Unexpectedly, a Symmetry on Unlabeled Graphs

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Abstract

We exhibit the joint symmetric distribution of the following two parameters on the set of unlabeled simple connected graphs with n vertices. The first parameter is the maximal number of leaves attached to a vertex. The second parameter is the size of the largest set of vertices sharing the same closed neighborhood minus 1.

Apparently, this is the first example of a natural non-trivial equidistribution of graph parameters on unlabeled simple connected graphs with a fixed set of vertices.

Our proof is enumerative, using the theory of species. Exhibiting an explicit bijection interchanging the two parameters remains an open problem.

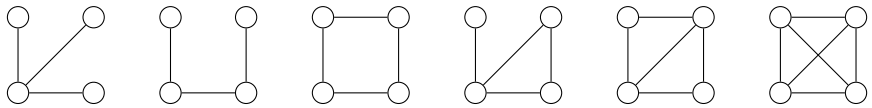
Mathematics Subject Classifications: 05C30

1 Introduction

Symmetries are an essential part of human life. Some seem obvious to us now, such as the rotational symmetry of a wheel, or the reflective symmetry of a balance scale. Other symmetries, such as the symmetry between area and bounce on Dyck paths are still mysterious [5, Open Problem 3.11].[1] In mathematical terms, a symmetry is a bijection on a set of objects. As the preceding example demonstrates, in some cases, we know about the existence of a symmetry but are unable to exhibit it explicitly.

There are many known bijections on sets classically studied in combinatorics, such as permutations, integer partitions or Dyck paths. However, to the best of our knowledge[2], there is not a single known 'natural' bijection from the set of all unlabeled simple connected graphs with a given finite set of vertices to itself. Enlarging the domain to all graphs we are aware of taking the complement of a graph. Alternatively, we can restrict the domain to three-connected planar graphs and remove the constraint that the number of vertices is preserved. Then a celebrated result of Whitney shows that mapping a graph to its planar dual is an involution [11, Thm. 11]. Of course, it is possible to modify these maps

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[1]Even in 2026, some people still ask why mirrors reflect horizontally but not vertically.
[2]https://mathoverflow.net/questions/313532



$s(G)=0$	$s(G)=0$	$s(G)=0$	$s(G)=1$	$s(G)=1$	$s(G)=3$
$t(G)=3$	$t(G)=1$	$t(G)=0$	$t(G)=1$	$t(G)=0$	$t(G)=0$

Figure 1: Sibling and tuft numbers of all unlabeled connected graphs with 4 vertices.

to obtain involutions preserving connectivity, but such a modification does not seem to be a very natural thing to do.

In fact[3], we do not even know of any pair of 'natural' equidistributed parameters on unlabeled simple connected graphs appearing in the literature. This may be surprising, since many graph parameters have been considered and studied, albeit mostly in terms of inequalities satisfied among them. The www.findstat.org database, as of 2025, lists about 300 such statistics, without any conjectural equidistributions.

Note that any equidistribution implies the existence of a bijection that maps one of the parameters to the other. Thus, our aim is to present a pair of non-trivial graph parameters which have the same distribution on the set of unlabeled simple connected graphs with a fixed number of vertices.

We consider only finite simple graphs. A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. Given a vertex v, the (open) *neighborhood* of v is the set $\mathrm{N}(v) := \{u \in V(G) \mid u \text{ adjacent to } v\}$, whereas the set $\bar{\mathrm{N}}(v) := \{v\} \cup \mathrm{N}(v)$ is the *closed neighborhood* of v. Two vertices are *siblings* if they share the same closed neighborhood. Finally, a *leaf* or *endpoint* is a vertex of degree one.

We consider the following two parameters on graphs. The *sibling number*

$$s(G) := \max_{v \in V(G)} \left|\{u \in V(G) \setminus \{v\} \mid \bar{\mathrm{N}}(u) = \bar{\mathrm{N}}(v)\}\right|$$

is the maximal number of other vertices sharing the same *closed* neighborhood with any given vertex. The *tuft number*[4] $t(G)$ is the maximal number of leaves adjacent to the same vertex.

An unlabeled graph is an isomorphism class of graphs. Figure 1 displays all unlabeled connected graphs with four vertices, together with their sibling and tuft numbers. Among all graphs with $n > 2$ vertices, the graph with maximal sibling number is the complete graph K_n, which has sibling number $n-1$ and tuft number 0. On the other hand, the unique graph maximizing the tuft number is the star graph S_n, which has $n-1$ leaves adjacent to a single vertex, and no siblings.

Our main theorem, initially conjectured by Per Alexandersson and the third author, exhibits a non-trivial equidistribution among graph parameters.

[3] https://mathoverflow.net/questions/312823
[4] www.findstat.org/St001826

Theorem 1. *The sibling number and the tuft number have joint symmetric distribution on the set of unlabeled connected graphs with n vertices. Put differently, the isomorphism type generating series $\sum_G x^{s(G)}y^{t(G)}$, where the sum is taken over all unlabeled connected graphs with n vertices, is symmetric in x and y.*

The sibling number and tuft number of a graph are the maximum sibling number and tuft number, respectively, of its connected components. Therefore, equidistribution of the parameters on connected graphs is a stronger property than equidistribution on the set of all graphs. The maximal number of vertices sharing the same open neighborhood and the tuft number do not have joint symmetric distribution.

To illustrate Theorem 1, the graphs with six vertices with sibling number 1 and tuft number 2 and those with sibling number 2 and tuft number 1 are displayed in Figure 2.

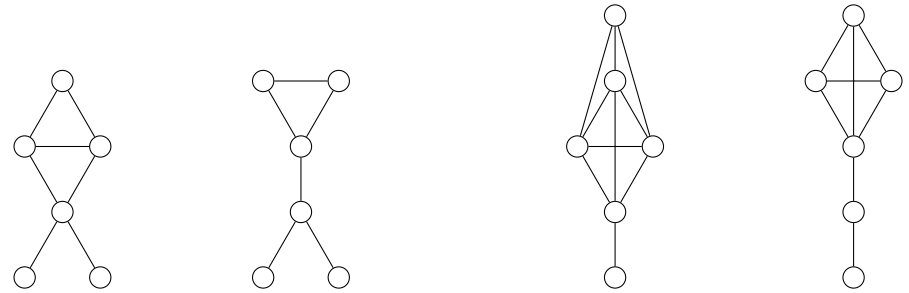


Figure 2: The two unlabeled connected graphs with 6 vertices with sibling number 1 and tuft number 2, and the two unlabeled connected graphs with 6 vertices with sibling number 2 and tuft number 1.

Graphs without siblings and graphs without vertices sharing the same open neighborhood were studied previously by several authors. Apparently, Sumner [10] was the first to formally introduce terminology. He calls a graph *point determining* if all of its vertices have distinct open neighborhoods, and *point distinguishing* if all of its vertices have distinct closed neighborhoods. He also notes that a graph is point distinguishing if and only if its complement is point determining.

Bull and Pease [2] re-introduced point determining graphs as 'mating graphs', to describe possible mating types of biological species. They provide the number of unlabeled point determining graphs with at most ten vertices, and ask for a general formula. Soon after, such a formula was supplied by Read [9], using the cycle index of graphs.

Jovović[5] then observed that the number of unlabeled connected point determining graphs with n vertices coincides with the number of unlabeled connected leafless graphs with n vertices, if $n \neq 2$. This was shown bijectively by Kilibarda [8]. A proof using

[5]cf. comments in www.oeis.org/A004108

combinatorial species building on Read's idea was then provided by Gessel and Li [4]. In fact, they show the following.

Theorem 2 (Kilibarda 2007, Gessel and Li 2011)**.** *The number of unlabeled connected point determining graphs with n vertices, the number of unlabeled connected point distinguishing graphs with n vertices, and the number of unlabeled connected leafless graphs with n vertices, coincide for $n \neq 2$.*

Gessel and Li used the language of combinatorial species that was introduced by Joyal [7, 6], and further developed by Bergeron, Labelle and Leroux [1], to provide an alternative proof of Kilibarda's result. We follow Gessel and Li's approach to prove Theorem 1. More precisely, we express the species of graphs with sibling number at most s and tuft number at most t as a composition of the species of graphs without siblings and a virtual species. It then turns out that this virtual species has an isomorphism type generating series which is obviously symmetric in s and t.

Since our main motivation was to exhibit a symmetry on graphs, let us mention some obstructions we encountered trying to find an explicit bijection. First of all, the sibling and the tuft number are not equidistributed on the set of (labeled) graphs. This fact also makes combinatorial species a natural tool to approach the problem. Although leaves cannot be adjacent to vertices having siblings in graphs other than K_2, it turns out that it is impossible to replace each group of siblings with a vertex having the appropriate number of leaves and vice versa. The reason is that the number of groups of siblings of maximal cardinality and the number of vertices adjacent to the maximal number of leaves are not equidistributed. In Section 10 we describe some tentative first steps towards a bijection.

However, we are able to prove the following refinement of Theorem 1. Let the *reduction* of a graph – other than K_2 – be the graph obtained by repeatedly removing all leaves and contracting each group of siblings to a single vertex. Trivially, the reduction is a leafless graph without siblings. Figure 3 provides an example of the reduction process.

