POTTS PARTITION FUNCTION AND ISOMORPHISMS OF TREES

MARTIN LOEBL AND JEAN-SÉBASTIEN SERENI

Abstract. We explore the well-known Stanley conjecture stating that the symmetric chromatic polynomial distinguishes non-isomorphic trees. The graph isomorphism problem has been extensively studied for decades. There are strong algorithmic advances, but our research concentrates on the following question: is there a natural function on graphs that decides graph isomorphism? Curiously, in mathematics and in physics the concepts of a "natural" graph function bear strong similarities: it essentially means that the function comes from the Tutte polynomial, which in physics is called the Potts partition function. Somewhat surprisingly, after decades of study, this bold project is still not infirmed. The aim of our research is to present a result that supports the project: we prove that the Stanley isomorphism conjecture holds for every *good class* of vertex-weighted trees. Good classes are rich: letting $\mathcal{C}$ be the class of all vertex-weighted trees, one can obtain for each weighted tree (T, w) a weighted tree (T', w') in polynomial time, so that $\mathcal{C}' := \{(T', w') : (T, w) \in \mathcal{C}\}$ is good and two elements (A, b) and (X, y) of $\mathcal{C}$ are isomorphic if and only if (A', b') and (X', y') are.

1. Introduction

We are interested in the classical question about the existence of a natural function on graphs that decides graph isomorphism. We start by introducing Stanley's conjecture along with related graph polynomials.

Stanley's conjecture. A *k-colouring* of a graph $G = (V, E)$ is a mapping $s\colon V \to \mathbf{N}$. The colouring s is a *k-colouring* if $f(V) = \{0, \ldots, k-1\}$,

---

Date: May 27, 2014.

2010 *Mathematics Subject Classification.* 05C31, 05C60.

Key words and phrases. U-polynomial, tree, graph isomorphism, graph reconstruction, Stanley's conjecture.

This work was done within the scope of the European Associated Laboratory STRUCO.

The authors were partially supported by the Czech Science Foundation under the contract number P202-13-21988S (M. L.) and by PHC Barrande 31231PF of the French MAE (J.-S. S.).

and it is *proper* if $s(u) \neq s(v)$ whenever $uv \in E$. We let $\mathrm{Col}(G;k)$ be the set of proper k-colourings of G and $\mathrm{Col}(G)$ be the set of all proper colourings of G, that is, $\mathrm{Col}(G) \coloneqq \cup_{k\in\mathbf{N}} \mathrm{Col}(G;k)$.

The *symmetric function generalisation of the chromatic polynomial* [8] is defined by

$$X_G(x_0, x_1, \dots) \coloneqq \sum_{s\in\mathrm{Col}(G)} \prod_{v\in V} x_{s(v)}.$$

Further, the *symmetric function generalisation of the bad colouring polynomial* [8] is defined by

$$XB_G(t, x_0, x_1, \dots) \coloneqq \sum_{s\colon V\to\mathbf{N}} (1+t)^{b(s)} \prod_{v\in V} x_{s(v)},$$

where $b(s) \coloneqq |\{uv \in E : s(u) = s(v)\}|$ is the number of monochromatic edges of f (note that the sum ranges over all (not necessarily proper) colourings of G).

The *Stanley isomorphism conjecture* proposes that X_G distinguishes non-isomorphic trees. As far as we know, the only result towards the Stanley's conjecture has been recently verified for the class of *proper caterpillars* [1]. (A caterpillar is a tree where the edges not-incident to a leaf form a path, and a caterpillar is proper if each vertex is a leaf or adjacent to a leaf.) Let us also mention that Conti, Contucci and Falcone [3] defined a polynomial P_T for each tree T so that $P_T = P'_T$ only if the trees T and T' are isomorphic. However, the polynomial P_T is not related to the Tutte polynomial.

Noble and Welsh's conjecture. Noble and Welsh [6] defined the *U-polynomial* and showed that it is equivalent to XB_G. Sarmiento [7] proved that the polychromate defined by Brylawski [2] is also equivalent to the U-polynomial. Hence the U-polynomial serves as 'the' mighty polynomial graph invariant. It is defined as follows. Given a partition $\tau = (C_1, \dots, C_\ell)$ of a set, we define $x(\tau)$ to be $x_{|C_1|} \dots x_{|C_\ell|}$.

$$U_G(z, x_1, x_2 \dots) \coloneqq \sum_{A\subseteq E(G)} x(\tau_A)(z-1)^{|A|-|V|+c(A)},$$

where $\tau_A = (C_1, \dots, C_\ell)$ is the partition of $|V|$ given by the components of the spanning subgraph (V, A) of G.

