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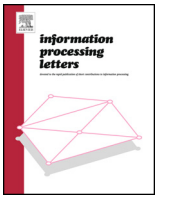

Polynomial invariants for cactuses

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ABSTRACT

Graph invariants are a useful tool in graph theory. Not only do they encode useful information about the graphs to which they are associated, but complete invariants can be used to distinguish between non-isomorphic graphs. Polynomial invariants for graphs such as the well-known Tutte polynomial have been studied for several years, and recently there has been interest to also define such invariants for phylogenetic networks, a special type of graph that arises in the area of evolutionary biology. Recently Liu gave a complete invariant for (phylogenetic) trees. However, the polynomial invariants defined thus far for phylogenetic networks that are not trees require vertex labels and either contain a large number of variables, or they have exponentially many terms in the number of reticulations. This can make it difficult to compute these polynomials and to use them to analyse unlabelled networks. In this paper, we shall show how to circumvent some of these difficulties for rooted cactuses and cactuses. As well as being important in other areas such as operations research, rooted cactuses contain some common classes of phylogenetic networks such phylogenetic trees and level-1 networks. More specifically, we define a polynomial F that is a complete invariant for the class of rooted cactuses without vertices of indegree 1 and outdegree 1 that has 5 variables, and a polynomial Q that is a complete invariant for the class of rooted cactuses that has 6 variables whose degree can be bounded linearly in terms of the size of the rooted cactus. We also explain how to extend the Q polynomial to define a complete invariant for leaf-labelled rooted cactuses as well as (unrooted) cactuses.

1. Introduction

Given a class $\mathcal{C}$ of graphs, and a polynomial $P(C)$ assigned to each element C in this class, we call P an *invariant* of $\mathcal{C}$ if $P(C) = P(C')$ when C is isomorphic to C' for all $C, C' \in \mathcal{C}$; if $P(C) = P(C')$ also implies that C is isomorphic to C' we call P a *complete invariant* for the class (see e.g. [15]). Polynomial invariants have been defined for various classes of graphs (see e.g. [4]), including the extensively studied *Tutte polynomial* (see e.g. [1] and the references therein). These usually encode useful information about the graph (e.g. number of edges, spanning forests), but they are not always complete invariants, and finding complete invariants for graphs remains an important area of research in graph theory and computer science [15].

Recently there has been interest in defining polynomial invariants for graphs that arise in the field of phylogenetics [13,17]. Such graphs are called *phylogenetic networks*, and they often come equipped with a leaf-labelling of the vertices corresponding to some collection of species (see e.g. [18, Chapter 10] for a recent overview). Phylogenetic networks are commonly used to elucidate the evolution-

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ary history for a collection of species that has undergone non-treelike evolution (such as e.g. bacteria or plants) [3], and an important problem asks to find ways to distinguish between distinct networks to compare evolutionary histories (see e.g. [5]). Hence finding complete invariants for special classes of phylogenetic networks could be useful as, for example, they would yield metrics on networks in question (see e.g. [14] where this approach has been recently used to study how the influenza virus evolves).

In this paper, we focus on the problem of finding complete polynomial invariants for the classes of rooted cactuses and cactuses (with or without leaf-labellings), two special classes of phylogenetic networks [7,8] which also arise in other areas such as operations research [12] and genome comparisons [16]. More specifically, recall that a *cactus* (also known as a *Husimi* tree) is a connected undirected graph in which any two cycles are edge disjoint [10]; a *rooted cactus* is a directed acyclic graph with a single source or root whose underlying undirected graph is a cactus, and such that there is a directed path from the root to any vertex in the graph [8] (see Fig. 1 for an example of a cactus and a rooted cactus). Observe that rooted cactuses are related to, but different from *directed cactuses*, which are strongly connected directed graphs where each edge is contained in exactly one directed cycle [2]. Also note that in general a rooted graph may also mean any type of graph that contains a distinguished vertex, which is slightly different from our meaning of rooted. If the underlying graph of a rooted cactus is an undirected tree (or, for brevity, a tree), we call it a *rooted tree* (also known as an *arborescence*). As well as trees, there are various other subclasses of unrooted and rooted cactuses such as (unlabelled) level-1 networks and galled trees (see e.g. [18, p.247]).

In previous related work, for trees, one of the first complete invariants for rooted trees was introduced in [6]. In fact, this polynomial is defined as the restriction of a certain greedoid polynomial (the Tutte polynomial of a greedoid) which arises from the fact that any rooted directed graph gives rise to a certain greedoid structure [6]. In [19] a modification was made to this polynomial to also give a complete invariant for rooted undirected unicyclic graphs (note that rooted undirected unicyclic graphs are similar but different from rooted cactuses, as the former is undirected and contains at most one cycle, while the latter is directed and can contain more than one cycle in the underlying graph). Interestingly, the problem of defining a complete invariant for (undirected) trees remained open until a solution was recently proposed in [13], in which Liu defined a new complete invariant B for rooted trees, which was extended to the class of (undirected) trees.

More recently, polynomial invariants have also been introduced for classes of phylogenetic networks, building on Liu's approach. In [13], Liu showed how to extend the polynomial invariant B to leaf-labelled trees, and more recently a polynomial invariant was introduced for rooted binary internally multi-labelled phylogenetic networks (where vertices with indegree at least 2, or *reticulations*, are distinctly labelled) in [17]. This was shown to be a complete invariant for a certain subclass of such partly-labelled networks. In [11], a polynomial invariant is defined for rooted unlabelled networks based on their spanning trees, and it is briefly mentioned that the polynomial is a complete invariant restricted to the class of so-called rooted, leaf-labelled[2] *tree-child* networks.