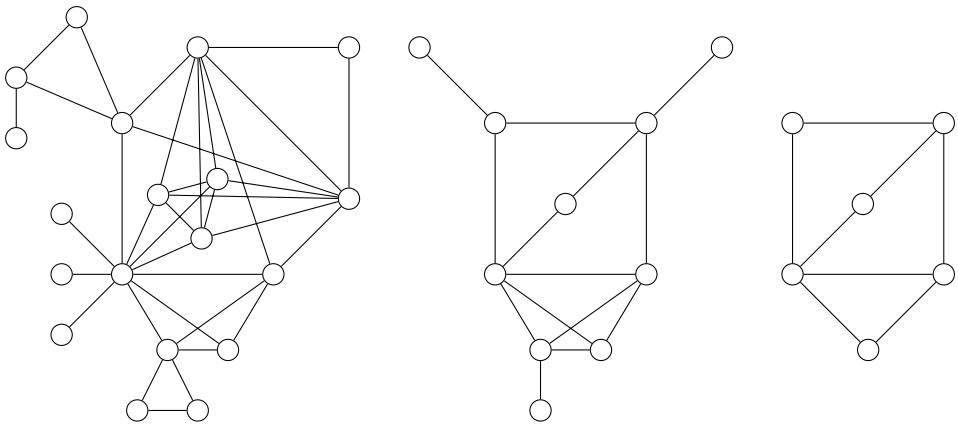


Figure 3: The graph on the left is reduced in two steps, each removing leaves and then contracting siblings, to the leafless point distinguishing graph depicted on the right.

Theorem 3. *Let R be a connected leafless point distinguishing graph. The sibling number and the tuft number have joint symmetric distribution on the set of unlabeled connected graphs with n vertices that reduce to R.*

The reduction operation has some attractive properties. For example, we show in Theorem 30 that a graph G contains an induced k-cycle if and only if the reduction of G contains an induced k-cycle, for $k \geqslant 4$. Together with the previous theorem, this implies that the sibling and the tuft number also have joint symmetric distribution on the set of connected chordal graphs, that is, graphs which do not contain an induced cycle with 4 or more vertices.

In a different direction, we show in Proposition 31 that the species of point distinguishing graphs reducing to a given leafless point distinguishing graph R can be expressed in terms of the species of point distinguishing graphs reducing to the single vertex graph. In particular, this implies that the enumeration of graphs with restricted sibling and restricted tuft number reducing to a graph R can be reduced to the case where R is the single vertex graph.

At the heart of our proof of Theorem 1 is a functional equation, expressing the species of graphs in terms of the species of point distinguishing graphs. As a further application, we exhibit another enumerative coincidence. A graph is *bi-point determining* if it is simultaneously point determining and point distinguishing. Equivalently, its automorphism group contains no transposition. Combining an expression for the species of bi-point determining graphs due to Gessel and Li [4, Cor. 4.7] with our functional equation, we find the following.

Theorem 4. *The number of unlabeled connected bi-point determining graphs with n vertices equals the number of unlabeled connected leafless point distinguishing graphs with n vertices.*

We do not have a bijective proof for this theorem, either.

Outline. In Section 2 we recall the main definitions and some results from the theory of combinatorial species, mostly to fix notation. In particular, in Examples 7, 8, 10 and 11 we introduce the species which appear in the following sections. In Section 3, we provide a decomposition of the species of graphs, essential for our approach, generalizing the functional equation used by Gessel and Li. As a first application, we prove Theorem 4 in Section 4. We use the decomposition again in Section 5 for the proof of Theorem 1. In the following two sections, we refine the decomposition to obtain Theorem 3. First, in Section 6, we show that removing leaves and contracting siblings in any order will produce the reduction of the graph. Then, in Section 7, we deduce Theorem 3. In Section 8, we show that induced cycles other than triangles are preserved by the reduction process. In particular, this implies that the sibling and the tuft number also have joint symmetric distribution on the set of unlabeled connected chordal graphs with n vertices. In Section 9, we provide a somewhat more explicit description of the species occurring in the decompositions used to prove our main theorems. Finally, in Section 10, we collect some observations that may help finding a bijective proof of Theorem 3.

2 Combinatorial Species

Combinatorial species were introduced by Joyal [6, 7] as a formal framework for enumeration. In this section, apart from briefly recalling the definitions, we also introduce the species appearing subsequently. For any details, we recommend Joyal's original articles and the textbook by Bergeron, Labelle and Leroux [1].

A *combinatorial species* is a functor from the category of finite sets with bijections to itself. Given a (finite) set of *labels* U, a species F produces a (finite) set $F[U]$ of *F-structures*. Moreover, given a bijection $\sigma : U \to V$ it produces a bijection $F[\sigma] : F[U] \to F[V]$, called the *relabeling* or *transport* of F-structures along σ. Often, the precise definition of relabeling for a particular species is obvious from context and therefore omitted. We regard two species F and G as *(combinatorially) equal*[6] if there is a natural isomorphism between F and G in the categorical sense.

The symmetric group $\mathfrak{S}_n$ acts on the set $F[n] \coloneqq F[\{1, 2, \ldots, n\}]$ by relabeling. The $\mathfrak{S}_n$-orbits under this action are called *isomorphism types of $F[n]$* or *unlabeled F-structures* of order (or size) n. Accordingly, two F-structures $a \in F[U]$ and $b \in F[V]$ are *isomorphic* if there is a bijection $\sigma : U \to V$ with $F[\sigma](a) = b$.

Example 5. The species of *(simple) graphs* is defined as follows. $\mathcal{G}[U]$ is the set of simple graphs with vertex set U. Unlabeled graphs are precisely the isomorphism types of $\mathcal{G}$.

The *exponential generating series* and the *isomorphism type generating series* associated with a species F are

$$F(x) \coloneqq \sum_{n \geqslant 0} \big|F[n]\big| \frac{x^n}{n!} \quad \text{and}$$
$$\widetilde{F}(x) \coloneqq \sum_{n \geqslant 0} \big|\{\text{isomorphism types of } F[n]\}\big| \, x^n,$$

respectively. Both are specializations of the *cycle index series*

$$Z_F \coloneqq \sum_{n \geqslant 0} \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} \operatorname{fix} F[\sigma] p_1^{\sigma_1} p_2^{\sigma_2} \ldots,$$

where $\operatorname{fix} F[\sigma]$ denotes the number of fixed points of $F[\sigma]$, p_k is the k-th power sum symmetric function, and σ_k is the number of k-cycles of σ.

Proposition 6. *The exponential generating series of a species is obtained from its cycle index series by specializing $p_1 = x$ and $p_k = 0$ for $k > 1$.*

The isomorphism type generating series of a species is obtained from its cycle index series by specializing $p_k = x^k$ for all $k \geqslant 1$.

A species F is a *subspecies* of a species G, if, for any set of labels, every F-structure is also a G-structure, and the relabeling bijections coincide. We denote the *restriction of*

[6] cf. [1, p. 21]

a species F to sets of cardinality m by F_m. The restrictions to sets of cardinality other than m, at least m, at most n and sets of cardinalities from m to n are denoted by $F_{\neq m}$, $F_{\geqslant m}$, $F_{\leqslant n}$ and $F_{m\leqslant\bullet\leqslant n}$, respectively.

Perhaps the most fundamental species is the *species of sets* E, which produces a single structure for any set of labels. The species E_0 is usually denoted by 1, and the species E_1 is usually denoted by X and referred to as the *singleton species*. We have $E(x) = \exp x$, $\widetilde{E}(x) = \frac{1}{1-x}$, and

$$Z_E = \exp\left(\sum_{k>0} \frac{p_k}{k}\right).$$

The zero species, producing no structure for any set of labels, is denoted by 0.

Example 7. Recall that a *point distinguishing graph* is a graph without siblings. We define $\mathcal{D}^{\mathrm{c}}[U]$ as the set of connected point distinguishing graphs with vertex set U. For a given connected point distinguishing graph $D \in \mathcal{D}^{\mathrm{c}}[U]$ and a bijection $\sigma : U \to V$, the graph $\mathcal{D}^{\mathrm{c}}[\sigma](D)$ is obtained from D by replacing the vertex labeled u with a vertex labeled $\sigma(u)$. Thus, the species of connected point distinguishing graphs $\mathcal{D}^{\mathrm{c}}$ is a subspecies of the species $\mathcal{G}^{\mathrm{c}}$ of connected graphs.

A *point determining graph* is a graph without vertices sharing the same open neighborhood. A *bi-point determining graph* is a graph which is point distinguishing and point determining. Thus, the species of bi-point determining graphs $\mathcal{B}^{\mathrm{c}}$ is the subspecies of $\mathcal{D}^{\mathrm{c}}$ whose structures are also point determining.

A *multisort species of k sorts* is a functor from the category whose objects are k-tuples of finite sets (short: 'k-sets') and whose morphisms are k-tuples of bijections, to the category of finite sets with bijections. Given a k-set $(U_1, \ldots, U_k)$, the elements of each set U_i are referred to as the *labels of sort i*. The concepts introduced for 1-sort species carry over to the multisort context in the obvious way.

We denote by X, Y, and Z the singleton species of three different sorts. That is, given a 3-set $U = (U_1, U_2, U_3)$, the set $X[U]$ contains a single structure if U_1 has one element and U_2 and U_3 are empty. Otherwise, $X[U]$ is empty. For convenience, we refer to labels of sort 1 as labels of sort X, etc. To emphasize that a species F has, for example, 3 sorts, we sometimes write $F(X, Y, Z)$. This notation is compatible with the composition of species defined below. However, we alert the reader that by abuse of notation X denotes both a 1-sort singleton species and a multisort singleton species.

In the following definitions, the addition of k-sets always refers to their component-wise disjoint union.

Example 8. The species $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, Y, Z)$ of *connected 3-sort graphs*, with leaves of sort Y and siblings of sort Z, is defined as follows. Given a 3-set $U = (U_1, U_2, U_3)$, let $\mathcal{G}^{\mathrm{c}}_{\neq 2}[U]$ be the set of connected graphs with vertex set $U_1 + U_2 + U_3$, such that the set of leaves is U_2, the set of vertices having siblings is U_3, and U_1 is the set of remaining vertices.

The complete graph with two vertices, K_2, is the unique connected graph that has a leaf which is simultaneously a sibling. Thus, there is no $\mathcal{G}^{\mathrm{c}}_{\neq 2}$-structure isomorphic to K_2.

The isomorphism types of $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, Y, Z)$ with at most three vertices and the corresponding isomorphism types of $\mathcal{G}^{\mathrm{c}}(X)$ are depicted in Figure 4.