Noble and Welsh conjectured that U_G distinguishes non-isomorphic trees. As observed by Thatte [9], it turns out that Stanley's and Noble and Welsh's conjectures are equivalent.

Loebl's conjectures. Let $k \in \mathbf{N}$. The *q-chromatic function* [5] of a graph $G = (V, E)$ is

$$M_G(k, q) := \sum_{s \in \mathrm{Col}(G;k)} q^{\sum_{v \in V} s(v)}. \tag{1.1}$$

It is known [5] that

$$M_G(k, q) = \sum_{A \subset E} (-1)^{|A|} \prod_{W \in \mathrm{C}(A)} (k)_{q^{|W|}},$$

where $\mathrm{C}(A)$ is the set of components of the spanning subgraph (V, A) and $|C|$ is the number of vertices in the component C. Moreover the *q-dichromate* is defined as

$$B_G(x, y, q) := \sum_{A \subset E} x^{|A|} \prod_{W \in \mathrm{C}(A)} (y)_{q^{|W|}}$$

and it is known that $B_G(x, y, q)$ is equal to the partition function of Potts model with certain magnetic field contribution.

Loebl conjectures that the q-dichromate is equivalent to the U-polynomial, and that q-dichromate distinguishes non-isomorphic chordal graphs. There is a close link between these strong conjectures and Stanley's conjecture, since chordal graphs have a very distinguished tree structure — in graph theory, they are often referred to as 'blown-up trees'. On the other hand, the isomorphism problem for general graphs is equivalent to the isomorphism problem restricted to chordal graphs: given a graph $G = (V, E)$, consider the chordal graph $G' = (V', E')$ so that $V' := V \cup E$ and $E' = \binom{V}{2} \cup \{\{u, e\}, \{v, e\} : \{u, v\} = e \in E\}$. It clearly holds that G and H are isomorphic if and only if G' and H' are isomorphic.

Recently a variant of the q-dichromate, $B_{r,G}(x, k, q)$, was proposed [4]:

$$B_{r,G}(x, k, q) := \sum_{A \subseteq E(G)} x^{|A|} \prod_{C \in \mathrm{C}(A)} \sum_{i=0}^{k-1} r^{|C| q^i}.$$

It is proved that if $(k, r) \in \mathbf{N}^2$ with $r > 1$ and $x := \mathrm{e}^{\beta J} - 1$, then

$$B_{r,G}(x, k, q) = \sum_{\sigma \colon V \to \{1,\ldots,k\}} \mathrm{e}^{\beta \sum_{uv \in E(G)} J\delta(\sigma(u),\sigma(v))} r^{\sum_{v \in V} q^{\sigma(v)}} \tag{1.2}$$

Hence $B_{r,G}(x, k, q)$ is the Potts partition function with variable (k) number of states and with magnetic field contribution $r^{\sum_{v \in V} q^{\sigma(v)}}$. Moreover, it is proved that $B_{r,G}$ is equivalent to U_G.

Summarising, establishing the conjecture that U_G distinguishes non-isomorphic chordal graphs would successfully finish the isomorphism project since U_G is equivalent to the Potts partition function with variable number of states and with magnetic field contribution, and the isomorphism problem for general graphs is equivalent to the isomorphism problem of the chordal graphs. Moreover the Stanley's conjecture is equivalent to the assertion that U_G distinguishes non-isomorphic trees.

The purpose of this work is to prove that the U-polynomial distinguishes non-isomorphic *weighted trees* in any *good family*. Good families are rich: we provide examples of good families F so that the isomorphism problem for general weighted trees is equivalent to the isomorphism problem in F. We hope that eventually it will be possible to introduce an analogous notion restricted to chordal graphs, relying on the extensively studied tree-decomposition theory.

1.1. **Main Results.** A weighted tree is a pair (T, w) where T is a tree and $w\colon V(T) \to \mathbf{N}^+$ is a positive integer vertex-weight function on T. Two weighted trees are isomorphic if there is an isomorphism of the trees that preserves the vertex weights. If (T, w) is a weighted tree then naturally

$$U_{(T,w)}(z, x_1, x_2 \dots) = \sum_{A \subset E(G)} x(\alpha_A)(z-1)^{|A| - \sum_v w(v) + c(A)},$$

where $\alpha_A = (V_1, \dots, V_\ell)$ is the partition of V determined by the components of the spanning subgraph (V, A) of G.

