FINITE SKEW BRACES WITH ISOMORPHIC NON-ABELIAN CHARACTERISTICALLY SIMPLE ADDITIVE AND CIRCLE GROUPS

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ABSTRACT. A skew brace is a triplet $(A,\cdot,\circ)$, where $(A,\cdot)$ and $(A,\circ)$ are groups such that the brace relation $x\circ(y\cdot z) = (x\circ y)\cdot x^{-1}\cdot(x\circ z)$ holds for all $x,y,z\in A$. In this paper, we study the number of finite skew braces $(A,\cdot,\circ)$, up to isomorphism, such that $(A,\cdot)$ and $(A,\circ)$ are both isomorphic to T^n with T non-abelian simple and $n\in\mathbb{N}$. We prove that it is equal to the number of unlabeled directed graphs on $n+1$ vertices, with one distingusihed vertex, and whose underlying undirected graph is a tree. In particular, it depends only on n and is independent of T.

CONTENTS

1. INTRODUCTION

A *skew brace* is a triplet $(A,\cdot,\circ)$, where $(A,\cdot)$ and $(A,\circ)$ are groups such that the so-called brace relation

$$x\circ(y\cdot z) = (x\circ y)\cdot x^{-1}\cdot(x\circ z)$$

holds for all $x,y,z\in A$, and here x^{-1} denotes the inverse of x in $(A,\cdot)$. We note that $(A,\cdot)$ and $(A,\circ)$ must have the same identity element. Often $(A,\cdot)$ is referred to as the *additive* group, and $(A,\circ)$ as the *circle* or *multiplicative* group, of the skew brace. Despite the terminology, the group $(A,\cdot)$ need not

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be abelian. A skew brace $(A,\cdot,\circ)$ with abelian additive group $(A,\cdot)$ is called a *brace* or sometimes a *classical brace*.

Braces were introduced by W. Rump [12] in order to study non-degenerate set-theoretic solutions of the Yang–Baxter equation which are involutive. L. Guarnieri and L. Vendramin [9] later extended this notion to skew braces to study all such solutions which are not necessarily involutive. Enumerating all skew braces (up to isomorphism) has thus become a problem of interest. As the reader would guess, an isomorphism between two skew braces $(A_1,\cdot_1,\circ_1)$ and $(A_2,\cdot_2,\circ_2)$ is a bijective map $\phi : A_1 \longrightarrow A_2$ such that

$$\phi(x \cdot_1 y) = \phi(x) \cdot_2 \phi(y)$$
$$\phi(x \circ_1 y) = \phi(x) \circ_2 \phi(y)$$

for all $x, y, \in A_1$. In [9], they also showed that there is a connection between skew braces and regular subgroups in the holomorph, as we shall explain.

We shall only consider skew braces with a finite underlying set. Given any finite groups G and N of the same order, define

$$b(G,N) = \#\left\{\begin{array}{c}\text{isomorphism classes of skew braces } (A,\cdot,\circ)\\ \text{such that } (A,\cdot)\simeq N \text{ and } (A,\circ)\simeq G\end{array}\right\}.$$

Recall that a subgroup of $\mathrm{Perm}(N)$, the group of permutations of N, is said to be *regular* if its action on N is both transitive and free. For example, both $\lambda(N)$ and $\rho(N)$ are regular, where

$$\begin{cases}\lambda : N \longrightarrow \mathrm{Perm}(N); & \lambda(\eta) = (x \mapsto \eta x),\\ \rho : N \longrightarrow \mathrm{Perm}(N); & \rho(\eta) = (x \mapsto x\eta^{-1}),\end{cases}$$

are the left and right regular representations of N. The *holomorph* of N is

$$\mathrm{Hol}(N) = \rho(N) \rtimes \mathrm{Aut}(N).$$

Let us further put

$$\mathcal{R}(G,N) = \{\text{regular subgroups of } \mathrm{Hol}(N) \text{ which are isomorphic to } G\}.$$

Note that $\mathrm{Aut}(N)$ acts on this set via conjugation in $\mathrm{Hol}(N)$.

Proposition 1.1. *For any finite groups G and N of the same order, we have*

$$b(G,N) = \#\left(\mathcal{R}(G,N)/\mathrm{Aut}(N)\right),$$

the number of orbits of $\mathcal{R}(G,N)$ under conjugation by $\mathrm{Aut}(N)$*.*

Proof. See [9, Theorem 4.2 and Proposition 4.3] or [13, Appendix]. □

Now, regular subgroups in the holomorph are also known to be related to Hopf–Galois structures. More specifically, define

$$e(G,N) = \#\left\{\begin{array}{c}\text{Hopf–Galois structures of type } N \text{ on a}\\ \text{Galois extension } L/K \text{ with } \mathrm{Gal}(L/K)\simeq G\end{array}\right\}.$$

We refer the reader to [6] for the definitions and background.