Note that $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X, X) = \mathcal{G}^{\mathrm{c}}_{\neq 2}(X)$, and $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X, 0)$ is the species of connected point distinguishing graphs $\mathcal{D}^{\mathrm{c}}$, whereas $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, 0, 0)$ is the species of connected leafless point distinguishing graphs.

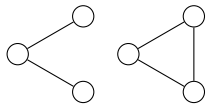
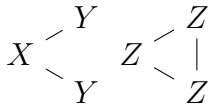
	0	1	2	3	⋯
$\mathcal{G}^{\mathrm{c}}(X)$	$\emptyset$				⋯
$\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, Y, Z)$	$\emptyset$	X	$\emptyset$		⋯

Figure 4: The first few isomorphism types of the species of connected graphs $\mathcal{G}^{\mathrm{c}}(X)$ and the species of connected 3-sort graphs $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, Y, Z)$. In the multisort case, we indicate the sorts in illustrations by the corresponding letters.

We will make use of the sum, the product and the composition of two species. The set of structures of the *sum* of two species F and G is the disjoint union of the set of F-structures and the set of G-structures,

$$(F + G)[U] \coloneqq F[U] + G[U].$$

The set of structures of the *product* of F and G is

$$(F \cdot G)[U] \coloneqq \sum_{U=V+W} F[V] \times G[W],$$

where the sum is over all ordered set partitions of U into two (possibly empty) parts. Finally, let F be a 1-sort species and let G be a k-sort species whose restriction to the empty set is zero. Then the set of structures on the k-set U of the *(partitional) composition* of F and G is

$$(F \circ G)[U] \coloneqq \sum_{\pi \in \mathrm{Par}[U]} F[\pi] \times \prod_{B \in \pi} G[B],$$

where the sum is over all set partitions of U into non-empty blocks. In other words, a structure in $\mathrm{Par}[(U_1, \ldots, U_k)]$ is a set of k-tuples, each of which has at least one non-empty component, whose component-wise union is U. The composition $F(G_1, \ldots, G_m)$ of an m-sort species F with m species $G_1, \ldots, G_m$ is defined similarly.

Example 9. Let F and G be species. Then $E(F) \cdot E(G) = E(F + G)$.

Example 10. A *tuft* is a structure consisting of a designated *root* of sort X and a non-empty set of leaves of sort Y. Thus, the species of tufts equals

$$\mathcal{T}(X, Y) \coloneqq X E_{\geqslant 1}(Y).$$



Figure 5: A tuft

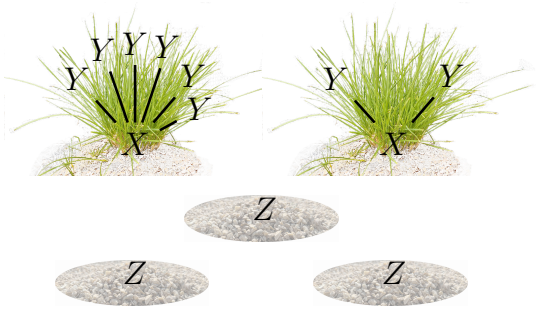


Figure 6: A patch

Example 11. A *patch* is a non-empty structure consisting of a possibly empty set of tufts together with a possibly empty set of additional leafless *roots*, subject to the following rule: if there is precisely one leafless root, it is of sort X, otherwise the leafless roots are of sort Z. In particular, the roots of a patch are exactly the vertices of sort X and Z. Thus, the species of patches equals

$$\mathcal{P}(X,Y,Z) \coloneqq (1 + X + E_{\geqslant 2}(Z)) \cdot (E \circ \mathcal{T}) - 1.$$

The following proposition summarizes how the operations on species interact with passing to the different types of generating series.

Proposition 12. *Let F and G be species. Then,*

$$\begin{aligned} (F+G)(x) &= F(x) + G(x), & (F \cdot G)(x) &= F(x)G(x), \\ \widetilde{(F+G)}(x) &= \widetilde{F}(x) + \widetilde{G}(x), & \widetilde{(F \cdot G)}(x) &= \widetilde{F}(x)\widetilde{G}(x), \\ Z_{F+G} &= Z_F + Z_G & Z_{F\cdot G} &= Z_F Z_G. \end{aligned}$$

Moreover, provided that the restriction of G to the empty set is zero, $(F \circ G)(x) = F(G(x))$ and $\widetilde{(F \circ G)}(x)$ is obtained from Z_F by substituting $\widetilde{G}(x^k)$ for p_k.[7]

A species F is *molecular* if any two F-structures are isomorphic. The zero species 0, producing no structure for any set of labels, is trivially molecular.

Example 13. Given a graph R, define a species $\mathcal{R}$ such that the structures $\mathcal{R}[U]$ are the graphs isomorphic to R with vertex set U. Then $\mathcal{R}$ is molecular. Note that the two species obtained in this way from the edgeless graph with n vertices and the complete graph with n vertices are equal.

Any species can be written as a sum of molecular species, and this *molecular decomposition* is uniquely determined. Put differently, two species are equal if and only if the

[7] More generally, $Z_{F\circ G}$ is known as the plethysm of the symmetric functions Z_F and Z_G, but we will not use this notion.

coefficients in their molecular expansions coincide. We define a *virtual (k-sort) species* as a formal difference of two (k-sort) species, up to the natural equivalence relation. Thus, the coefficients of the molecular expansion of a virtual species can be arbitrary integers.

Similar to the common practice of providing the first few Taylor coefficients of a formal power series, it may be helpful for developing some intuition to display the first few terms of the molecular decomposition of a species.

Virtual species allow us to define the *multiplicative inverse* and *compositional inverse* of a species, subject to a natural condition.

Theorem 14 ([1, Exc. 2.5.7., Prop. 2.5.19])**.** *A virtual species has a multiplicative inverse if its restriction to the empty set equals the species* 1 *or* -1*. A* 1*-sort virtual species* F *has a compositional inverse* $F^{(-1)}$ *if its restriction to the empty set is the zero species and its restriction to sets of cardinality* 1 *is the species* X *or* $-X$*.*

Example 15.

1. The species of sets E satisfies the condition of the first part of the theorem, so its multiplicative inverse exists. By Example 9, it is given by $E(-X)$. Its molecular decomposition begins with

$$1 - X - E_2 + X^2 - E_3 + 2XE_2 - X^3 - E_4 + 2XE_3 + E_2^2 - 3X^2E_2 + X^4 + \dots$$

2. The molecular decomposition of the compositional inverse of the species of non-empty sets $E_{\geqslant 1}$, also known as the *combinatorial logarithm* Ω, begins with

$$X - E_2 - E_3 + XE_2 - E_4 + E_2 \circ E_2 + XE_3 - X^2E_2 + \dots$$

   The isomorphism type generating series of Ω is $\widetilde{\Omega}(x) = x - x^2$, by the following reasoning. Note that $\big(E_{\geqslant 1}(X - X^2)\big)^{\sim}(x) = \widetilde{E}(x)/\widetilde{E}(x^2) - 1 = \frac{1-x^2}{1-x} - 1 = x$. Taking into account that the isomorphism type generating series of a composition $F \circ G$ only depends on $\widetilde{G}(x)$ by Proposition 12, we obtain

$$\widetilde{\Omega}(x) = \big(\Omega \circ E_{\geqslant 1}(X - X^2)\big)^{\sim}(x) = x - x^2.$$

3. The compositional inverse of $X - X^2$ is the species of ordered rooted trees $\mathcal{A}$ with labels on all vertices [1, Eq. (1.1.27)]. This follows from the decomposition of an ordered rooted tree as a root and a tuple of ordered rooted trees, which gives the equality of species $\mathcal{A} = X/(1 - \mathcal{A})$. Rearranging gives $\mathcal{A} - \mathcal{A}^2 = X$.

3 A Decomposition of Graphs

In this section, we generalize a functional equation discovered by Gessel and Li to take siblings into account. Using the notation introduced in Section 2, the two intermediate steps [9, Eq. (2.2)] and [4, Thm. 2.2], and [4, Thm. 3.1] on which Gessel and Li's argument is based, read as follows.

Proposition 16 (cf. Read 1989)**.** *The species of connected point distinguishing graphs $\mathcal{D}^{\mathrm{c}}$ and the species of connected graphs $\mathcal{G}^{\mathrm{c}}$ are related by the equality*

$$\mathcal{D}^{\mathrm{c}} \circ E_{\geqslant 1} = \mathcal{G}^{\mathrm{c}}.$$

Proposition 17 (Gessel & Li 2011)**.** *The species of connected graphs other than K_2, with leaves of sort X or Y, and other vertices of sort X equals*

$$\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X+Y, X) = \mathcal{G}^{\mathrm{c}}\big(XE(Y)\big) - XY - E_2(X).$$

We remark that the two error terms on the right-hand side differ from the result of Gessel and Li only because we restrict the species $\mathcal{G}^{\mathrm{c}}_{\neq 2}$ to structures whose size is not equal to 2.

Combining Propositions 16 and 17 we obtain the equation

$$\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X+Y, X) = \mathcal{D}^{\mathrm{c}} \circ E_{\geqslant 1}\big(XE(Y)\big) - XY - E_2(X),$$

which is the key ingredient of Gessel and Li's proof of Theorem 2. Our goal is to generalize this decomposition so that we can also keep track of siblings. Recall that $\mathcal{P}$ denotes the species of patches defined in Example 11.

Theorem 18 (Patch Decomposition of Graphs)**.** *The species of connected graphs other than K_2, with leaves of sort X or Y, siblings of sort Z, and other vertices of sort X equals*

$$\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X+Y, Z) = \mathcal{D}^{\mathrm{c}} \circ \mathcal{P} - XY - E_2(Z).$$

This functional equation reflects the fact that the vertices of any graph can be partitioned into leaves, siblings and other vertices. In principle, this partition can be refined to also distinguish non-leaf vertices which share the same open neighborhood with some other vertex [3]. It would be interesting to find a functional equation that exploits this refinement.