The polynomial invariants defined thus far for phylogenetic networks (that are not trees) require vertex labels and either contain a large number of variables, or they have exponentially many terms in the number of reticulations. This can make it difficult to compute these polynomials and to use them to analyse unlabelled networks. In this paper, we shall show how to circumvent some of these difficulties for rooted cactuses and cactuses. More specifically, we begin in Section 2 by introducing a complete invariant for a certain class of vertex-labelled trees (which we call *special pairs*), which generalizes the tree polynomial presented in [13]. We then use this new invariant to introduce two new polynomial invariants for rooted cactuses.

Our first polynomial invariant F given in Section 3 is based on *unfolding* a network, a technique used in [17] and inspired by [9]. When unfolding a rooted cactus, copies of the subnetwork rooted at every reticulation are created. Labels are subsequently added to the unfolded network, which is a directed tree, to create a special pair. In Theorem 3.3 we give a one-to-one correspondence between a rooted cactus and its labelled unfolded network. This immediately gives a polynomial invariant F for rooted cactuses using the special pair definition from before. The polynomial F has 5 variables when leaves are unlabelled, and at most $n+4$ variables when its n leaves are labelled. In addition, as we shall show, F is a complete invariant for the class of rooted cactuses without elementary vertices, that is vertices with indegree and outdegree one. Note that in phylogenetics this is not a strong assumption since elementary vertices are commonly excluded from phylogenetic networks as they do not correspond to evolutionary events such as speciation or hybridization.

Our second polynomial invariant Q for rooted cactuses which is given in Section 4, is based on *expanding* a rooted cactus, a process in which we encode every reticulation with two appended leaves and an added edge. Each iteration of the expansion removes one reticulation vertex from the network; labelling the vertices creates a special pair, that uniquely encodes the original rooted cactus. As we prove in Theorem 4.3, this gives a complete invariant for the class of rooted cactuses (where we now allow for elementary vertices), which we call Q. The Q polynomial has 6 variables when leaves are unlabelled, and at most $n+5$ variables when its n leaves are labelled. We also show that the degree of the Q polynomial is linear in the number of leaves and the reticulations of the network.

In Section 5, we show how to define a complete invariant for the class of leaf-labelled rooted cactuses, by generalising an approach used in [13]. We also explain how to use Q to obtain a complete invariant for (undirected) cactuses, either with or without leaf-labels. Finally, in Section 6, we discuss our findings and give suggestions for future research.

[2] In [11] this result is stated to hold for unlabelled networks, but in a personal correspondence with the authors we were informed that it should be stated to hold for labelled networks.

2. Liu's polynomial revisited

In this section, we define a polynomial invariant P for rooted trees with certain vertex labellings which generalizes Liu's polynomial for rooted (leaf-labelled) trees. We shall use this polynomial to define our new invariants for cactuses in the following sections.

Let $\mathcal{T}$ denote the class of rooted trees. For $T \in \mathcal{T}$ we let ρ_T denote the root of T, $V(T)$ and $L(T)$ be the vertex and leaf-sets of T respectively, and $\bullet$ denote the single vertex tree in $\mathcal{T}$. The *stem* of a tree $T \in \mathcal{T}$ is the shortest directed path in T that starts at the root of T and does not end in a vertex of outdegree 1. We call a stem *trivial* if it consists only of the root. Note that if T is the single vertex tree we regard it as a root and a leaf. Given a set $\{T_1, \ldots, T_k\}$, $k \geq 1$, of rooted trees we let $\wedge(T_1, \ldots, T_k)$ denote the rooted tree obtained by taking a single vertex v and joining this vertex to the root ρ_i of each tree T_i by an arc (v, ρ_i).

Now, given an arbitrary rooted tree $T = \wedge(T_1, \ldots, T_k)$ where $T_i \in \mathcal{T}$, define the 2-variable polynomial $B(T) \in \mathbb{Z}[x, y]$ by recursively applying the following rules [13, Def. 2.1]:

(1) $B(\bullet) = x$, and
(2) $B(T) = y + \prod_{i=1}^{k} B(T_i)$.

In [13, Theorem 2.8] it is shown that B is a complete invariant for $\mathcal{T}$. Moreover in [13, Corollary 3.5], it is proven that a complete invariant B_l for the class of leaf-labelled, rooted trees can be defined as follows. For $T = \wedge(T_1, \ldots, T_k)$ where $T_i \in \mathcal{T}$, and $\bullet_j$ denoting the single vertex tree with label x_j, define $B_l(T)$ by replacing rules (1) and (2) with [13, Def. 3.4]:

(1') $B_l(\bullet_j) = x_j$, and
(2') $B_l(T) = y + \prod_{i=1}^{k} B_l(T_i)$.

Note that different leaf vertices in T may have the same label.

We now generalize these polynomial invariants to rooted trees whose vertices are labelled. We call a maximal directed path of outdegree-1 vertices a *string*.

For any set of variables K, we call a pair (T, λ) a *vertex-labelled rooted tree* if $T \in \mathcal{T}$ and $\lambda : V(T) \to K$. Let $K \subseteq \{x_1, x_2 \ldots\} \cup \{y, z\} \cup \{s\}$, be a fixed set of variables (possibly infinite). We call the pair (T, λ) *special* if:

(i) $\lambda(L(T)) \in \{x_1, x_2 \ldots\}$,
(ii) If $W = (w_1, \ldots, w_p)$ is a string in T, then $\lambda(w_1) \in \{y, z\}$ and if $p > 1$, then $\lambda(w_i) = y$ for all $2 \leq i \leq p$, and
(iii) For every vertex $v \in V(T)$ that is not in $L(T)$ or in a string, $\lambda(v) \in \{y, z\} \cup S$.