Let (T, w) be a weighted tree. If $e \in E(T)$, then $T - e$ is the disjoint union of two trees, which we consider to be weighted and rooted at the endvertex of e that they contain. A rooted weighted tree (S, w_S) is a *shape* of (T, w) if $2 \leqslant |V(S)| \leqslant |V(T)| - 2$ and there exists an edge $e \in E(T)$ such that S is one of the two components of $T - e$; moreover w_S is the restriction of w to the vertices of S. We consider S rooted at the endvertex of e. We usually shorten the notation and write S for the shape (S, w_S). In a tree, a vertex of degree one is called a *leaf.*

Definition 1.1. A set $\mathcal{T}$ of weighted trees (T, w) is *good* if it satisfies the following properties:

(1) If a vertex of T is adjacent to a leaf, then all its neighbours but one are leaves.
(2) If v is a leaf or has a neighbour that is a leaf, then $w(v) = 1$.
(3) Let $(T, w), (T', w') \in \mathcal{T}$ and let S be a shape of T and such that $w(S) \leqslant w(T)/2$. Let S' be a shape of T' such that the multi-set of the vertex weights with multiplicities of S is equal to the multi-set of the vertex weights with multiplicities of S'. Then S is isomorphic to S'.

Definition 1.2. A set S of weighted trees is *relevant* if there is an efficient algorithm that computes, for each weighted tree (T, w), a weighted tree $(T', w') \in S$ so that whenever (T_1, w_1) and (T_2, w_2) are weighted trees, (T_1, w_1) is isomorphic to (T_2, w_2) if and only if (T'_1, w'_1) is isomorphic to (T'_2, w'_2).

An example of a good relevant set of weighted trees is that composed of all weighted single vertices. Indeed, the classical isomorphism test for trees can easily be extended to the weighted trees; it amounts to coding n-vertex-weighted trees by 0-1 vectors of length polynomial in n. This can be seen as assigning a non-negative integer weight to a single vertex. Such weighted single vertices are of course distinguished by the U-polynomial.

Our purpose is to provide a wide generalisation of this fact, by proving the next statement.

Theorem 1. *The U-polynomial distinguishes non-isomorphic weighted trees in any good set.*

Our proof of Theorem 1 is not constructive in the sense that we are not able to reconstruct the weighted tree T from U_T.

We illustrate the richness of good sets of weighted trees by our next theorem. Let $\mathcal{C}$ be the class of all vertex-weighted trees (T, w) with $\max\{w(v) : v \in V(T)\} \leqslant 2^{|V(T)|}$, where we assume for convenience that each weight is given as a binary number with exactly $|V(T)|$ bits. For each tree T we define T' to be the tree obtained from T by identifying each leaf h with the root of one new star S_h with three vertices.

Theorem 2. *For each $(T, w) \in \mathcal{C}$, one can construct a weight function w' for the vertices of T' such that two elements (T_1, w_1) and (T_2, w_2) of $\mathcal{C}$ are isomorphic if and only if the corresponding elements (T'_1, w'_1) and (T'_2, w'_2) are isomorphic. Furthermore, the set $C' := \{(T', w') : (T, w) \in \mathcal{C}\}$ is good.*

Proof. Let $(T, w) \in \mathcal{C}$. We start by showing how to construct a weight function w' for T'. First, we let the weight of each leaf of T', that is, each vertex of $T' \setminus T$, be 1. Next we perform, to $(T, w) \subset (T', w)$, a variant of the coding for the classical isomorphism test for weighted trees mentioned above. The coding gradually assigns a binary vector $w''(v)$ to each vertex v, starting with the neighbours of the leaves of T', i.e., the leaves of T, which are all assigned (01) in the first step. We assume binary vectors to be ordered according to the positive integer they code.

In each further step $t > 1$, we let S_t be the set of the vertices v with exactly one neighbour that has not been assigned its w''-code before step t. For each $v \in S_t$, we define $c(v)$ to be obtained from $w(v)$ and from the constructed w''-codes $z_1 \geqslant z_2 \geqslant \dots z_m$ of all but one of the neighbours of v, as follows:

$$c(v) := (0z_1 \dots z_m 1w(v)).$$

We choose one vertex x in S_t such that $c(x) = \min\{c(v) : v \in S_t\}$ and we set $w''(x) := c(x)$. This finishes step t.

We observe that the following hold after each step t.

(i) If a vertex x is assigned its code $w''(x)$ in step t and its neighbour y is assigned its code $w''(y)$ in an earlier step, then $w''(x) > w''(y)$.

(ii) If a vertex x is assigned its code $w''(x)$ in step t, then there is exactly one shape $S(x)$ rooted at x such that each vertex v of $S(x) \setminus x$ has been assigned its w''-code before step t.

The coding terminates if there is a vertex r such that all of its neighbours have been assigned a w''-code. We observe that when the coding terminates, each vertex but r has been assigned its w''-code.

Finally, if $v \neq r$, then $w'(v)$ is the positive integer coded by $w''(v)$ and we set $w'(r) := w(r) + \sum_{v \neq r} w'(v)$. The vertex r is the *root* of (T', w'). This finishes the construction of (T', w').