At the heart of the patch decomposition are the underlying point distinguishing graph and the corresponding patch partition of a $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X+Y, Z)$-structure G. Before stating precise definitions, we provide an informal description. The underlying point distinguishing graph of G is obtained by removing all leaves of sort Y, and then contracting each group of siblings in the resulting graph, ignoring whether vertices are of sort X or Z, to a single vertex. Each block of the patch partition corresponds to a vertex in this graph and consists of the siblings contracted to this vertex together with the adjacent leaves that were removed in the first step. A visualisation is provided in Figure 7.

Note that the underlying point distinguishing graph of a $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X+Y, Z)$-structure may have leaves, but cannot have siblings. Consider, for example, the path graph with $n \geqslant 4$ vertices with both leaves of sort Y and inner vertices of sort X. If $n \geqslant 5$, the underlying point distinguishing graph is the path graph with $n-2$ vertices. By contrast, if $n = 4$, removing the leaves we obtain K_2, which consists of two siblings. Thus, the underlying point distinguishing graph is a single vertex.

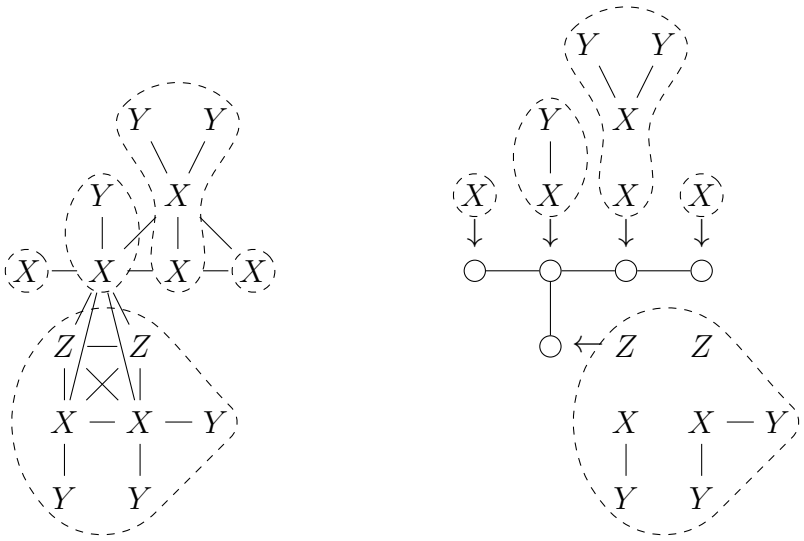


Figure 7: Decomposing a $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X+Y, Z)$-structure into its underlying point distinguishing graph and an assignment of patches to its vertices.

To define the underlying point distinguishing graph and the patch partition precisely, we introduce two maps. For a set L of leaves of a graph G, let $\lambda_L(G)$ be the graph obtained from G by removing L. Moreover, let $\rho(G)$ be the graph obtained from G by contracting each group of siblings to a single vertex. Note that $\rho(G)$ is point distinguishing.

Given $G \in \mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X+Y, Z)[U]$, with $U = (U_1, U_2, U_3)$, its *patch partition* $\left(\pi, (P_B)_{B\in\pi}\right)$ consists of a set partition $\pi \in \mathrm{Par}[U]$ and, for each block $B \in \pi$, a patch $P_B \in \mathcal{P}[B]$. Each block B corresponds to a triple (A, L, R) with $A \subseteq U_1$, $L \subseteq U_2$, $R \subseteq U_3$, such that $A + R$ is a maximal group of siblings of $\lambda_{U_2}(G)$, and L are the leaves of sort Y adjacent in G to a vertex in A. The patch P_B has leaves L and roots $A + R$. The adjacencies in the patch are precisely the adjacencies in G between vertices in A and L. Finally, the *underlying point distinguishing graph* of G is $\rho \circ \lambda_{U_2}(G) \in \mathcal{D}^{\mathrm{c}}[\pi]$.

Proof of Theorem 18, the Patch Decomposition. Let $U = (U_1, U_2, U_3)$ be a 3-set of labels. By the definition of composition, a structure in $(\mathcal{D}^{\mathrm{c}} \circ \mathcal{P})[U]$ is a triple $\left(\pi, D, (P_B)_{B\in\pi}\right)$ with $\pi \in \mathrm{Par}[U]$, $D \in \mathcal{D}^{\mathrm{c}}[\pi]$ and $P_B \in \mathcal{P}[B]$ for each $B \in \pi$.

We have to exhibit an equivariant bijection between these triples and graphs $G \in \mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X + Y, Z)[U]$, whose leaves can be of sort X or Y, with exceptions for $|U_1| = |U_2| = 1$, $U_3 = \emptyset$ and for $U_1 = U_2 = \emptyset$, $|U_3| = 2$.

Given the triple, the graph G is obtained from the disjoint union of the patches $(P_B)_{B\in\pi}$ as follows. For each block $B \in \pi$, we add edges between all the roots of P_B. Additionally, we add edges between all roots of P_B and $P_{B'}$ if B and B' are adjacent in D.

Let us first check that this yields an element G in $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X + Y, Z)[U]$. By the definition of a patch, only leaves may be of sort Y.

Since a patch P_B contains either no, or at least two vertices of sort Z, vertices of sort Z cannot be leaves in G, provided that there is at least one other root in the same

patch or in a patch adjacent to P_B. The exceptional case of an $\mathcal{D}^{\mathrm{c}} \circ \mathcal{P}$-structure whose image has leaves of sort Z and thus does not correspond to a $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X+Y, Z)$-structure is illustrated on the left of Figure 8.

Thus, it remains to show that precisely the vertices of sort Z within a block are siblings in G. Two vertices in the same block B are siblings in G if and only if they are both of sort Z, unless D is a single vertex and P_B is a single tuft with a single leaf. The exceptional case of an $\mathcal{D}^{\mathrm{c}} \circ \mathcal{P}$-structure whose image has siblings of sort other than Z is illustrated on the right of Figure 8.

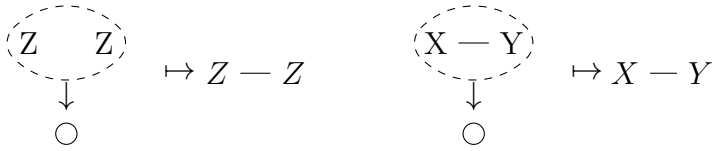


Figure 8: The two types of $\mathcal{D}^{\mathrm{c}} \circ \mathcal{P}$-structures that do not correspond to $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X+Y, Z)$-structures.

So it suffices to show that $u \in B$ and $u' \in B'$ with $B \neq B'$ are not siblings in G. If one of them is a leaf of its patch, its only neighbor lies in the same block, so they are not siblings. We may therefore assume that both are roots. If B and B' are not adjacent in D, then u and u' are not adjacent in G and therefore not siblings. If B and B' are adjacent in D, the closed neighborhoods of B and B' must be distinct because D has no siblings. Without loss of generality, suppose that B'' is a neighbor of B but not of B'. Then, any root in $P_{B''}$ is a neighbor of u but not of u', so u and u' are not siblings.

Next, we check that the patch partition of G is $\big(\pi, (P_B)_{B\in\pi}\big)$, and the underlying point distinguishing graph of G equals D. Recall that $\lambda_{U_2}(G)$ is obtained from G by removing the leaves of sort Y. Since the adjacencies in $\lambda_{U_2}(G)$ of roots of sort X and roots of sort Z within a block are exactly the same, each maximal group of siblings in $\lambda_{U_2}(G)$ consists exactly of the roots of one block. It follows that D equals $\rho \circ \lambda_{U_2}(G)$.

Conversely, the patch partition and the underlying point distinguishing graph determine, for each $\mathcal{G}_{\neq 2}$-structure, a triple $\big(\pi, D, (P_B)_{B\in\pi}\big)$. It is clear that assembling the patches in the patch partition according to the adjacencies of the underlying point distinguishing graph reconstructs the original graph. Hence, we have a bijection between $\mathcal{D}^{\mathrm{c}} \circ \mathcal{P}$-structures and $\mathcal{G}^{\mathrm{c}}_{\neq 2}$-structures. The bijection intertwines with relabeling, since its definition does not involve any choice depending on the labels. □

4 Bi-Point-Determining Graphs

Gessel and Li also study bi-point determining graphs. In particular, they provide the following expression for the species of connected bi-point determining graphs [4, Cor. 4.7].

Theorem 19 (Gessel & Li 2011)**.** *The species $\mathcal{B}^{\mathrm{c}}$ of connected bi-point determining graphs equals*

$$\mathcal{B}^{\mathrm{c}} = \mathcal{G}^{\mathrm{c}}(2\Omega - X) - \Omega + X.$$

Combining the patch decomposition with this theorem we can deduce Theorem 4, that is, the number of unlabeled connected leafless point distinguishing graphs coincides with the number of bi-point-determining graphs. It would be interesting to find an explicit bijection demonstrating this fact.

Proof of Theorem 4. The species of connected leafless point distinguishing graphs is equal to $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X,0,0)$. We want to compare its isomorphism type generating series with the isomorphism type generating series of $\mathcal{B}^{\mathrm{c}} = \mathcal{G}^{\mathrm{c}}(2\Omega - X) - \Omega + X$. Setting $Y = -X$ and $Z = 0$ in the Patch Decomposition from Theorem 18 and using Proposition 16 we obtain

$$\begin{aligned}\mathcal{G}^{\mathrm{c}}_{\neq 2}(X,0,0) &= \mathcal{D}^{\mathrm{c}} \circ \mathcal{P}(X,-X,0) + X^2 \\ &= \mathcal{G}^{\mathrm{c}} \circ \Omega \circ \mathcal{P}(X,-X,0) + X^2.\end{aligned}$$

By Proposition 12, the isomorphism type generating series of two compositions $F \circ G$ and $F \circ H$ are equal if $\widetilde{G}(x) = \widetilde{H}(x)$. Thus, comparing with Theorem 19, it suffices to show that

$$\begin{aligned}\big(2\Omega - X\big)^{\sim}(x) &= \big(\Omega \circ \mathcal{P}(X,-X,0)\big)^{\sim}(x) \quad \text{and} \\ \big(-\Omega + X\big)^{\sim}(x) &= x^2.\end{aligned}$$

Recall from Example 15 (2) that $\widetilde{\Omega}(x) = x - x^2$, which implies the second equality. To show the first equality we will additionally use $\big(E(X - X^2)\big)^{\sim}(x) = 1 + x$ and $\big(XE_{\geqslant 1}(-X)\big)^{\sim}(x) = -x^2$ from the same example.