Hence, basically, the vertices of a special pair can be labelled arbitrarily as long as the labelling of the leaves is disjoint from the labelling of the internal vertices and strings are labelled $(z, y, y, \ldots)$ or $(y, y, \ldots)$. Moreover, we shall see below, given any $T \in \mathcal{T}$, there is some λ so that (T, λ) is a special pair. Note also that if $T = \wedge(T_1, \ldots, T_k)$ where $T_i \in \mathcal{T}$, then $(T_i, \lambda_i = \lambda|_{V(T_i)})$ is a special pair for all $1 \leq i \leq k$.

We now define a polynomial invariant P_K for the class of vertex-labelled trees. Given a vertex-labelled tree (T, λ) define $P_K(T, \lambda)$ recursively as follows:

- If $T = (\{v\}, \emptyset)$, set $P_K(T, \lambda) = \lambda(v)$.
- If $T = \wedge(T_1, \ldots, T_k)$, set $P_K(T, \lambda) = \lambda(\rho_T) + \prod_{i=1}^{k} P_K(T_i, \lambda_i)$.

To ease notation, in case the set K is clear from the context, we denote $P_K(T, \lambda)$ by $P(T, \lambda)$.

An example of a special pair is given by setting $x = x_1$ and $K = \{x, y\}$, and, for any rooted tree $T \in \mathcal{T}$, defining $\lambda : V(T) \to K$ by $\lambda(v) = y$ if v is an internal vertex and $\lambda(v) = x$ if v is a leaf. Then $P(T, \lambda) = B(T)$ is in fact Liu's polynomial for T.

For another example, set $K = \{x_1, x_2, \ldots\} \cup \{y\}$ (note this is an infinite set). Suppose $T \in \mathcal{T}$ is a leaf-labelled tree with $\phi : L(T) \to \{x_1, x_2, \ldots, x_n\}$ where $n \geq 1$. Then define $\lambda_L : V(T) \to K$, by setting $\lambda_L(v) = y$ if v is an internal vertex and $\lambda_L(v) = \phi(v)$ if v is a leaf. Then $P(T, \lambda_L) = B_l(T)$ is Liu's polynomial for T with leaf-labels.

We say that special pairs (T, λ) and (T', λ') are *isomorphic* if T is isomorphic to T' via a map $\psi : V(T) \to V(T')$ such that $\lambda(v) = \lambda'(\psi(v))$ for all $v \in V(T)$. We now show that P is a complete invariant for special pairs.

Theorem 2.1. *Suppose that (T, λ) and (T', λ') are special pairs. $P(T, \lambda) = P(T', \lambda')$ if and only if (T, λ) is isomorphic to (T', λ').*

Proof. It is straight-forward to check that P is an invariant for special pairs using a similar proof to [13, Prop 2.2]. To show that P is also a complete invariant, we use a similar proof to [13, Cor. 3.5].

Suppose $P(T, \lambda) = P(T', \lambda')$. We want to show that (T, λ) is isomorphic to (T', λ'). Assume $\lambda(V(T)) = \{s_1, \ldots, s_k\} \subseteq \{x_1, x_2 \ldots\} \cup \{y, z\} \cup S$, where $k \geq 2$. Since $P(T, \lambda) = P(T', \lambda')$, it follows that $\lambda(V(T')) = \{s_1, \ldots, s_k\}$ (i.e., $P(T, \lambda)$ and $P(T', \lambda')$ are both polynomials in the same variables).

Consider the polynomial P' in $\mathbb{Z}[x, y]$ obtained from the polynomial $P(T, \lambda)$ in $\mathbb{Z}[s_1, \ldots, s_k]$ by replacing each variable x_i by x and each variable in $S \cup \{z\}$ by y. Then P' is Liu's polynomial for T, i.e. $B(T)$, and so P' is irreducible in $\mathbb{Z}[x, y]$ [13, Lem. 2.6]. It follows that $P(T, \lambda)$ is irreducible in $\mathbb{Z}[s_1, \ldots, s_k]$.

We now use strong induction on n, the number of leaf vertices in T.

If $n = 1$, then $T = (w_1, \ldots, w_l)$, where $l \geq 1$, is a directed path of length $l-1$. If $l > 1$, then $(w_1, w_2, \ldots, w_{l-1})$ is a string in T. If $l = 1$, then $P(T, \lambda) = x_i$, and if $l \geq 2$, then $P(T, \lambda) = (l-1)y + x_i$ or $P(T, \lambda) = z + (l-2)y + x_i$, for some $i \geq 1$. In either case it is straight-forward to check that $P(T, \lambda) = P(T', \lambda')$ implies (T, λ) is isomorphic to (T', λ').

Now suppose that T has $N > 1$ leaves and that the result holds for trees with n leaves where $1 \leq n \leq N - 1$. First note that if T has a stem $(w_1, \ldots, w_l, v)$ with length greater than 0 (with outdegree of v at least 2), then

$(w_1, \ldots, w_l)$ is a string with $l \geq 1$. It follows that the degree 1 terms in $P(T, \lambda)$ are either $ly + \lambda(v)$ or $z + (l-1)y + \lambda(v)$, where $\lambda(v) \in \{y, z\} \cup S$. Hence, as $P(T, \lambda) = P(T', \lambda')$, it follows that T' has a stem of the same length as T and that λ and λ' restricted to the stems are the same.