Let us observe that (T, w) can be reconstructed from (T', w'): first, notice that T is obtained from T' by deleting all the leaves. In particular, we thus know $|V(T)|$. Next, the vertex r is the unique vertex of T' with the largest weight. Moreover, $w(r) = w'(r) - \sum_{v \in V(T') \setminus \{r\}} w'(v)$. In addition, for each vertex $v \neq r$ the weight $w(v)$ can be deduced from $w'(v)$ as follows: the binary representation of $w(v)$ is equal to the last $|V(T)|$ digits of the binary representation of $w'(v)$. This proves the first part of the statement of Theorem 2.

It remains to show that $\mathcal{C}'$ is a good class of weighted trees. Clearly, Properties (1) and (2) of Definition 1.1 hold and so it remains to show that so does (3). Let (A', b') be an element of $\mathcal{C}'$ and let S be a shape of A' such that $b'(S) \leqslant b'(A)/2$. Then the root of (A', b') does not belong to S. Hence, letting s be the root of S we infer that $S = S(s)$ thanks to Property (ii). It follows that s is the unique vertex of S with maximum b'-weight and S can be uniquely reconstructed from $b''(s)$. This shows the second part of the statement of Theorem 2, thereby ending the proof. $\square$

2. The Structure of the Proof of Theorem 1.

We fix a good set of weighted trees and, from now on, we say that a weighted tree is *good* if it belongs to this set. We write down a procedure and with its help prove Theorem 1. The rest of the paper then describes our realisation of the procedure.

A *j-Shape* is an isomorphism class of rooted weighted trees with total weight j. We note that a shape is a weighted rooted subtree, while a j-Shape is an isomorphism class. We start with an observation.

Observation 2.1. *Let (T, w) be a weighted tree. Assume that for each j-Shape S and each $j \leqslant w(T)/2$, we know the number of shapes of (T, w) that are isomorphic to S. Then we know T.*

Proof. We use an easy but important observation that two shapes of T are either disjoint or one is contained in the other. Let us order the shapes of (T, w) of weight at most $w(T)/2$ decreasingly according to their weight. Let m be the maximum weight of a shape of T and let $S_1, \ldots, S_a$ be the shapes with weight m. Clearly, either the shapes $S_1, \ldots, S_a$ are joined in T to the same vertex, or $a = 2$ and $m = w(T)/2$. In the latter case, T is determined. In the former case, let r be the vertex of T to which each of $S_1, \ldots, S_a$ is joined. The shapes of T of weight equal to $m - 1$, if any, are either shapes of $S_1, \ldots, S_a$, which we know, or joined by an edge to r. Continuing in this way with weights $m - 2, m - 3, \ldots$, we gradually increase the tree containing r until we reach weight $w(T)$. The resulting tree is T. $\square$

2.1. **Isomorphism of good weighted trees is U-recognisable.** Let (T, w) be a good weighted tree. Let $\alpha(T) = (\alpha_1, \ldots, \alpha_n)$ be the weights of the shapes of T, with $\alpha_1 < \ldots < \alpha_n$. The definition of a shape implies that $\alpha_1 \geqslant 2$. We shall consider both partitions of the integer $w(T)$ and partitions of the tree T. To distinguish between them clearly, partitions of an integer are referred to as *expressions*. For each partition P of T, the weights of the parts of T form an expression E of $w(T)$, which we call the *characteristic* of P.

- A *j-expression* of an integer W is a partition of W in which one of the part has size $W - j$.
- A *j-partition* of T is a partition of T whose characteristic is a j-expression of $w(T)$.
- A j-partition $(T_0, \ldots, T_k)$ of T with $w(T_0) = w(T) - j$ is *shaped* if there exists an edge e of T such that T_0 is one of the components of $T - e$.

For an expression E of a positive integer, we let $\mathcal{U}(T, w, E)$ be the number of partitions of (T, w) with characteristic E. Note that this number is 0 if E is not an expression of $w(T)$. We notice that, for each expression E, the polynomial $U_{(T,w)}$ determines $\mathcal{U}(T, w, E)$.

We note that among the partitions of T corresponding to an expression, some are shaped and others are not. The proof of Theorem 1 relies on the following procedure.

Procedure 1.
INPUT: The polynomial $U_{(T,w)}$, an integer $j \in \{\alpha_1 + 1, \dots, w(T)/2\}$, a j-expression E and, for each $j' < j$ and each j'-Shape S, the number of shapes of T that are isomorphic to S.
OUTPUT: The number of shaped j-partitions of T with characteristic E.

Let us see how this procedure allows us to establish Theorem 1.

