1. Here, the green path differences generate the ideal

\[
I_{\text{green}} = \langle p_{[v_3]}p_{[v_a]} - p_{[v_4]}p_{[v_3]} \rangle = \langle p_{000+}p_{011+} - p_{010+}p_{001+} \rangle
\]

in the obvious notation for marginal probabilities. This result extends the results of both of Garcia Puente et al. (2005b), Geiger et al. (2006) who do not study context-specific Bayesian networks.

Using Theorem 10, we can see again that \( I_{\text{F}} \) is not toric. This is because even though now \( v_3 \) and \( v_4 \) are in the same position, implying that \( t(v_3) = t(v_4) \), we still have \( t(v_5) \neq t(v_6) \). So \( t(v_3)t(v_6) \neq t(v_4)t(v_5) \) and condition \( \Box \) is not fulfilled.
Because in the staged tree $T$ tree path differences can be extended, we find that in this case the ideal of model invariants is not equal to the kernel of the algebraic parametrisation, $I_T \neq \ker \varphi$. In fact $I_T$ is not radical and has five associated primes, one of them being $\ker \varphi$. We can computationally check in this case that the kernel of $\varphi$ is equal to the ideal of maximal paths: $\ker \varphi = \text{Imaths}$. This observation, together with all of the examples presented in this paper, is strong evidence for Theorem 16 which we formulate in the discussion at the end of this paper.

In a final step, we observe that many of the unfoldings in the graph of $T$ as given in Fig. 4a are logically impossible. For instance, the measure of recovery for cells which have died is nonsensical. In the same fashion, the problem description states that within the cell culture, cells get damaged only if the surrounding environment was hostile. This implies that the measure of survival is nonsensical in benign environments. As a result, many of the atomic probabilities in the context-specific Bayesian network need to be assigned probability zero. We can avoid this redundancy by directly modelling the given situation using the staged tree depicted in Fig. 4d. We denote this tree $T_{>0}$ because all of its labels are strictly positive. The dimension of the corresponding model $M_{T_{>0}}$ is much smaller: the model variety is of dimension four in seven-dimensional space, rather than of dimension six in sixteen-dimensional space, as was the case for $M_T$.

The ideal of model invariants for the staged tree $T_{>0}$ can be calculated in exactly the same fashion as presented above, now resulting in

$$I_{T_{>0}} = I'_{\text{yellow}} + I'_{\text{green}} + I'_{\text{blue}}$$

$$= \langle p_2 p_6 - p_5 p_3 \rangle + \langle p_1 (p_5 + p_6) - p_4 (p_2 + p_3) \rangle + \langle (p_1 + p_2 + p_3) p_8 - p_7 (p_4 + p_5 + p_6) \rangle$$

where we read the atomic probabilities from top to bottom in Fig. 4d. This ideal is toric because all paths fully extend. Again, we can calculate that $I_{T_{>0}} \neq \ker \varphi$ but that the kernel of the algebraic parametrisation is given by the maximal paths:

$$\text{Imaths} = \ker \varphi = \langle p_3 p_5 - p_2 p_6, p_2 p_4 - p_3 p_5, p_3 p_4 - p_1 p_6, p_4 p_7 - p_1 p_8, p_5 p_7 - p_2 p_8, p_6 p_7 - p_3 p_8 \rangle.$$

These generators form a Gröbner basis with respect to the reverse lexicographical term order.

7. Discussion

Throughout this text we have analysed the algebraic and geometric properties of the ideal $I_T$ of model invariants of $M_T$. We have seen that this ideal has a distinguished prime component, namely $\ker \varphi$, and we have fully characterised in Theorem 10 conditions under which this ideal is toric. Although we have not always explicitly stated it, all of the examples we have seen in this paper have the property that $\ker \varphi$ is equal to the ideal $\text{Imaths}$. This leads us to:

**Conjecture 16.** Let $T$ be a staged tree. Then the kernel of $\varphi$ is exactly the ideal generated by maximal paths,

$$\ker \varphi = \text{Imaths}.$$ 

For brevity, we decided not to discuss the algorithmic properties of the ideal $\text{Imaths}$ in this text. However, the available nested polynomial representations of staged trees, as in (4) and (5) and analysed by Gørgen et al. (2018), provide a promising computational tool to find $\text{Imaths}$. This is because using these, we can recursively relate extensions of path differences to the polynomials $t(v)$ for any $v \in V$. 

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Restricting our study to toric staged tree models in Section 5.2, we saw that the algebraic characterisation of these is closely related to condition (⋆) which is necessary for paths to extend. In the context of decomposable graphical models, we know that the ideal of model invariants given by conditional independence statements is the toric ideal defining the kernel of the associated parameterisation, and that moreover the generators of this ideal form a Gröbner basis. In the analysis conducted in Section 6 of this paper, we saw that for decomposable models the ideal \(I_{\text{paths}}\) is exactly the ideal obtained by Geiger et al. (2006) and that therefore its generators form a Gröbner basis. In the toric model represented by the tree \(T_{>0}\) from Fig. 4d, we can see that not only \(\ker \varphi = I_{\text{paths}}\) but the binomial generators of \(I_{\text{paths}}\) form a Gröbner bases of the ideal they generate. This leads is to state a variation of Theorem 16 for toric staged tree models.

**Conjecture 17.** Let \(T = (V, E)\) be a staged tree and suppose that condition (⋆) holds for all vertices \(v, w \in V\) which are in the same stage. Then

\[
\ker \varphi = I_{\text{paths}}
\]

and the generators of \(I_{\text{paths}}\) corresponding to path differences of maximal extensions form a Gröbner basis of \(\ker \varphi\).

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