It follows that we can assume that T and T' both have trivial stems consisting of a root with outdegree at least 2, and hence that $\lambda(\rho_T), \lambda'(\rho_{T'}) \in \{y, z\} \cup S$. So $T = \wedge(T_1, \ldots, T_i)$ where $i > 1$, and $T' = \wedge(T'_1, \ldots, T'_j)$ where $j > 1$. But then

$$P(T, \lambda) = \lambda(\rho_T) + \prod_{k=1}^{i} P(T_k, \lambda_k)$$

$$= \lambda'(\rho_{T'}) + \prod_{l=1}^{j} P(T'_l, \lambda'_l) = P(T', \lambda').$$

Since $i, j > 1$, the products are polynomials in which all terms have degree 2 or higher, and so $\lambda(\rho_T) = \lambda'(\rho_{T'})$ as these are both degree 1 polynomials. Moreover, (T_k, λ_k), $1 \leq k \leq i$, and (T'_l, λ'_l), $1 \leq j \leq l$, are all special pairs and so their polynomials must be irreducible. It follows that $i = j$ and after reordering of indices, $P(T_k, \lambda_k) = P(T'_k, \lambda'_k)$ for all $1 \leq k \leq i$. Since the trees T_i and T'_i have fewer than N leaves, it follows by the induction hypothesis that T_i and T'_i must be isomorphic. Therefore (T, λ) is isomorphic to (T', λ'). □

3. A rooted cactus invariant based on unfolding

In this section we modify the technique used in [17] to obtain a complete polynomial invariant for a special subclass of rooted cactuses. To define this polynomial we first require some additional notation. Recall that a rooted cactus is a directed acyclic graph with a single root ρ whose underlying undirected graph is a cactus, and such that there is a directed path from the root to any vertex in the graph. Note that from this definition, it follows that ρ is the only vertex with indegree 0 and that all vertices of V have indegree at most 2. Note that cycles of the underlying cactus may overlap in a vertex. We call a vertex *elementary* if it has indegree 1 and outdegree 1. A vertex with outdegree 0 is called a *leaf* and a vertex with indegree 2 is called a *reticulation* (so we allow a vertex to be both a leaf and a reticulation). A *reticulation cycle* for a reticulation v in a cactus is a pair of internally vertex-disjoint paths ending in v and with the same origin vertex w; we call w the *top vertex* of the reticulation cycle.

We now define a polynomial invariant for the class of rooted cactuses, which we will show to be complete for rooted cactuses without elementary vertices. First, we associate a vertex-labelled pair (U_N, λ_N) to a rooted cactus N as follows (see Fig. 1 for an example):

(A) For every vertex v in N that is the top vertex for $c \geq 1$ reticulation cycles, resolve the vertex v as follows. Let $w_1, w'_1, \ldots, w_c, w'_c$ be children of v such that each pair (w_i, w'_i) is in the same reticulation cycle. For $1 \leq i \leq c$, add a new vertex v_i with an arc (v, v_i), replace the arcs $(v, w_i), (v, w'_i)$ by arcs $(v_i, w_i), (v_i, w'_i)$ and give v_i label s, i.e., set $\lambda_N(v_i) = s$. Call the resulting network N'.

(B) Unfold the network N' to get U_N as follows. While there exists a lowest reticulation v, make a copy of the tree rooted at v and replace one incoming arc (w, v) of v by an arc (w, v') with v' the root of the copy of v. If v and v' are leaves, label them r. Otherwise, label them z.

(C) Give all leaf vertices in U_N, that are not already labelled, label x. Give all remaining unlabelled vertices in U_N label y.

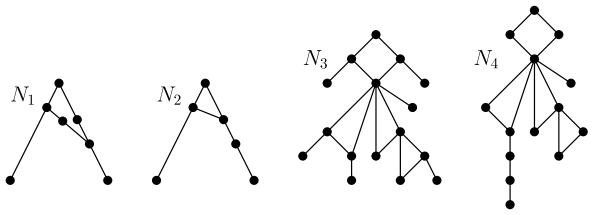

Fig. 1. Example of four rooted cactuses. All arcs are directed downwards. The networks N_1 and N_2 have the same F polynomials $F(N_1) = F(N_2) = y + s + [y + x(y + z + x)][y + z + x]$, but different Q polynomials, since $Q(N_1) = y + s + [y + x(y + q)](z + x)(y + q)$ and $Q(N_2) = y + s + (y + xq)(z + y + x)q$ (for example, $Q(N_1)$ has an $xyzq$ term while $Q(N_2)$ does not).

Observe that each vertex of U_N that corresponds to a reticulation of N is either an internal vertex labelled z or a leaf labelled r. We now show that (U_N, λ_N) is a special pair if N has no elementary vertices.

Lemma 3.1. *Let N be a rooted cactus without elementary vertices. Then (U_N, λ_N) is a special pair with $K \subseteq \{x_1 = x, x_2 = r\} \cup \{y, z\} \cup \{s\}$.*

Proof. Each string consists of exactly one vertex, which is labelled z. In addition, each leaf is labelled x or r and each internal vertex is labelled y, z or s. □

Note that Lemma 3.1 would not be true if we allowed N to contain elementary vertices, as then (U_N, λ_N) could contain a string with a sequence of labels $(y, z, \ldots)$. See Fig. 1 for two non-isomorphic networks that have the same F polynomials. We now define operations that undo the unfolding described above. The *lowest common ancestor (LCA)* of two vertices u and v of a rooted cactus is the unique lowest vertex that has a path to both u and v. Given (U_N, λ_N), for a rooted cactus N without elementary vertices, we construct a digraph $M(U_N, \lambda_N)$ from the rooted tree U_N as follows.

(a) While there exists a pair of vertices a, b in U_N that are either both internal vertices labelled z or both leaves labelled r, choose such a pair with lowest LCA v_t. Fold-up the two rooted cactuses below a and b by adding an arc from the parent of b to a and then deleting b and all its descendants. Remove the label (r or z) from a.

(b) Contract all arcs of the form (v, u) where u has label s.

Observe that this digraph $M(U_N, \lambda_N)$ is unlabelled as it does not come with a labelling map.