Proof of Theorem 1. Let (T, w) and (T', w') be good weighted trees with $U_{(T,w)} = U_{(T',w')}$. The vector $\alpha(T) = (\alpha_1, \dots, \alpha_n)$ can be computed from the U-polynomial, since its coordinates correspond to the partitions of T into two subtrees, each of weight at least 2. (The same applies for T'.)

Recall that $\alpha_1 \geqslant 2$. Furthermore, a shape S of T or T' is isomorphic to an α_1-Shape if and only if S is the star S^1 on α_1 vertices rooted at its centre. This is because the leaves and their neighbours have weight 1. It follows that the number of shapes of T of weight α_1 can be calculated from $U_{(T,w)}$ and thus this number is the same for (T', w').

By Observation 2.1, (T, w) and (T', w') are isomorphic if $w(T) = w'(T')$ and the numbers of all their shapes isomorphic to any given j-Shape of weight $j \leqslant 1/2w(T)$ are the same. To prove this we apply Procedure 1 inductively for each $j \leqslant 1/2w(T)$, starting with $j = \alpha_1 + 1$. By its validity we know that for each j-expression E, the numbers of shaped j-partitions with characteristic E of T and of T' are the same. In order to move to $j + 1$, we need to show the following.

Assertion 2.2. *For any given j-Shape S, the numbers of shapes of T and of T' isomorphic to S are the same.*

This can be argued as follows. A j-expression E is *valid* if there is a shaped j-partition of T with characteristic E. If E is a j-expression, then we let $W(E)$ be the multi-set consisting of all the parts of E. We define $S(E)$ to be the j-Shape isomorphic to a shape of T whose vertex weights are given by $W(E)$, which can be done thanks to (3) of Definition 1.1 since T is good. It is possible that $S(E)$ does not exist in which case E is redefined as invalid. (Indeed, $S(E)$ does not exist when the following holds: if S is a shape of T with shaped partition W, then at least one part of W does not correspond to a single vertex of S.)

A valid j-expression E is *minimal* if no proper refinement of E is valid. If E is minimal, then the number of shaped j-partitions of T with characteristic E is equal to the number of shapes of T isomorphic to $S(E)$. We note that we do not know $S(E)$, but we do know that T and T' have the same number of shapes isomorphic to $S(E)$.

Finally, consider a valid j-expression E such that for each valid refinement E' of E, we know that T and T' have the same number $n(E')$ of shapes isomorphic to $S(E')$. Now, the number of shapes of T (and of T') isomorphic to $S(E)$ is equal to the number of shaped j-partition of T with characteristic E minus a non-negative integer linear combination of $n(E')$, where E' is a valid refinement of E. Again we note that we do not know the coefficients $n(E')$, since we do not know the Shapes $S(E')$. But we do know that these coefficients are the same in T' as well, and so we can conclude that the numbers of shapes of T and of T' isomorphic to $S(E)$ are the same. $\square$

3. Designing Procedure 1

An *α_j-situation* σ is a tuple $((\sigma_1, w_1), \dots, (\sigma_{t(\sigma)}, w_{t(\sigma)}))$ of disjoint weighted rooted trees with $t(\sigma) \geqslant 2$ such that $w_1(\sigma_1) \leqslant \dots \leqslant w_{t(\sigma)}(\sigma_{t(\sigma)})$ and $\sum_{i=1}^{t(\sigma)} w_i(\sigma_i) = \alpha_j$. An α_j-situation σ is said to *occur* in a tree T if there exists a subtree T' of T and $t(\sigma)$ distinct edges $e_1, \dots, e_{t(\sigma)}$ with exactly one end in $V(T')$ such that, for each $i \in \{1, \dots, t(\sigma)\}$, there is an isomorphism preserving the root and the weights between σ_i and the component of $T - e_i$ different from T'. Note that if σ occurs in T, then for each $i \in \{1, \dots, t(\sigma)\}$ the tree T has a shape isomorphic to σ_i.

We proceed in steps, the first one being an exhaustive listing that depends only on α_j.

Step 1. Explicitly list all α_j-situations for $\alpha_j \leqslant w(T)/2$.

Step 2. For each $\alpha_j \leqslant w(T)/2$ and each α_j-situation σ from Step 1, compute the number $m_T(\sigma)$ of times σ occurs in T.

Before designing Step 2, we show how Steps 1 and 2 accomplish Procedure 1. Suppose that the two steps are completed. Let $E = \{E_1, \dots, E_k\}$ be an α_j-expression of $w(T)$.