Proposition 1.2. *For any finite groups G and N of the same order, we have*

$$e(G,N) = \frac{|\mathrm{Aut}(G)|}{|\mathrm{Aut}(N)|}\cdot \#\mathcal{R}(G,N).$$

Proof. This follows from work of [8] and [2], or see [6, Chapter 2]. □

From Propositions 1.1 and 1.2, we see that

$$b(G,N) = 0 \text{ if and only if } e(G,N) = 0.$$

However, the numbers $b(G,N)$ and $e(G,N)$ need not be equal, and the calculation of the former is more difficult in general, because one also needs to take the conjugation action of $\mathrm{Aut}(N)$ into account.

Assumption. In this rest of this paper, we shall take G to be a finite non-abelian characteristically simple group. Equivalently, this means $G = T^n$ for some finite non-abelian simple group T and $n \in \mathbb{N}$.

By drawing tools from graph theory and some consequences of the classification of finite simple groups (CFSG), in [15] the author obtained a closed formula for the number $e(G,G)$.

Theorem 1.3. *We have the formula*

$$e(G,G) = 2^n(n|\mathrm{Aut}(T) + 1)^{n-1}.$$

For $n = 1$, by Proposition 1.2 and Theorem 1.3, we have

$$e(G, G) = \#\mathcal{R}(G, G) = 2 \text{ and so } \mathcal{R}(G, G) = \{\lambda(G), \rho(G)\}.$$

This fact was first shown in [5]; also see [14, Theorem 1.4] for generalization to quasisimple groups. From this and Proposition 1.1, we get $b(G, G) = 2$.

For $n \geq 2$, however, the size of $\mathcal{R}(G, G)$ becomes much larger, and it is no longer obvious what the value of $b(G, G)$ ought to be simply from Theorem 1.3. Nonetheless, we are still able to determine $b(G, G)$. To state our result, we first need to introduce some definitions.

Recall that a *tree* is a connected graph which has no cycle, or equivalently, a graph in which any two vertices can be connected by a unique simple path. It is known that a graph on $n+1$ vertices is a tree if and only if it has exactly n edges and is connected.

Definition 1.4. In this paper, we shall use *directed tree* to mean a directed graph whose underlying undirected graph is a tree. For brevity, put

$$\mathbb{N}_n = \{1, \dots, n\} \text{ and } \mathbb{N}_{0,n} = \mathbb{N}_n \sqcup \{0\}.$$

Let $\mathcal{T}(n)$ be the set of all labeled directed trees on $n + 1$ vertices, labeled by $\mathbb{N}_{0,n}$. Two directed graphs $\Gamma_1, \Gamma_2 \in \mathcal{T}(n)$ are *equivalent* if there is a bijection

$$\xi \in \mathrm{Map}(\mathbb{N}_{0,n}, \mathbb{N}_{0,n}) \text{ with } \xi(0) = 0$$

such that for any $v, v' \in \mathbb{N}_{0,n}$, there is an arrow $v \longrightarrow v'$ in Γ_1 precisely when there is an arrow $\xi(v) \longrightarrow \xi(v')$ in Γ_2. We shall write $\Gamma_1 \sim \Gamma_2$ in this case.

While $e(G, G)$ depends on both n and T, the number $b(G, G)$ turns out to depend only on n. Our main theorem is the following.

Theorem 1.5. *We have the equality*

$$b(G, G) = \#\left(\mathcal{T}(n)/\sim\right),$$

the number of equivalence classes of $\sim$ on the set $\mathcal{T}(n)$.

Observe that unlike Theorem 1.3, here we do not have a closed formula for $b(G, G)$. Let us briefly explain why this is expected to be difficult.