Lemma 3.2. *If N is a rooted cactus without elementary vertices, then N is isomorphic to $M(U_N, \lambda_N)$.*

Proof. We will show that (a) reverses (B). Since it is clear that (b) reverses (A), and since the vertices of N and $M(U_N, \lambda_N)$ are unlabelled, it will follow that $M(U_N, \lambda_N)$ is isomorphic to N.

We now show that (a) reverses (B). Each iteration of (B), acting on a reticulation v of a reticulation cycle with top vertex v_t, creates a pair a, b of vertices that are either both internal vertices labelled z or both leaves labelled r. In either case, their lowest common ancestor is v_t. Call such a triple (a, b, v_t) a *good triple*. Future iterations may make copies of such good triples, which will also all be good. We will show that (a) only selects good triples.

To do so, we first observe that, for any pair of good triplets $(a, b, v_t), (a', b', v'_t)$ (with $\{a, b\} \neq \{a', b'\}$), the paths from v_t to a and b are vertex disjoint from the paths from v'_t to a' and b'. This follows from the observation that, after step (A), all reticulation cycles are vertex disjoint. We now show that (a) only selects good triples. Suppose (a) selects a triple (a, b, v_t) that is not good. Since a is labelled z or r, it is also in a good triple (a, c, w_t). Note that w_t is not strictly below v_t because then (a) would not select (a, b, v_t). So either $w_t = v_t$ or w_t is above v_t.

Now note that also b is in a good triple (b, d, u_t). Moreover, u_t is below v_t, and $u_t \neq v_t$, because otherwise the paths from u_t to b and d would not be vertex disjoint from the paths from w_t to a and c. This gives a contradiction because in this case (a) would not select (a, b, v_t).

We conclude that (a) only selects good triples. Hence, each iteration of (a) undoes an iteration of (B) on one copy of the created good triple. It follows that (a) reverses (B). □

Now define a polynomial F for a rooted cactus N by setting

$$F(N) = P(U_N, \lambda_N).$$

Note that if $N \in \mathcal{T}$ is a rooted tree, then $F(N) = B(T)$, i.e., Liu's polynomial for T. Moreover, if N is *binary*, i.e., if all vertices have outdegree at most 2 and all reticulations have outdegree 1, then F is a polynomial in the four variables x, y, z and s, and otherwise in the five variables x, y, z, r and s.

We now show that $F(N)$ is a complete invariant for the class of rooted cactuses without elementary vertices.

Theorem 3.3. *If N and N' are rooted cactuses without elementary vertices, then $F(N) = F(N')$ if and only if N is isomorphic to N'.*

Proof. It is straight-forward to check that if N is isomorphic to N', then (U_N, λ_N) is isomorphic to $(U_{N'}, \lambda_{N'})$. So by Theorem 2.1 $F(N) = F(N')$.

Conversely, suppose $F(N) = F(N')$. By Lemma 3.1, (U_N, λ_N) and $(U_{N'}, \lambda_{N'})$ are both special pairs. Therefore by Theorem 2.1, (U_N, λ_N) is isomorphic to $(U_{N'}, \lambda_{N'})$. So $M(U_N, \lambda_N)$ is isomorphic to $M(U_{N'}, \lambda_{N'})$. By Lemma 3.2 it now follows that N is isomorphic to N'. □

Remark 3.4. Observe that the polynomial $F(N)$ can be obtained directly from N by defining a polynomial $F(N, v)$ for each vertex v of $N = (V, A)$ as follows, and letting $F(N) = F(N, \rho)$.

- If v is a leaf, then
$$F(N, v) = \begin{cases} r & \text{if } v \text{ is a reticulation,} \\ x & \text{otherwise.} \end{cases}$$
- Otherwise, v is the top vertex of $c \geq 0$ reticulation cycles, with $w_1, w'_1, \ldots, w_c, w'_c$ children of v such that each pair (w_i, w'_i) is in the same reticulation cycle, and $w_{c+1}, \ldots, w_{d-c}$ the other children of v (with d the outdegree of v). Let $G(N, v) = \prod_{i=1}^{c} \left[s + F(N, w_i)F(N, w'_i)\right] \prod_{i=c+1}^{d-c} F(N, w_i)$. Then,
$$F(N, v) = \begin{cases} z + G(N, v) & \text{if } v \text{ is a reticulation} \\ y + G(N, v) & \text{otherwise.} \end{cases}$$

4. A rooted cactus invariant based on expanding

In the last section, we defined a polynomial F that is a complete invariant for the special class of rooted cactuses without elementary vertices. Although this polynomial has the advantage of being in at most 5 variables, it is not a complete invariant for all rooted cactuses, and F could have degree that is exponentially dependent on the number of reticulations (observe that copies of networks rooted at each reticulation are created when obtaining the special pair). In this section, we introduce a polynomial invariant Q for the class of rooted cactuses, which has the advantages of not needing to exclude elementary vertices and having a linearly bounded degree.

To define Q and show that it is a complete invariant for cactuses, we use a similar approach to the one used for F. Suppose that $N = (V, E)$ is a rooted cactus. We begin by associating a vertex-labelled tree (T_N, μ_N) to N as follows (see Fig. 2 for an example):

(A) As in page 4.
(B') Expand the network N' to get T_N as follows. While there exists a reticulation, take a lowest reticulation cycle in N', with top vertex v_t and with reticulation v having parents u, u'. Remove arcs (u, v), (u', v). Add vertices p, p' and arcs (u, p), (u', p'). Add arc (v_t, v). Give both of the vertices p, p' (which are leaves) label q. Give v the label z if it is an internal vertex and r if it is a leaf.
(C) As in page 4.

The following lemma is straight-forward to prove.