For each α_j-situation $\sigma = ((\sigma_1, w_1), \dots, (\sigma_{t(\sigma)}, w_{t(\sigma)}))$, let Ψ_σ be the collection of all surjections from the expression $\{E_1, \dots, E_k\}$ to $\{\sigma_1, \dots, \sigma_{t(\sigma)}\}$. We observe that the number X of non-shaped j-partitions of T with characteristic E is

$$\sum_{\alpha_j\text{-situation } \sigma} m_T(\sigma) \sum_{f \in \Psi_\sigma} \sum_{i=1}^{t(\sigma)} \mathcal{U}(\sigma_i, f^{-1}(\sigma_i)),$$

where $f^{-1}(\sigma_i)$ is naturally interpreted as an expression. Notice that this formula allows us to compute X: for each $i \in \{1, \dots, t(\sigma)\}$, the tree σ_i

is given by σ, hence the U-polynomial of σ_i can be computed. Consequently, we can compute the number of shaped α_j-partitions of T with characteristic E, which is

$$\mathcal{U}(T, w, E) - X.$$

This accomplishes Procedure 1.

It remains to design Step 2. Fix a situation $\sigma = ((\sigma_1, w_1), \dots, (\sigma_t, w_t))$.

Observation 3.1. *For every pair $(i, j) \in \{1, \dots, t\}^2$, if T_i and T_j are two shapes of a tree T that are isomorphic to σ_i and σ_j, respectively, then either $T_i \subseteq T_j$ or $T_j \subseteq T_i$ or $T_i \cap T_j = \varnothing$.*

To see this, let e_k be the edge of T such that T_k is a component of $T - e_k$ for $k \in \{i, j\}$. Then, either $e_j \in E(T_i)$ or $e_j \in E(T - T_i)$. If $e_j \in E(T - T_i)$, then either $T_j \subseteq T_i$ or $T_j \subseteq T - T_i$, in which case $T_j \cap T_i = \varnothing$. If $e_j \in E(T_i)$, then $T_j \subseteq T_i$: otherwise, $T_j \cap T_i \neq \varnothing$ and $T - T_i \subset T_j$, so that $w(T_i) + w(T_j) > w(T)$. This would contradict the hypothesis that $\sum_{k=1}^{t(\sigma)} w_k(\sigma_k) = \alpha_j$, since $\alpha_j \leqslant w(T)/2$. This concludes the proof of Observation 3.1.

Define Λ to be the set of all t-tuples $(T_1, \dots, T_t)$ such that for each $i \in \{1, \dots, t\}$,

- T_i is a shape of T that is isomorphic to (σ_i, w_i), and
- if $j \in \{1, \dots, t\} \setminus \{i\}$, then T_i is not a subtree of T_j.

Observation 3.2. *The number of times that σ occurs in T is equal to $|\Lambda|$.*

Proof. We prove that the elements of Λ are exactly occurrences of σ in T. By the definition, each occurrence of σ gives rise to an element of Λ.

Conversely, let $(T_1, \dots, T_t)$ be an element of Λ. Observation 3.1 implies that the shapes T_i are mutually disjoint. For each $k \in \{1, \dots, t\}$, let e_k be the edge of T associated to the shape T_k and let v_k be the endvertex of e_k that does not belong to T_k. Note that $v_k \notin \cup_{j=1}^{t} T_j$ since no tree T_i is a subtree of another tree T_j and $\alpha_j \leqslant w(T)/2$. Set $T'_k \coloneqq T'_{k-1} - T_k$, where $T'_0 \coloneqq T$.

Observe that each of $T_{k+1}, \dots, T_t$ is a shape of T'_k. Hence, T'_k is connected and contains all vertices $v_1, \dots, v_t$. Therefore, setting $T' \coloneqq T'_t$ shows that $(T_1, \dots, T_t)$ occurs in T. $\square$

Our goal is to compute $|\Lambda|$. For a tree T', define $\Lambda_0(T')$ to be the set of all t-tuples $(T_1, \dots, T_t)$ such that T_i is a shape of T' that is isomorphic to (σ_i, w_i) for each $i \in \{1, \dots, t\}$. Set $\Lambda_0 \coloneqq \Lambda_0(T, w)$. In this notation, the weight shall be omitted when there is no risk of confusion. The advantage of Λ_0 is that its size can be computed. Indeed,

$$|\Lambda_0| = \prod_{i=1}^{t} \sharp((\sigma_i, w_i) \hookrightarrow T),$$

where $\sharp((\sigma_i, w_i) \hookrightarrow T)$ is the number of shapes of T that are isomorphic to (σ_i, w_i). This number is given in the input of Procedure 1, since $w_i(\sigma_i) < \alpha_j$.