Remark 1.6. The equivalence relation $\sim$ in Definition 1.4 simply means that we can forget about the labeling of the vertices except the vertex 0. We then see that $\#(\mathcal{T}(n)/\sim)$ is equal to the size of the set

$$\mathcal{T}^\star(n) = \left\{ \begin{array}{c} \text{unlabeled directed trees on } n+1 \text{ vertices} \\ \text{with a distinguished vertex (root)} \end{array} \right\}.$$

The underlying undirected graph of an element $\Gamma \in \mathcal{T}^\star(n)$ may be regarded as an (unordered) rooted tree.[1] Now, the famous Cayley's formula tells us that the number of labeled trees on $n+1$ vertices is $(n+1)^{n-1}$. It was also shown in [7] that for each $1 \leq d \leq n$, we have

$$\#\left\{ \begin{array}{c} \text{labeled trees on } n+1 \text{ vertices in} \\ \text{which a specified vertex has degree } d \end{array} \right\} = \binom{n-1}{d-1} n^{n-d}. \tag{1.1}$$

The formula for $e(G,G)$ in Theorem 1.3 was obtained using (1.1). However, to compute $b(G,G)$, we need to consider unlabeled trees, and so far there is no known closed formula for the number of unlabeled (rooted) trees; see [11, A000055 and A000081]. We also need to take the orientation of the directed trees into account, which adds even more complexity into the problem. It is possible that there does not even exist a closed formula for $b(G,G)$.

2. Description of endomorphisms

The endomorphisms of G play an important role in the proof of both Theorems 1.3 and 1.5. Following the notation in [15], let us give a description of these endomorphisms.

For each $i \in \mathbb{N}_n$, we shall write

$$T^{(i)} = 1 \times \cdots \times 1 \times T \times 1 \times \cdots \times 1 \ (T \text{ is in the } i\text{th position}),$$

and use $x^{(i)}$ to denote an arbitrary element of $T^{(i)}$. For convenience, let $T^{(0)}$ denote the trivial subgroup and $x^{(0)}$ the identity element.

Proposition 2.1. *Elements of* $\mathrm{End}(G)$ *are precisely the maps*

$$(x^{(1)}, \ldots, x^{(n)}) \mapsto (\varphi_1(x^{(\theta(1))}), \ldots, \varphi_n(x^{(\theta(n))})),$$

[1] We did not refer to elements of $\mathcal{T}^\star(n)$ as "directed rooted trees" because it has a different meaning.

where $\theta \in \mathrm{Map}(\mathbb{N}_n, \mathbb{N}_{0,n})$*, and* $\varphi_i \in \mathrm{Hom}(T^{(\theta(i))}, T^{(i)})$ *for each* $i \in \mathbb{N}_n$*. Moreover, the above map lies in* $\mathrm{Aut}(G)$ *precisely when* θ *is injective with image equal to* $\mathbb{N}_n$ *and* φ_i *is bijective for each* $i \in \mathbb{N}_n$*.*

Proof. This basically follows from the proof of [3, Lemma 3.2], which gives a description of elements of $\mathrm{Aut}(G)$. □

In view of Proposition 2.1, we introduce the following notation.

Definition 2.2. Given any $f \in \mathrm{End}(G)$, we shall write

$$f(x^{(1)}, \dots, x^{(n)}) = (\varphi_{f,1}(x^{(\theta_f(1))}), \dots, \varphi_{f,n}(x^{(\theta_f(n))})),$$

where $\theta_f \in \mathrm{Map}(\mathbb{N}_n, \mathbb{N}_{0,n})$, and $\varphi_{f,i} \in \mathrm{Hom}(T^{(\theta_f(i))}, T^{(i)})$ for each $i \in \mathbb{N}_n$. To ensure that θ_f is uniquely determined by f, we shall assume that

$$\varphi_{f,i} \text{ is non-trivial when } \theta_f(i) \neq 0. \tag{2.1}$$

Note that in this case $\varphi_{f,i}$ is necessarily bijective because T is simple. Let us define $\theta_f(0) = 0$, so that we may regard $\theta_f \in \mathrm{Map}(\mathbb{N}_{0,n}, \mathbb{N}_{0,n})$. Also, we shall write $\varphi_{f,0} \in \mathrm{Hom}(T^{(0)}, T^{(0)})$ for the trivial map for convenience.

3. Characterization of regular subgroups

In [15], the present author computed $e(G, G)$ by first giving a characterization of $\mathcal{R}(G, G)$ in terms of trees. Let us recall this characterization.

Using a combinatorial argument, it was shown in [15, Section 3] that

$$\text{every element of } \mathcal{R}(G, G) \text{ lies in } \mathrm{InHol}(G) = \rho(G) \rtimes \mathrm{Inn}(G), \tag{3.1}$$

where $\mathrm{Inn}(G)$ denotes the inner automorphism group of G. We remark that the proof of (3.1) requires the fact that T has solvable outer automorphism group, which is known as Schreier conjecture and is a consequence of CFSG.