By definition, $\mathcal{P}(X,-X,0) = (1+X) \cdot E\big(XE_{\geqslant 1}(-X)\big) - 1$. Therefore, again substituting different species with the same isomorphism type generating series in the equation,

$$\begin{aligned}\big(\mathcal{P}(X,-X,0)\big)^{\sim}(x) &= \big(E(X - X^2) \cdot E(-X^2) - 1\big)^{\sim}(x) \\ &= \big(E_{\geqslant 1}(X - 2X^2)\big)^{\sim}(x).\end{aligned}$$

This implies $\big(\Omega \circ \mathcal{P}(X,-X,0)\big)^{\sim}(x) = x - 2x^2 = (2\Omega - X)^{\sim}(x)$. □

5 Symmetry of the Sibling Number and the Tuft Number

In this section, we prove Theorem 1. Let us first refine the Patch Decomposition from Theorem 18 to take the sibling number into account. To do so, let $\mathcal{G}^{\mathrm{c},s}_{\neq 2}$ be the subspecies of the species of connected 3-sort graphs $\mathcal{G}^{\mathrm{c}}_{\neq 2}$ with sibling number at most s and let $\mathcal{P}^s$ be the subspecies of the species of patches with sibling number at most s:

$$\mathcal{P}^s(X,Y,Z) \coloneqq (1 + X + E_{2 \leqslant \bullet \leqslant 1+s}(Z)) \cdot (E \circ \mathcal{T}) - 1.$$

Moreover, we use the Iverson bracket $[s > 0] \coloneqq \begin{cases} 1 & \text{if } s > 0, \\ 0 & \text{otherwise.} \end{cases}$

Corollary 20. *The species of connected graphs other than K_2, with leaves of sort X or Y, siblings of sort Z, other vertices of sort X, and restricted sibling number equals*

$$\mathcal{G}^{\mathrm{c},s}_{\neq 2}(X, X+Y, Z) = \mathcal{D}^{\mathrm{c}} \circ \mathcal{P}^s - XY - [s>0]E_2(Z).$$

Proof. Let $U = (U_1, U_2, U_3)$ be a 3-set of labels. By the Patch Decomposition from Theorem 18 we have an equivariant bijection between graphs $G \in \mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X+Y, Z)[U]$ and triples $\big(\pi, D, (P_B)_{B\in\pi}\big)$ with $\pi \in \mathrm{Par}[U]$, $D \in \mathcal{D}^{\mathrm{c}}[\pi]$ and $P_B \in \mathcal{P}[B]$ for each $B \in \pi$, with the exception of $(\mathcal{D}^{\mathrm{c}} \circ \mathcal{P})$-structures of size 2.

We have shown that each group of siblings of G correspond to the roots of sort Z in a patch. Thus, the sibling number of G is at most s if and only if $P_B \in \mathcal{P}^s[B]$ for each $B \in \pi$.

The exceptional $(\mathcal{D}^{\mathrm{c}} \circ \mathcal{P}^s)$-structures of size 2 are depicted in Figure 8. If $s = 0$, the unique $(\mathcal{D}^{\mathrm{c}} \circ \mathcal{P}^s)$-structure of size 2 is a single tuft. Otherwise, if $s > 0$, there is an additional structure consisting of two vertices of sort Z. □

It remains to take into account the tuft number. One might expect that this can be achieved by restricting the tuft number of each tuft appearing in $\mathcal{P}^s$. This is not the case, because $\mathcal{G}^{\mathrm{c},s}_{\neq 2}(X, X+Y, Z)$ may have leaves of sort X.

Instead, we first reduce the problem to the enumeration of connected 3-sort graphs with bounded sibling number and tuft number equal to 1, using a suitable substitution of virtual species. In a second step, we replace each tuft in a graph with tuft number 1 with a tuft having at most t leaves.

Lemma 21. *Let H be a set of connected graphs other than K_2, closed under replacing each set of leaves adjacent to the same vertex with any positive number of leaves adjacent to this vertex, provided that the resulting graph is different from K_2. Let $\mathcal{H}_{\neq 2}$ be the subspecies of $\mathcal{G}^{\mathrm{c}}_{\neq 2}$ whose structures are isomorphic to a graph in H. Let $\mathcal{H}^t_{\neq 2}$ be the subspecies of $\mathcal{H}_{\neq 2}$ whose structures have tuft number at most t. Finally, let $\mathcal{Y}_t = E_{1\leqslant\bullet\leqslant t}(Y)$.*

Then, if H contains the star graphs with at least three vertices,

$$\mathcal{H}^t_{\neq 2}(X, Y, Z) = \mathcal{H}_{\neq 2}(X, \Omega(\mathcal{Y}_t), Z) + X\Omega(\mathcal{Y}_t) - [t>0]XY,$$

whereas otherwise,

$$\mathcal{H}^t_{\neq 2}(X, Y, Z) = \mathcal{H}_{\neq 2}(X, \Omega(\mathcal{Y}_t), Z).$$

Proof. Suppose first that H contains the star graphs with at least three vertices. Then any graph in $\mathcal{H}^t_{\neq 2}[U]$, with the exception of the star graphs, can be obtained from a graph in $\mathcal{H}^1_{\neq 2}$ by replacing each tuft with a tuft having at least one and at most t leaves. The star graphs in $\mathcal{H}^t_{\neq 2}[U]$ consist of a single vertex of sort X together with at least two and at most t leaves of sort Y. Therefore, setting $\mathcal{Y}_t \coloneqq E_{1\leqslant\bullet\leqslant t}(Y)$ and using that $E_{2\leqslant\bullet\leqslant t}(Y) = \mathcal{Y}_t - [t>0]Y$, we obtain

$$\mathcal{H}^t_{\neq 2}(X, Y, Z) = \mathcal{H}^1_{\neq 2}(X, \mathcal{Y}_t, Z) + X\mathcal{Y}_t - [t>0]XY. \tag{1}$$

Setting $t = \infty$ in this equation yields

$$\mathcal{H}_{\neq 2}(X, Y, Z) = \mathcal{H}^1_{\neq 2}(X, E_{\geqslant 1}(Y), Z) + XE_{\geqslant 1}(Y) - XY.$$

Substituting $\Omega(\mathcal{Y}_t)$ for Y we obtain

$$\mathcal{H}_{\neq 2}(X, \Omega(\mathcal{Y}_t), Z) = \mathcal{H}^1_{\neq 2}(X, \mathcal{Y}_t, Z) + X\mathcal{Y}_t - X\Omega(\mathcal{Y}_t). \tag{2}$$

Therefore,

$$\begin{aligned}\mathcal{H}^t_{\neq 2}(X, Y, Z) &\overset{(1)}{=} \mathcal{H}^1_{\neq 2}(X, \mathcal{Y}_t, Z) + X\mathcal{Y}_t - [t > 0]XY \\ &\overset{(2)}{=} \mathcal{H}_{\neq 2}(X, \Omega(\mathcal{Y}_t), Z) + X\Omega(\mathcal{Y}_t) - [t > 0]XY.\end{aligned}$$

If H does not contain the star graphs on at least three vertices the computation simplifies, and we obtain

$$\mathcal{H}^t_{\neq 2}(X, Y, Z) = \mathcal{H}_{\neq 2}(X, \Omega(\mathcal{Y}_t), Z). \qquad \square$$

Lemma 22. *Let $\mathcal{Q}^{s,t}$ be the virtual species*

$$\mathcal{Q}^{s,t}(X, Y, Z) \coloneqq \big(1 + X + E_{2\leqslant\bullet\leqslant 1+s}(Z)\big)E\Big(X\big(E_{\leqslant t}(Y)E(-X) - 1\big)\Big) - 1.$$

Then

$$\mathcal{P}^s\big(X, \Omega(\mathcal{Y}_t) - X, Z\big) = \mathcal{Q}^{s,t}(X, Y, Z).$$

Proof. Recall that $\mathcal{P}^s(X, Y, Z) = (1 + X + E_{2\leqslant\bullet\leqslant 1+s}(Z)) \cdot (E \circ \mathcal{T}) - 1$ with $\mathcal{T}(X, Y) = XE_{\geqslant 1}(Y)$. Thus, we compute using Example 9

$$\begin{aligned}E_{\geqslant 1}\big(\Omega(\mathcal{Y}_t) - X\big) &= E\big(\Omega(\mathcal{Y}_t) - X\big) - 1 \\ &= E\big(\Omega(\mathcal{Y}_t)\big)E(-X) - 1 \\ &= (1 + \mathcal{Y}_t)E(-X) - 1 \\ &= E_{\leqslant t}(Y)E(-X) - 1,\end{aligned}$$

which implies the claim. $\square$

Theorem 23. *The species of connected graphs other than K_2, with leaves of sort Y, siblings of sort Z, other vertices of sort X, and with restricted sibling and tuft number equals*

$$\mathcal{G}^{\mathrm{c},s,t}_{\neq 2}(X, Y, Z) = \mathcal{D}^{\mathrm{c}} \circ \mathcal{Q}^{s,t}(X, Y, Z) + X^2 - [t > 0]XY - [s > 0]E_2(Z).$$

Proof. We apply Lemma 21 in the case where $\mathcal{H}_{\neq 2} = \mathcal{G}^{\mathrm{c},s}_{\neq 2}$ is the species of connected graphs other than K_2 with sibling number at most s. The closure property holds because replacing a positive number of leaves adjacent to a vertex by another positive number does not affect the sibling number, unless the resulting graph is a K_2.