Next, we compute $|\Lambda|$ using the principle of inclusion and exclusion. Setting $I \coloneqq \{1, \dots, t\}^2 \setminus \{(i,i) : 1 \leqslant i \leqslant t\}$, we have

$$|\Lambda| = |\Lambda_0| - \left| \bigcup_{(i,j)\in I} \Lambda_{(i,j)} \right|,$$

where $\Lambda_{(i,j)}$ is the subset of Λ_0 composed of the elements $(T_1, \dots, T_t)$ with $T_i \subseteq T_j$.

By the principle of inclusion-exclusion, we deduce that the output of Step 2 is equal to

$$|\Lambda_0| - \sum_{\varnothing \neq F \subseteq I} (-1)^{|F|-1} \left| \bigcap_{(i,j)\in F} \Lambda_{(i,j)} \right|.$$

It remains to compute $\left|\bigcap_{(i,j)\in F} \Lambda_{(i,j)}\right|$ for each non-empty subset F of I. We start with an observation, which characterises the sets F for which the considered intersection is not empty.

Observation 3.3. *Let $F \subseteq I$. Then, $\bigcap_{(i,j)\in F} \Lambda_{(i,j)} \neq \varnothing$ if and only if for every $(i,j) \in F$, either σ_i is isomorphic to σ_j, or σ_j has a shape that is isomorphic to σ_i.*

From now on, we consider only contributing sets F. We construct four directed graphs W_0, W_1, W_2 and W_3 that depend on F. Each vertex x of W_k is labeled by a subset $\ell(x)$ of $\{(\sigma_1, w_1), \dots, (\sigma_t, w_t)\}$. These labels will have the following properties.

(1) $(\ell(x))_{x\in V(W_k)}$ is a partition of $\{(\sigma_1, w_1), \dots, (\sigma_t, w_t)\}$.
(2) For each vertex x of W_k, all weighted trees in $\ell(x)$ are isomorphic.
(3) $\left|\cap_{(i,j)\in F}\Lambda_{(i,j)}\right|$ is equal to the number of elements $(T_1, \dots, T_t)$ of Λ_0 such that
   - for each vertex x of W_k, if $(\sigma_i, w_i), (\sigma_j, w_j) \in \ell(x)$ then $T_i = T_j$; and

- for every arc (x, y) of W_k, if $((\sigma_i, w_i), (\sigma_j, w_j)) \in \ell(x) \times \ell(y)$, then $T_i \subseteq T_j$.

The directed graph W_0 is obtained as follows. We start from the vertex set $\{z_1, \ldots, z_t\}$. For each $i \in \{1, \ldots, t\}$, the label $\ell(z_i)$ of z_i is set to be $\{(\sigma_i, w_i)\}$. For each $(i, j) \in F$, we add an arc from z_i to z_j. Thus W_0 satisfies properties (1)–(3). Note that W_0 may contain directed cycles, but by Observation 3.3, if C is a directed cycle then all elements in $\cup_{x \in V(C)} \ell(x)$ are isomorphic.

Now, W_1 is obtained by the following recursive operation. Let (x, y, z) be a triple of vertices such that (x, y) and (x, z) are arcs, but neither (y, z) nor (z, y) are arcs. Let $(\sigma_y, w_y) \in \ell(y)$ and $(\sigma_z, w_z) \in \ell(z)$. We add the arc (y, z) if $|V(\sigma_y)| \leqslant |V(\sigma_z)|$, and the arc (z, y) if $|V(\sigma_z)| \leqslant |V(\sigma_y)|$. (In particular, if $|V(\sigma_y)| = |V(\sigma_z)|$, then both arcs are added.)

We observe that W_1 satisfies (1)–(3). Since neither the vertices nor the labels were changed, the only thing that we need to show is that if the arc (y, z) was added, then for all tuples $(T_1, \ldots, T_t) \in \cap_{(i,j) \in F} \Lambda_{(i,j)}$ and all $((\sigma_i, w_i), (\sigma_j, w_j)) \in \ell(y) \times \ell(z)$, it holds that $T_i \subseteq T_j$. This follows from Observation 3.1: since (y, z) was added, there exists $s \in \{1, \ldots, t\}$ such that T_s is contained in both T_i and T_j.

The directed graph W_2 is obtained by recursively contracting all directed cycles of W_1. Specifically, for each directed cycle C, all the vertices of C are contracted into a vertex z_C (parallel arcs are removed, but not directed cycles of length 2), and $\ell(z_C) := \cup_{x \in V(C)} \ell(x)$. We again observe that W_2 satisfies properties (1)–(3).

Finally, W_3 is obtained from W_2 by recursively deleting transitivity arcs, that is, the arc (y, z) is removed if there exists a directed path of length greater than 1 from y to z. Note that W_2 and W_3 have the same vertex-set, and every arc of W_3 is also an arc in W_2. Again, W_3 readily satisfies properties (1)–(3).