Lemma 4.1. *(T_N, μ_N) is a special pair with $K \subseteq \{x_1 = x, x_2 = r, x_3 = q\} \cup \{y, z\} \cup \{s\}$.*

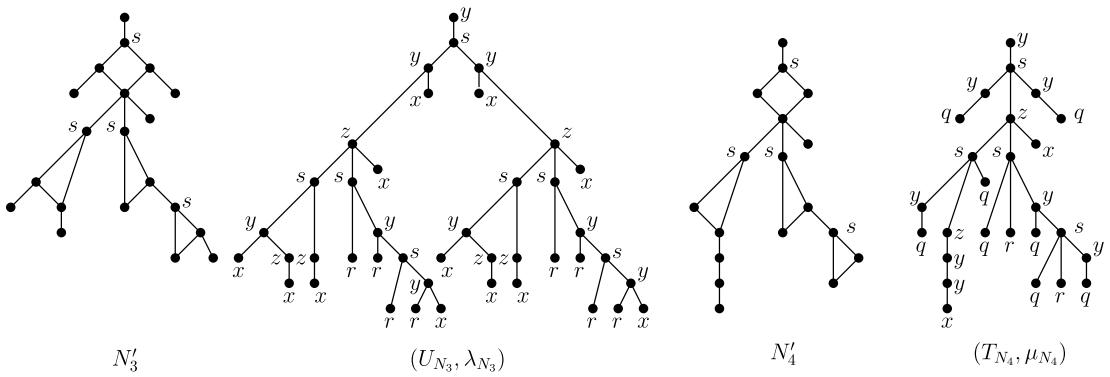

Fig. 2. Example of how the special pairs (U_{N_3}, λ_{N_3}) and (T_{N_4}, μ_{N_4}) are obtained from rooted cactuses N_3 and N_4 of Fig. 1, respectively. All arcs are directed downwards.

Now, given (T_N, μ_N), we construct a digraph $M(T_N, \mu_N)$ from the rooted tree T_N as follows:

(a') While there exists a pair of leaves p, p' labelled q in T_N, choose such a pair with lowest LCA v_t. Let u, u' be the (necessarily unique) parents of p and p', respectively. Let v be the (necessarily unique) child of v_t labelled z or r. Remove leaves p, p' and arc (v_t, v). Add arcs $(u, v), (u', v)$.
(b) Contract all arcs of the form (v, u) where u has label s.

Lemma 4.2. *If N is a rooted cactus, then N is isomorphic to $M(T_N, \mu_N)$.*

Proof. The proof follows from observing that (a') reverses (B), that (b) reverses (A) and that the vertices of both N and $M(T_N, \mu_N)$ are unlabelled. □

Now define a polynomial Q for a rooted cactus N by setting

$$Q(N) = P(T_N, \mu_N). \tag{1}$$

Note that if $N \in \mathcal{T}$ is a rooted tree, then $Q(N) = F(N) = B(T)$. Moreover, if N is binary, then Q is a polynomial in the five variables x, y, z, q, s and otherwise in the six variables x, y, z, q, r and s.

We now show that $Q(N)$ is a complete invariant for rooted cactuses.

Theorem 4.3. *If N and N' are rooted cactuses, then $Q(N) = Q(N')$ if and only if N is isomorphic to N'.*

Proof. This is analogous to the proof of Theorem 3.3, by replacing Lemmas 3.1 and 3.2 with Lemmas 4.1 and 4.2. □

Note that, in contrast to the polynomial F, Q less directly reflects the structure of a cactus. Indeed, with the construction of Q, we add two additional leaves for every reticulation. On the other hand, with the construction used for F, every leaf of the unfolded tree corresponds to a leaf of the original network. However, as we shall now show, unlike F, the degree of Q can linearly bounded in terms of the number of leaves and reticulations.

Theorem 4.4. *Let N be a rooted cactus with n leaves and k reticulations. Then $Q(N)$ is a polynomial of degree $n + 2k$.*

Proof. We have defined $Q(N)$ as the polynomial P of the special pair (T_N, μ_N). By a similar argument to the one presented in [[13], Lemmas 2.3 and 2.4], each term of the polynomial $Q(N)$ corresponds to a rooted subtree S_N of T_N, where S_N and T_N share the same root, and any leaf of T_N is a leaf of S_N or a descendant of a leaf of S_N (for example, the term $cx^a r^b q^d y^e z^f s^g$ in $Q(N)$ corresponds to a primary subtree of T_N that contains $a+b+d+e+f+g$ leaves: a labelled x, b labelled r, d labelled q, e labelled y, f labelled z, and g labelled s). Such rooted subtrees are called *primary subtrees*. The coefficient c of the term counts exactly how many primary subtrees exist with matching leaves. The degree of the polynomial $Q(N)$ is then the greatest number of leaves across all primary subtrees of T_N. This corresponds to, amongst possibly other primary subtrees, the primary subtree that is isomorphic to T_N. To count the number of leaves in T_N, observe that we add two leaves labelled q every time we expand a reticulation cycle. It follows that the number of leaves in T_N, and therefore the degree of the polynomial $Q(N)$, is $n+2k$. □

Remark 4.5. As with the polynomial F, we observe that the polynomial $Q(N)$ can be obtained directly from N by defining a polynomial $Q(N, v)$ for each vertex v of $N = (V, A)$ as follows, and letting $Q(N) = Q(N, \rho)$.