The star graphs with at least three vertices have sibling number zero, so the first equation in Lemma 21 applies. After setting $Y = \Omega(\mathcal{Y}_t) - X$ in Corollary 20, the claim follows from Lemma 22. $\square$

We can now prove that the sibling and the tuft number have joint symmetric distribution on the set of unlabeled connected graphs with n vertices. In fact, we show that the isomorphism type generating series of $\mathcal{G}_{\neq 2}^{\mathrm{c},s,t}(X,X,X)$ is symmetric in s and t.

Lemma 24. *The isomorphism type generating series of the virtual species $\mathcal{Q}^{s,t}(X,X,X)$ is*

$$\widetilde{\mathcal{Q}^{s,t}}(x) = \frac{(1-x^{s+2})(1-x^{t+2})}{1-x} - 1.$$

The isomorphism type generating series of the virtual species

$$X^2 - [t>0]X^2 - [s>0]E_2$$

is $x^2 - [t>0]x^2 - [s>0]x^2$.

In particular, these generating series are symmetric in s and t.

Proof. The first factor in $\mathcal{Q}^{s,t}(X,X,X)+1$ is $1+X+E_{2\leqslant\bullet\leqslant 1+s} = E_{\leqslant 1+s}$ and its isomorphism type generating series is

$$\widetilde{E_{\leqslant 1+s}}(x) = (1-x^{s+2})/(1-x).$$

To compute the isomorphism type generating series of the second factor, we first set $\mathcal{F}^t \coloneqq X(E_{\leqslant t}(X)\cdot E(-X)-1)$ and find that

$$\widetilde{\mathcal{F}^t}(x) = x\left(\frac{1-x^{t+1}}{1-x}\cdot(1-x)-1\right) = -x^{t+2}.$$

We now recall that the cycle index series of E equals $Z_E = \exp\left(\sum_{k>0}\frac{p_k}{k}\right)$. Substituting $p_k = -x^{k(t+2)}$ we obtain, in accordance with Proposition 12,

$$\widetilde{E(\mathcal{F}^t)}(x) = \exp\left(-\sum_{k>0}\frac{x^{k(t+2)}}{k}\right) = 1-x^{t+2},$$

which finishes the computation of $\widetilde{\mathcal{Q}^{s,t}}(x)$. □

Proof of Theorem 1. By Theorem 23 and Lemma 24, the isomorphism type generating series of $\mathcal{G}_{\neq 2}^{\mathrm{c},s,t}(X,X,X)$ is symmetric in s and t.

Since the species of graphs other than K_2 with sibling number s and tuft number t equals

$$\mathcal{G}_{\neq 2}^{\mathrm{c},s,t} - \mathcal{G}_{\neq 2}^{\mathrm{c},s-1,t} - \mathcal{G}_{\neq 2}^{\mathrm{c},s,t-1} + \mathcal{G}_{\neq 2}^{\mathrm{c},s-1,t-1},$$

the claim follows for $n \neq 2$. For $n=2$, we have $s(K_2) = t(K_2) = 1$. □

6 The Reduction of a Graph

In this section, we show that the reduction of a graph, as defined in the introduction, and the reduction of the same graph with some leaves removed coincide. In particular, we show that the reduction of the underlying point distinguishing graph equals the reduction of the original graph.

In fact, we will prove a slight generalization of this statement. Recall from Section 3 that $\lambda_L(G)$ is the graph obtained from G by removing a set of leaves L, and $\rho(G)$ is the graph obtained from G by contracting each group of siblings to a single vertex. For convenience, let λ without subscript denote the map removing all leaves of a graph. Note that $\rho(G)$ cannot be isomorphic to K_2 and that $\lambda_L(G)$ has at least one vertex if G is not isomorphic to K_2.

Theorem 25. *Let G be a connected graph other than K_2 and let U be a subset of its leaves. Then there exists a set of leaves V of $\rho \circ \lambda(G)$ such that*

$$\rho \circ \lambda \circ \rho \circ \lambda_U(G) = \rho \circ \lambda_V \circ \rho \circ \lambda(G).$$

One can actually show that the reduction of a graph can also be obtained by repeatedly cutting off any single leaf from a graph other than K_2 and reducing the size of any group of siblings by one, in any order. However, we do not need this statement, so we content ourselves with the above.

Theorem 25 is a simple consequence of the following lemma.

Lemma 26. *Let H be a connected graph other than K_2 and let L be a subset of its leaves. Then*

$$\rho \circ \lambda_L(H) = \rho \circ \lambda_L \circ \rho(H).$$

Proof. We partition the set of vertices of $\lambda_L(H)$ into maximal groups of siblings $\{S_i \mid i \in I\}$. Each set S_i corresponds to a triple (P_i, L_i, R_i) of (possibly empty) sets of vertices in H, where $L_i \subseteq L$ is the set of leaves in L of H adjacent to S_i, $P_i \subseteq S_i$ is the set of vertices adjacent to a leaf in L_i in H and $R_i = S_i \setminus P_i$. These sets partition the set of vertices of H.

Let us first show that R_i is a maximal group of siblings of H for all $i \in I$. Let $x \in R_i$ and let $y \neq x$ be a sibling in H. In a graph other than K_2, siblings cannot be leaves, so x and y are both vertices in $\lambda_L(H)$. Moreover, in a graph other than K_2, siblings cannot be adjacent to leaves. Thus, the map λ_L preserves neighborhoods of siblings, and x and y are also siblings in $\lambda_L(H)$. Since $S_i = P_i \cup R_i$ is a maximal group of siblings in $\lambda_L(H)$, $y \in S_i$. Finally, $y \notin P_i$ because it is a sibling of x in H.

It follows that the vertices of $\rho(H)$ can be partitioned into pairs of sets (L_i, S_i'), with

$$S_i' = \begin{cases} P_i & \text{if } R_i = \emptyset \\ P_i \cup \{r_i\} & \text{otherwise,} \end{cases}$$

where r_i is the vertex obtained by contracting the maximal group of siblings R_i. Consequently, the sets S_i' partition $\lambda_L \circ \rho(H)$.

We now show that each set S'_i is a maximal group of siblings in this graph. Consider the surjective map

$$\iota : \lambda_L(H) \to \lambda_L \circ \rho(H)$$
$$z \mapsto \begin{cases} r_i & \text{if } z \in R_i \text{ for some } i \\ z & \text{otherwise.} \end{cases}$$

For any two vertices x and y in $\lambda_L(H)$ we have that x and y are equal or adjacent if and only if $\iota(x)$ and $\iota(y)$ are equal or adjacent in $\lambda_L \circ \rho(H)$. Put differently,

$$\bar{\mathrm{N}}_{\lambda_L(H)}(x) = \bar{\mathrm{N}}_{\lambda_L(H)}(y) \Leftrightarrow \bar{\mathrm{N}}_{\lambda_L \circ \rho(H)}(\iota(x)) = \bar{\mathrm{N}}_{\lambda_L \circ \rho(H)}(\iota(y)).$$

Since each set S'_i is a maximal group of siblings, it is contracted to a single vertex s'_i when applying ρ to $\lambda_L \circ \rho(H)$. On the other hand, applying ρ to $\lambda_L(H)$ contracts each set S_i to a single vertex s_i by definition. Finally, s'_i and s'_j are adjacent if and only if s_i and s_j are adjacent for any pair $i, j \in I$, because ρ preserves adjacency between the groups of siblings it contracts. □

Proof of Theorem 25. If $\lambda_U(G)$ is isomorphic to K_2 then $\lambda(G)$ is either isomorphic to K_2 or a single vertex graph. Thus we choose $V = \emptyset$ and find that both sides of the equation

$$\rho \circ \lambda \circ \rho \circ \lambda_U(G) = \rho \circ \lambda_V \circ \rho \circ \lambda(G). \tag{3}$$

correspond to the single vertex graph.

Otherwise, let U^c be the complement of U in the set of leaves of G. Since this is a subset of leaves of $\lambda_U(G)$, and $\lambda_U(G)$ is not isomorphic to K_2, we can apply Lemma 26 with $H = \lambda_U(G)$ and obtain

$$\rho \circ \lambda(G) = \rho \circ \lambda_{U^c} \circ \lambda_U(G) = \rho \circ \lambda_{U^c} \circ \rho \circ \lambda_U(G). \tag{4}$$

If $\lambda_{U^c} \circ \rho \circ \lambda_U(G)$ is isomorphic to K_2, it follows that $\rho \circ \lambda(G)$ is the single vertex graph, and that $\lambda \circ \rho \circ \lambda_U(G)$ is either isomorphic to K_2 or the single vertex graph. We choose $V = \emptyset$ and find that both sides of Equation (3) yield the single vertex graph.

Finally, suppose that neither $\lambda_U(G)$ nor $\lambda_{U^c} \circ \rho \circ \lambda_U(G)$ are isomorphic to K_2. Since siblings in a graph other than K_2 cannot be leaves and cannot be adjacent to leaves, U^c is a subset of the set of leaves of $\rho \circ \lambda_U(G)$. Let V be the complement of U^c in the set of leaves of $\rho \circ \lambda(G)$.

Applying Lemma 26 and taking into account that $V \cup U^c$ is the set of leaves of $\rho \circ \lambda_U(G)$, we have

$$\rho \circ \lambda_V \circ \rho \circ \lambda_{U^c} \circ \rho \circ \lambda_U(G) = \rho \circ \lambda_V \circ \lambda_{U^c} \circ \rho \circ \lambda_U(G) = \rho \circ \lambda \circ \rho \circ \lambda_U(G).$$

Combining this with Equation (4), the theorem follows. □

Corollary 27. *Let U be a subset of leaves of a connected graph $G \neq K_2$. Then $\rho \circ \lambda_U(G)$ and G have the same reduction.*

Proof. Recall that each step in the reduction of G consists of applying $\rho \circ \lambda$. We induct on the minimal integer n such that $(\rho \circ \lambda)^n(G)$ is reduced. The base case $n = 0$, in which U is necessarily empty, is trivial.