Now, let us prove that each component of W_3 is an arborescence, that is a directed acyclic graph with each out-degree at most one. We only need to show that every vertex of W_3 has outdegree at most 1.

Assume that (x, y) and (x, z) are two arcs of W_3. First, note that, in W_2, there is no directed path from y to z or from z to y, for otherwise the arc (x, y) or the arc (x, z) would not belong to W_2, respectively. Therefore, regardless whether y and z arose from contractions of directed cycles in W_1, there exist three vertices x', y' and z' in W_1 such that both (x', y') and (x', z') are arcs but neither (y', z') nor (z', y') is an arc. This contradicts the definition of W_1. Consequently, every vertex of W_3 has outdegree at most 1, as wanted.

Set

$$\tau(T) \coloneqq \big\{\sharp((\sigma_i, w_i) \hookrightarrow H) : \\ H \in \{(T, w), (\sigma_1, w_1), \ldots, (\sigma_t, w_t)\} \text{ and } 1 \leqslant i \leqslant t\big\}.$$

We recall that $\tau(T)$ is known from the assumptions of Procedure 1. Step 2 is completed by the following procedure.

Procedure 2.
INPUT: A labeled directed forest W of arborescences and the set $\tau(T)$.
OUTPUT: For each $H \in \{(T, w), (\sigma_1, w_1), \ldots, (\sigma_t, w_t)\}$, the number $\mathcal{P}_3(H, W, \tau(T))$ of elements $(T_1, \ldots, T_t)$ of $\Lambda_0(H)$ such that

- for each vertex x of W, if $(\sigma_i, w_i), (\sigma_j, w_j) \in \ell(x)$ then $T_i = T_j$; and
- for every arc (x, y) of W, if $((\sigma_i, w_i), (\sigma_j, w_j)) \in \ell(x) \times \ell(y)$, then $T_i \subseteq T_j$.

The output of Procedure 2 can be recursively computed as follows. Let $W_{\max}$ be the set of vertices of W with outdegree 0. For each vertex x of W, let (σ^x, w^x) be a representative of $\ell(x)$.

$$\mathcal{P}_3(H, W, \tau(T)) = \prod_{x \in W_{\max}} (\sharp((\sigma^x, w^x) \hookrightarrow H)) \cdot \mathcal{P}_3((\sigma^w, w^x), \tilde{W}(w), \tau(T)),$$

where $\tilde{W}(w)$ is obtained from the component of W that contains x by removing x, and $\sharp((\sigma^x, w^x) \hookrightarrow H)$ is known thanks to the set $\tau(T)$.

By property (3) of the labels, the output $\mathcal{P}_3(T, W_3, \tau(T))$ is equal to $\left|\bigcap_{(i,j) \in F} \Lambda_{(i,j)}\right|$. This concludes the design of Procedure 1.

References

[1] J. Aliste-Prieto and J. Zamora, *Proper caterpillars are distinguished by their chromatic symmetric function*, Discrete Math. **315** (2014), 158–164.

[2] T. Brylawski, *Intersection theory for graphs*, J. Combin. Theory Ser. B **30** (1981), no. 2, 233–246.

[3] R. Conti, P. Contucci, and C. Falcolini, *Polynomial invariants for trees: a statistical mechanics approach*, Discrete Appl. Math. **81** (1998), no. 1-3, 225–237.

[4] M. Klazar, M. Loebl, and I. Moffatt, *The Potts model and chromatic functions of graphs*, Ann. Inst. Henri Poincaré D **1** (2014), no. 1, 47–60.

[5] M. Loebl, *Chromatic polynomial, q-binomial counting and colored Jones function*, Adv. Math. **211** (2007), no. 2, 546–565.

[6] S. D. Noble and D. J. A. Welsh, *A weighted graph polynomial from chromatic invariants of knots*, Ann. Inst. Fourier (Grenoble) **49** (1999), no. 3, 1057–1087, Symposium à la Mémoire de François Jaeger (Grenoble, 1998).

[7] I. Sarmiento, *The polychromate and a chord diagram polynomial*, Ann. Comb. **4** (2000), no. 2, 227–236.

[8] R. P. Stanley, *A symmetric function generalization of the chromatic polynomial of a graph*, Adv. Math. **111** (1995), no. 1, 166–194.
[9] B. D. Thatte, *Subgraph posets, partition lattices, graph polynomials and reconstruction*, arXiv:0609574, 2006.

Dept. of Applied Mathematics, Charles University, Praha, Czech Republic.
E-mail address: loebl@kam.mff.cuni.cz

CNRS, (LORIA, Orpailleur), Vandœuvre-lès-Nancy, France.
E-mail address: sereni@kam.mff.cuni.cz