- If v is a leaf then
$$Q(N, v) = \begin{cases} r & \text{if } v \text{ is a reticulation,} \\ x & \text{otherwise} \end{cases}$$
- Otherwise, v is the top vertex of $c \geq 0$ reticulation cycles, with $w_1, w_1', \ldots, w_c, w_c'$ children of v such that each pair (w_i, w_i') is in the same reticulation cycle with reticulation v_i, and $w_{c+1}, \ldots, w_{d-c}$ the other children of v (with d the outdegree of v). Let $R(N, v) = \prod_{i=1}^{c}[s + Q'(N, w_i)Q'(N, w_i')Q(N, v_i)]\prod_{i=c+1}^{d-c} Q'(N, w_i)$ where
$$Q'(N, v) = \begin{cases} q & \text{if } v \text{ is a reticulation,} \\ Q(N, v) & \text{otherwise.} \end{cases}$$

Then we have

$$Q(N,v) = \begin{cases} z + R(N,v) & \text{if } v \text{ is a reticulation,} \\ y + R(N,v) & \text{otherwise,} \end{cases}$$

See Fig. 1 for an example of a Q polynomial for a given network.

5. Cactuses and leaf-labellings

In this section, we show that the invariant Q can be used to give an invariant for cactuses (which are undirected), and that it is relatively simple to extend its definition so as to give an invariant for partially leaf-labelled rooted cactuses and cactuses (note that for cactuses a leaf is a vertex with degree 1).

First, recall, that a cactus is an (undirected) graph in which any two cycles are edge-disjoint. For a cactus G, let $R(G)$ be the set of all rooted cactuses that can be obtained from G by picking some vertex to be the root and choosing some orientation for each edge in G. Note that $R(G)$ may contain isomorphic rooted cactuses. The following observation follows a similar idea to the one used in [13, Lemma 3.1].

Lemma 5.1. *Suppose that G, G' are undirected cactuses. Then G and G' are isomorphic if and only if $R(G) \sim R(G')$ (i.e., there is a bijection $f : R(G) \to R(G')$ such that $f(D)$ is isomorphic to D for all $D \in R(G)$).*

Proof. If G and G' are isomorphic, then clearly $R(G) \sim R(G')$. Conversely, if $R(G) \sim R(G')$ then pick any $D \in R(G)$. Then there is a $D' \in R(G')$ that is isomorphic to D. Since G and G' are the underlying undirected graphs of D and D', respectively, it follows that G and G' are isomorphic. □

Now suppose that C is any complete polynomial invariant for rooted cactuses with $C(N) \in \mathbb{Z}[t_1, \ldots, t_m]$ for some variables $t_1, \ldots, t_m$, and $C(N)$ is irreducible in $\mathbb{Z}[t_1, \ldots, t_m]$, for any rooted cactus N. Given a cactus G, we define the polynomial C_u by

$$C_u(G) = \prod_{D \in R(G)} C(D).$$

Note that this polynomial can have large degree in general, depending on the number of cycles and the size of each cycle (larger sizes lead to more rootings). The following result is related to the observation following [13, Theorem 3.2].

Theorem 5.2. *The polynomial C_u is a complete invariant for cactuses.*

Proof. By assumption, for each $D \in R(G)$, $C(D)$ is an irreducible polynomial in $\mathbb{Z}[t_1, \ldots, t_m]$. The result now follows from Lemma 5.1 and the fact that $\mathbb{Z}[t_1, \ldots, t_m]$ is a unique factorization domain. □

Corollary 5.3. *For the polynomial Q defined in (1), Q_u is a complete invariant for cactuses.*

Note that Q_u restricted to the class of rooted trees is not the same as Liu's polynomial since our rooting procedure differs the one in [13].

We now consider *leaf-labelled* rooted cactuses (see e.g. [8]). As mentioned in the introduction, in phylogenetics it is common to consider (di)graphs in which the leaves are labelled by some set of species (see e.g. [18, Section 10.3]). Using our results on special pairs it is straightforward to obtain a complete invariant for partially leaf-labelled rooted cactuses (i.e. ones in which some subset of the leaves is labelled), in a similar way used to deal with leaf-labelled trees in [13]. Indeed, given a rooted cactus N and a map $\phi : L' \to \{x_1, x_2, \ldots, x_p\}$ from a subset L' of the leaves of N to some collection of species $\{x_1, x_2, \ldots x_p\}$, we can define a special pair (T_N, μ_N) as in the definition of Q above, except that in step (C), we give all remaining leaf vertices v the label x_i (instead of x) if $\phi(v) = x_i$ and label x (as before) if $v \notin L'$. Then using the same argument as in Theorem 4.3, it can be seen that this leads to a complete invariant for the class of partially leaf-labelled rooted cactuses. Moreover, using a partially leaf-labelled version of Lemma 5.1 (in which we only select roots at vertices that are unlabelled), it is possible to also define a polynomial invariant for the collection of partially leaf-labelled cactuses (see e.g. [7]), and to show that it is a complete invariant for this class.

6. Discussion

We have introduced a new complete polynomial invariant Q for the class of rooted cactuses which has at most 6 variables, and also shown how to use Q to obtain a complete invariant for cactuses. In addition, we have shown that the degree of the Q polynomial for a rooted cactus with n leaves and k reticulations is $n + 2k$ [Theorem 4.4]. We have also introduced a polynomial invariant F for rooted cactuses which has only 5 variables regardless of the number of reticulations in the network, and more naturally respects the structure of the network. However, F is only a complete invariant for rooted cactuses without elementary vertices and the degree of F for a rooted cactus may be exponential in the number of reticulations in the rooted cactus.

It could be of interest to look for other polynomial invariants of rooted cactuses/cactuses which shed different light on their structure. For example, in [6] it is asked if the greedoid polynomial invariant introduced for rooted trees gives a complete invariant for larger classes of directed rooted graphs, and so it is natural to ask if it gives a complete invariant for rooted cactuses. However, in recent work [20] it is shown that, even for a simple example of a rooted cactus [20, Fig. 3], the polynomial does not reflect the structure of the directed graph, so this seems unlikely to be the case. Another possibility would be to consider the TVT polynomial in [19] or the "B-polynomial" for digraphs introduced in [1]; the TVT polynomial gives a complete invariant for rooted trees [19, p. 569] but it is not known whether this is the case for the B-polynomial [1, Question 10.6].