Suppose that $(\rho\circ\lambda)^{n+1}(G)$ is reduced, with n minimal. Let $G' = \rho\circ\lambda(G)$. In particular $R(G) = R(G')$. By induction, $\rho \circ \lambda_V(G')$ and G' have the same reduction for any set of leaves V of G'.

By Theorem 25, there exists a set of leaves V of $G' = \rho \circ \lambda(G)$ such that

$$\rho \circ \lambda \circ \rho \circ \lambda_U(G) = \rho \circ \lambda_V(G').$$

Thus, denoting the reduction of a graph G with $R(G)$, we have

$$R\big(\rho \circ \lambda_U(G)\big) = R\big(\rho \circ \lambda \circ \rho \circ \lambda_U(G)\big) = R\big(\rho \circ \lambda_V(G')\big) = R(G') = R(G). \qquad \square$$

7 Refined Symmetry of the Sibling and the Tuft number

In this section, we prove Theorem 3 by further refining the Patch Decomposition from Theorem 18 and Corollary 20.

Let R be a connected leafless point distinguishing graph. Let $\mathcal{G}^{R,s}_{\neq 2}$, $\mathcal{G}^{R,s,t}_{\neq 2}$ and $\mathcal{D}^R$ be the subspecies of $\mathcal{G}^{c,s}_{\neq 2}$, $\mathcal{G}^{c,s,t}_{\neq 2}$ and $\mathcal{D}^{\mathrm{c}}$ respectively, whose structures, regarded as graphs, reduce to a graph isomorphic to R.

Corollary 28. *For the single vertex graph* $\bullet$*, we have*

$$\mathcal{G}^{\bullet,s}_{\neq 2}(X, X + Y, Z) = \mathcal{D}^{\bullet} \circ \mathcal{P}^s - XY - [s > 0]E_2(Z),$$

whereas, for $R \neq \bullet$*, we have*

$$\mathcal{G}^{R,s}_{\neq 2}(X, X + Y, Z) = \mathcal{D}^R \circ \mathcal{P}^s.$$

Proof. By the Patch Decomposition from Theorem 18 we have an equivariant bijection between graphs $G \in \mathcal{G}^{\mathrm{c}}_{\neq 2}(X, X + Y, Z)[U]$ and triples $\big(\pi, D, (P_B)_{B\in\pi}\big)$, where D is the underlying point distinguishing graph of G. By Corollary 20, this bijection preserves the sibling number. Corollary 27 applied to the set of leaves of sort Y of G implies that G and its underlying point distinguishing graph D reduce to the same graph R.

If R is not the single vertex graph, G has at least 4 vertices, so the exceptional cases corresponding to XY and $E_2(Z)$ depicted in Figure 8 do not occur. $\square$

Theorem 29. *For the single vertex graph* $\bullet$*, we have*

$$\mathcal{G}^{\bullet,s,t}_{\neq 2}(X, Y, Z) = \mathcal{D}^{\bullet} \circ \mathcal{Q}^{s,t} + X^2 - [t > 0]XY - [s > 0]E_2(Z),$$

whereas, if $R \neq \bullet$*, we have*

$$\mathcal{G}^{R,s,t}_{\neq 2}(X, Y, Z) = \mathcal{D}^R \circ \mathcal{Q}^{s,t}.$$

Proof. We apply Lemma 21 in the case where $\mathcal{H}_{\neq 2} = \mathcal{G}_{\neq 2}^{R,s}$ is the species of connected graphs other than K_2 with sibling number at most s which reduce to R. The closure property holds because replacing a positive number of leaves adjacent to a vertex by a positive number of leaves neither affects the reduction of the graph nor its sibling number, unless the resulting graph is a K_2.

The star graphs with at least three vertices have sibling number zero and reduce to a single vertex. Thus, the first equation in Lemma 21 applies if and only if R is the single vertex graph. After setting $Y = \Omega(\mathcal{Y}_t) - X$ in Corollary 28, the claim follows from Lemma 22. □

Proof of Theorem 3. This follows from Theorem 29 in the same way as Theorem 1 follows from Theorem 23. □

8 Induced Cycles and Graph Reduction

An *induced subgraph* of a graph G consists of a subset V of vertices of G together with all edges of G connecting vertices within V. An *induced k-cycle* is an induced subgraph that is isomorphic to a cycle graph with k vertices. In this section, we show that induced cycles with at least 4 vertices are essentially preserved by reduction.

Theorem 30. *For $k \geqslant 4$, a graph G contains an induced k-cycle if and only if the reduction of G contains an induced k-cycle.*

In particular, the sibling number and the tuft number have joint symmetric distribution on the set of connected chordal graphs, i.e., on graphs which do not contain an induced cycle with 4 or more vertices.

Proof. We show that induced cycles are preserved when removing leaves and when contracting any maximal group of siblings to a single vertex. The former is true, because an induced cycle of a graph cannot contain a leaf.

To prove the latter, we first show that a group of siblings S and an induced k-cycle C with $k \geqslant 4$ can have at most one vertex in common. Let v be such a vertex and let u and w be its neighbors on the induced k-cycle. Because $k \geqslant 4$ the vertices u and w cannot be adjacent. Thus, neither of them can be a sibling of v.

Let G' be the graph obtained by contracting the vertices in a maximal group of siblings S to a single vertex. If S and C have no vertices in common, C is also an induced cycle of G'. If S and C have a single vertex v in common, contracting the group of siblings S to a single vertex v', the vertices of $(C \setminus \{v\}) \cup \{v'\}$ form an induced cycle of G'.

Conversely, $\lambda(G)$ is an induced subgraph of G, and $\rho(G)$ is isomorphic to the subgraph induced on one representative of each maximal group of siblings. Thus, the reduction of G is isomorphic to an induced subgraph of G. □

9 Point Distinguishing Graphs Reducing to a Given Graph

In this section, we show that the species $\mathcal{D}^R$ of point distinguishing graphs which reduce to a given connected leafless point distinguishing graph R can be obtained from the

species $\mathcal{D}^\bullet$ of point distinguishing graphs which reduce to the single vertex graph with little computational effort. Additionally, we provide the first few terms of the molecular decompositions of the species $\mathcal{D}^\bullet$ and the species of leafless point distinguishing graphs $\mathcal{G}^c_{\neq 2}(X,0,0)$.

Recall from Example 15 (3) that the compositional inverse of $X - X^2$ is the species of ordered rooted trees $\mathcal{A}$.

Proposition 31. *Let R be a connected leafless point distinguishing graph and let $\mathcal{R}$ be the species whose unique isomorphism type is R. Then*

$$\mathcal{D}^\bullet = (X - X^2) \circ \mathcal{P}(X, -X, 0)^{(-1)}$$

whereas, if $R \neq \bullet$,

$$\mathcal{D}^R = \mathcal{R} \circ \mathcal{P}(X, -X, 0)^{(-1)}.$$

In particular, if $R \neq \bullet$, we have that

$$\mathcal{D}^R = \mathcal{R} \circ \mathcal{A} \circ \mathcal{D}^\bullet.$$

It is remarkable that the compositional inverse $\mathcal{P}(X, -X, 0)^{(-1)} = \mathcal{A} \circ \mathcal{D}^\bullet$ of the virtual species $P(X, -X, 0) = (1+X) \cdot E\big(XE_{\geqslant 1}(-X)\big) - 1$ is a proper (that is, non-virtual) species.

Proof. For any connected leafless point distinguishing graph R we have $\mathcal{G}^{R,s}_{\neq 2}(X,0,0) = \mathcal{R}$, because the only leafless point distinguishing graph reducing to R is R itself. Thus, setting $Y = -X$ and $Z = 0$ in Corollary 28, we obtain

$$X = \mathcal{D}^\bullet \circ \mathcal{P}^s(X, -X, 0) + X^2,$$

if R is the single vertex graph, and

$$\mathcal{R} = \mathcal{D}^R \circ \mathcal{P}^s(X, -X, 0),$$

otherwise. Since $\mathcal{P}^s(X, -X, 0) = \mathcal{P}(X, -X, 0)$ the claim follows. □

Using these identities and the `SageMath` implementation of species,[8] it is easy to compute the first few terms of the molecular decompositions and isomorphism type generating series of the species $\mathcal{D}^\bullet$ and $\mathcal{P}(X, -X, 0)^{(-1)}$. The molecular decomposition of the species $\mathcal{D}^\bullet$ begins with[9]

$$\begin{aligned} &X + XE_2 + XE_3 + E_2(X^2) + XE_4 + 2X^3E_2 + 2XE_2(X^2) \\ &\quad + XE_5 + E_2(XE_2) + X^2E_2^2 + E_2E_2(X^2) + 3X^4E_2 \end{aligned}$$

[8] developed by Mainak Roy and the third author, included since version 10.7
https://doc.sagemath.org/html/en/reference/combinat/sage/rings/lazy_species.html

[9]
```
L.<X> = LazyCombinatorialSpecies(QQ)
E = L.Sets(); P = E(X*E(-X)-X)*(1+X)-1; (X-X^2)(P.revert())
```

$$+ E_2(X^3) + E_3(X^2) + X^2E_2(X^2) + 2X^3E_3 + 2X^6 + \dots$$

The corresponding isomorphism type generating series begins with

$$x + x^3 + 2x^4 + 5x^5 + 14x^6 + 43x^7 + 141x^8 + 491x^9 + 1778x^{10} + \dots$$

The molecular decomposition of $\mathcal{P}(X, -X, 0)^{(-1)}$ begins with

$$\begin{aligned} X &+ X^2 + XE_2 + 2X^3 + XE_3 + 2X^2E_2 + E_2(X^2) + 5X^4 \\ &+ XE_4 + 2X^2E_3 + 8X^3E_2 + 4XE_2(X^2) + 14X^5 \\ &+ XE_5 + 2X^2E_4 + E_2(XE_2) + 2X^2E_2^2 + 8X^3E_3 + E_2E_2(X^2) \\ &+ 27X^4E_2 + E_2(X^3) + E_3(X^2) + 11X^2E_2(X^2) + 44X^6 + \dots \end{aligned}$$