Another natural question is to look for complete invariants for broader classes of (di)graphs that are of interest in

phylogenetics. For example, we could consider the classes $\mathcal{C}$ and $\mathcal{C}'$ that consist of directed acyclic graphs that are uniquely determined by the graphs obtained by applying steps (A), (B), and (C) or (A), (B'), and (C), used to obtain a special pair in the definition of F and Q, respectively. It would be interesting to know if we could obtain complete invariants for $\mathcal{C}$ and $\mathcal{C}'$ in a similar way to F and Q and, if so, which well-known classes of (non leaf-labelled) phylogenetic networks are contained in these classes (note that for generalizing the approach used to obtain F, results on so-called stable networks in [9] might be relevant). More specifically, it would be interesting to know for which $k \geq 0$ is the collection of level-k networks (network in which every biconnected component contains at most k reticulations) contained in either $\mathcal{C}$ or $\mathcal{C}'$? Note that (non-leaf-labelled) level-0 and level-1 networks are rooted trees and cactuses, respectively, so $k = 2$ is the first case of interest. Extra care must be taken in this $k = 2$ case, as reticulation cycles may have more than one top vertex. In particular, this means unfolding and expanding will have to be redefined, perhaps depending on the comparability of top vertices of reticulation cycles.

As we have seen, different constructions of polynomials give rise to advantages and disadvantages with respect to the number of variables, the polynomial size, and the graph classes for which it is complete. Ideally, it would be useful to find complete invariants that can be computed in polynomial time for special classes of phylogenetic networks.[3] However, even if it is not possible to find such invariants, it could still be interesting to look for polynomials like the Tutte polynomial which may not provide complete invariants but may be easier to compute and can still provide useful information about the underlying structure of the network.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

[3] This may be too much to ask in general in light of the fact DAG isomorphism checking is at least as hard as the graph isomorphism problem.

References

[1] J. Awan, O. Bernardi, Tutte polynomials for directed graphs, J. Comb. Theory, Ser. B 140 (2020) 192–247.
[2] R. Balaji, R.B. Bapat, S. Goel, Resistance distance in directed cactus graphs, Electron. J. Linear Algebra 36 (2020) 277–292.
[3] E. Bapteste, L. van Iersel, A. Janke, S. Kelchner, S. Kelk, J.O. McInerney, D.A. Morrison, L. Nakhleh, M. Steel, L. Stougie, et al., Networks: expanding evolutionary thinking, Trends Genet. 29 (2013) 439–441.
[4] B. Bollobás, Modern Graph Theory, vol. 184, Springer Science & Business Media, 1998.
[5] G. Cardona, M. Llabrés, F. Rosselló, G. Valiente, Metrics for phylogenetic networks I: generalizations of the Robinson-Foulds metric, IEEE/ACM Trans. Comput. Biol. Bioinform. 6 (2008) 46–61.
[6] G. Gordon, E. McMahon, A greedoid polynomial which distinguishes rooted arborescences, Proc. Am. Math. Soc. 107 (1989) 287–298.
[7] M. Hayamizu, K.T. Huber, V. Moulton, Y. Murakami, Recognizing and realizing cactus metrics, Inf. Process. Lett. 157 (2020) 105916.
[8] K.T. Huber, V. Moulton, M. Owen, A. Spillner, K.S. John, The space of equidistant phylogenetic cactuses, arXiv preprint, arXiv:2111.06115, 2021.
[9] K.T. Huber, V. Moulton, M. Steel, T. Wu, Folding and unfolding phylogenetic trees and networks, J. Math. Biol. 73 (2016) 1761–1780.
[10] K. Husimi, Note on Mayer's' theory of cluster integrals, J. Chem. Phys. 18 (1950) 682–684.
[11] R. Janssen, P. Liu, Comparing the topology of phylogenetic network generators, J. Bioinform. Comput. Biol. 19 (2021) 2140012.
[12] L. Kang, C. Bai, E. Shan, K. Nguyen, The 2-maxian problem on cactus graphs, Discrete Optim. 13 (2014) 16–22.
[13] P. Liu, A tree distinguishing polynomial, Discrete Appl. Math. 288 (2021) 1–8.
[14] P. Liu, P. Biller, M. Gould, C. Colijn, Analyzing phylogenetic trees with a tree lattice coordinate system and a graph polynomial, Syst. Biol. 71 (6) (2022) 1378–1390.
[15] S. Liu, Generalized permanental polynomials of graphs, Symmetry 11 (2019) 242.
[16] B. Paten, M. Diekhans, D. Earl, J.S. John, J. Ma, B. Suh, D. Haussler, Cactus graphs for genome comparisons, J. Comput. Biol. 18 (2011) 469–481, https://doi.org/10.1089/cmb.2010.0252.
[17] J.C. Pons, T.M. Coronado, M. Hendriksen, A. Francis, A polynomial invariant for a new class of phylogenetic networks, PLoS ONE 17 (2022) e0268181.
[18] M. Steel, Phylogeny: Discrete and Random Processes in Evolution, SIAM, 2016.
[19] S.J. Tedford, A Tutte polynomial which distinguishes rooted unicyclic graphs, Eur. J. Comb. 30 (2009) 555–569.
[20] K.S. Yow, C.Y. Chen, W.J. Leong, F. Ismail, Discovering factors of graph polynomials, Menemui Mat. 41 (2019) 88–95.