The corresponding isomorphism type generating series begins with

$$x + x^2 + 3x^3 + 9x^4 + 29x^5 + 99x^6 + 353x^7 + 1300x^8 + 4913x^9 + 18945x^{10} + \dots$$

The isomorphism types of the species $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, 0, 0)$, the species of graphs having no siblings or leaves, are precisely the graphs R that arise as the reduction of some graph. The molecular decomposition of this species seems to be significantly harder to compute. A naive approach, enumerating all graphs, yields the following.

$$\begin{aligned} X &+ P_4 + E_2E_3 + P_5 + XP_4 + 2XE_2(X^2) \\ &+ E_2E_4 + E_3(E_2) + 3E_2E_2(X^2) + E_2(E_3) + 4X^4E_2 + 2P_6 + E_2(XE_2) \\ &+ 2\big(X^2E_2(X^2)\big)/\mathbb{Z}_2 + E_3(X^2) + XE_2E_3 + X^2E_2^2 + XP_5 + 8X^2E_2(X^2) + 2E_2(X^3) \\ &+ 2X^6 + \dots \end{aligned}$$

Here, P_n denotes the species of polygons of size n, corresponding to a graph whose automorphism group is the dihedral group of degree n and order $2n$. Moreover, $\big(X^2E_2(X^2)\big)/\mathbb{Z}_2$ is the species of polygons on six vertices with a single diameter which connects two opposite vertices. The corresponding isomorphism type generating series begins with

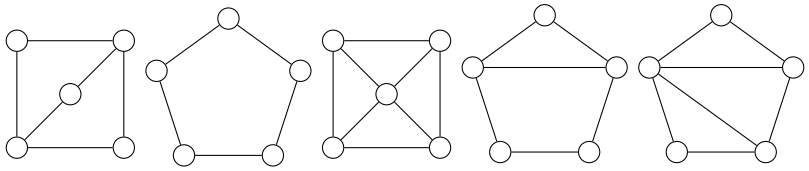
$$x + x^4 + 5x^5 + 31x^6 + 293x^7 + 4986x^8 + 151096x^9 + 8264613x^{10} + \dots$$

By Theorem 4 this generating series coincides with the generating series of bi-point-determining graphs.[10] Figure 9 shows the connected leafless point distinguishing graphs with five vertices corresponding to the five terms of size 5 in the molecular decomposition of $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, 0, 0)$.

10 Towards a Bijection

To prove Theorem 1 and Theorem 3 bijectively, one might hope to construct an involution on the set of unlabeled connected graphs with a given number of vertices, which

[10] www.oeis.org/A129586



E_2E_3 P_5 XP_4 $XE_2(X^2)$ $XE_2(X^2)$

Figure 9: All unlabeled connected leafless point distinguishing graphs with 5 vertices and their corresponding term in the molecular decomposition of $\mathcal{G}^{\mathrm{c}}_{\neq 2}(X, 0, 0)$.

interchanges groups of siblings with tufts and preserves the reduction. In this section, we will discuss this idea and its pitfalls.

To an unlabeled connected graph G other than K_2 we associate the (unlabeled) *decorated graph* G_{dec} as follows:

- we tag each vertex of G that is adjacent to k leaves with T_k, and remove all leaves from G,
- we replace each maximal group of siblings of size $k+1$ of G by a single vertex, which we tag with S_k.

An example for this process is displayed in Figure 10. Since a vertex adjacent to a leaf cannot have siblings, G_{dec} is well-defined and each of its vertices has at most one tag.[11] The sibling number $s(G)$ is the maximal number s such that S_s appears as a tag, and the tuft number $t(G)$ is the maximal number t, such that T_t appears as a tag.

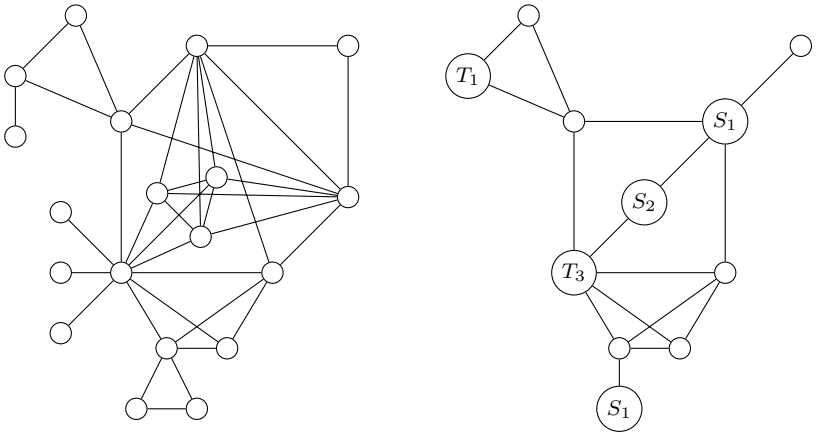


Figure 10: An unlabeled graph and its associated decorated graph.

Let a *tagged graph* be an unlabeled graph each of whose vertices may be untagged, have a tag T_k or a tag S_k for some positive integer k. We can, in fact, characterize the tagged graphs that occur as decorated graphs.

[11] a very similar idea appears in [3]

Proposition 32. *Given an unlabeled connected graph G other than K_2, its decorated graph G_{dec} satisfies the following conditions:*

1. *An isolated vertex is not tagged S_1 or T_1.*
2. *If two vertices of G_{dec} are siblings, at least one of them is tagged T_k, for some k.*
3. *Every untagged leaf is a neighbor of a vertex with tag S_k, for some k.*

Conversely, any connected tagged graph satisfying these conditions is the decorated graph of an unlabeled connected graph other than K_2.

Proof. The first condition accounts for the fact that we exclude K_2.

To show that the second condition holds, let u and v be two siblings of G_{dec}, such that neither of them has a tag T_k for any k. By construction, the preimages of u and v in G cannot be siblings, that is they have distinct closed neighborhoods. Let w be any vertex of G which is, without loss of generality, in the open neighborhood of the preimage of u but not in the open neighborhood of the preimage of v. The vertex w cannot be a leaf because u has no tag T_k in G_{dec}. Thus, its image in G_{dec}, which is distinct from u and v, is in the neighborhood of u but not in the neighborhood of v, contradicting the assumption that u and v are siblings.

For the third condition, let u be an untagged vertex in G_{dec}. Then, by construction, its preimage cannot be a leaf of G. Thus, if u is a leaf in G_{dec}, its preimage must have multiple neighbors in G which necessarily are siblings.

Conversely, suppose that a tagged graph satisfies all three conditions. Replacing the tags with their corresponding structures and then constructing its decorated graph, results in the original tagged graph, because vertices which are leaves or adjacent to leaves cannot have siblings. □

One might hope that changing each tag S_n to a tag T_n and vice versa provides a bijection interchanging the sibling and the tuft number. However, the validity of the conditions given in Proposition 32 is not preserved by this operation. For example, the tagged graph on the left in Figure 11 is a valid decorated graph, whereas the tagged graph on the right violates the third condition.

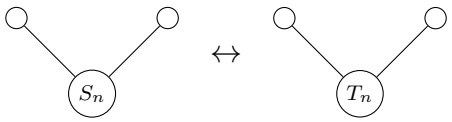


Figure 11: A tagged graph satisfying the conditions of Proposition 32 on the left and an invalid tagged graph on the right.

Because of Theorem 3, we want to find an involution ι on the set of unlabeled connected graphs that interchanges the sibling and the tuft number, and is equivariant with respect to reduction. Additionally, we may require that ι replaces any tag S_k with a tag T_k and conversely, on the corresponding decorated graph, whenever the result is a valid decorated

graph. Under these assumptions, Figure 12 displays pairs of sets of decorated graphs that are necessarily in bijection. Note that these examples demonstrate that a bijection cannot preserve the number of tags.

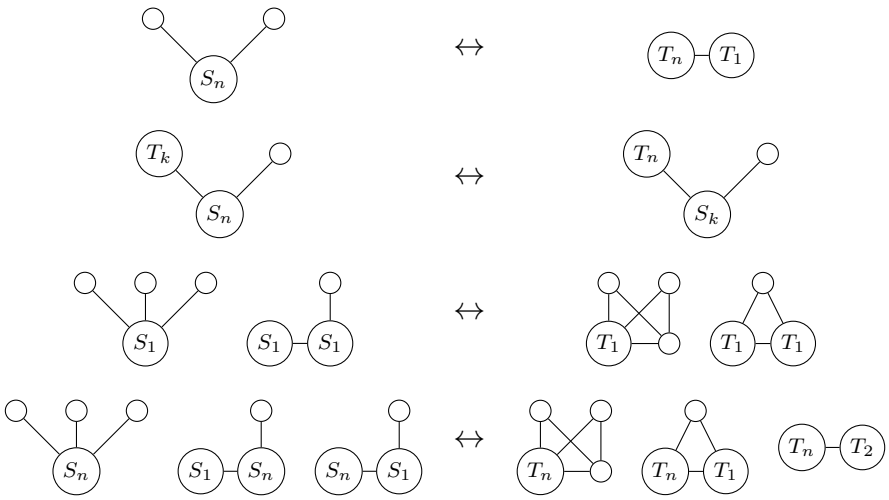


Figure 12: Some sets of decorated graphs that reduce to a single vertex necessarily corresponding to each other by Theorem 3. The last set requires $n > 1$.

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