Recall that a pair (f, g), with $f, g \in \mathrm{End}(G)$, is *fixed point free* (fpf) if

$$f(x) = g(x) \text{ holds exactly when } x = 1.$$

Given any $f, g \in \mathrm{End}(G)$, we can define a subgroup of $\mathrm{InHol}(G)$ by setting

$$\mathcal{G}_{(f,g)} = \{\rho(g(x))\lambda(f(x)) : x \in G\}. \tag{3.2}$$

It is not hard to check that $\mathcal{G}_{(f,g)}$ is regular if and only if (f,g) is fpf; see [4, Proposition 1]. Since G has trivial center, all regular subgroups of $\mathrm{InHol}(G)$ (which are isomorphic to G) arise in this way by [4, Proposition 6], so

$$\mathcal{R}(G,G) = \{\mathcal{G}_{(f,g)} : f,g \in \mathrm{End}(G) \text{ such that } (f,g) \text{ is fpf}\}. \tag{3.3}$$

We are thus reduced to the problem of determining when a pair (f,g), with $f,g \in \mathrm{End}(G)$, is fpf. Plainly (f,g) is fpf if and only if the equations

$$\varphi_{f,i}(x^{(\theta_f(i))}) = \varphi_{g,i}(x^{(\theta_g(i))}), \tag{3.4}$$

for i ranging over $\mathbb{N}_n$, has no common solution except

$$x^{(1)} = \cdots = x^{(n)} = 1.$$

Here the notation is as in Definition 2.2. To study this system of equations, in [15] the author developed a graph-theoretic method, as follows.

Definition 3.1. Given any $f,g \in \mathrm{End}(G)$, define $\Gamma_{\{f,g\}}$ to be the undirected multigraph with vertex set $\mathbb{N}_{0,n}$, and we draw one edge $\mathfrak{e}_i$ between $\theta_f(i)$ and $\theta_g(i)$ for each $i \in \mathbb{N}_{0,n}$. Note that $\Gamma_{\{f,g\}}$ has $n+1$ vertices and n edges, so it is a tree precisely when it is connected.

The vertices of $\Gamma_{\{f,g\}}$ should be viewed as the identity element $x^{(0)}$ and the variables $x^{(1)},\dots,x^{(n)}$. For each $i \in \mathbb{N}_n$, the edge $\mathfrak{e}_i$ represents (3.4), and

$$\begin{cases} \text{(3.4) is equivalent to } x^{(\theta_f(i))} = (\varphi_{f,i}^{-1} \circ \varphi_{g,i})(x^{(\theta_g(i))}) & \text{if } \theta_f(i) \neq 0, \\ \text{(3.4) is equivalent to } x^{(\theta_g(i))} = (\varphi_{g,i}^{-1} \circ \varphi_{f,i})(x^{(\theta_f(i))}) & \text{if } \theta_g(i) \neq 0, \end{cases} \tag{3.5}$$

by condition (2.1). Thus, we can solve the equations (3.4) by "following the edges" in the graph $\Gamma_{\{f,g\}}$. Let us illustrate the idea via two examples.

Example 3.2. Take $n = 3$ and let $f,g \in \mathrm{End}(G)$ be such that

$$f(x^{(1)},x^{(2)},x^{(3)}) = (\varphi_{f,1}(x^{(2)}), \varphi_{f,2}(x^{(0)}), \varphi_{f,3}(x^{(1)})),$$
$$g(x^{(1)},x^{(2)},x^{(3)}) = (\varphi_{g,1}(x^{(1)}), \varphi_{g,2}(x^{(3)}), \varphi_{g,3}(x^{(0)})).$$

The associated graph $\Gamma_{\{f,g\}}$ is given by

$$2 \text{ —— } 1 \text{ —— } 0 \text{ —— } 3$$

and is a tree. If $f(x^{(1)}, x^{(2)}, x^{(3)}) = g(x^{(1)}, x^{(2)}, x^{(3)})$ holds, then based on the observations in (3.5), we see that:

- The edge $0 - 1$ tells us that $x^{(1)} = (\varphi_{f,3}^{-1} \circ \varphi_{g,3})(x^{(0)}) = 1$.
- The edge $0 - 3$ tells us that $x^{(3)} = (\varphi_{g,2}^{-1} \circ \varphi_{f,2})(x^{(0)}) = 1$.
- The edge $1 - 2$ tells us that $x^{(2)}$ is determined by $x^{(1)}$ with

$$x^{(2)} = (\varphi_{f,1}^{-1} \circ \varphi_{g,1})(x^{(1)}).$$

Since we already know that $x^{(1)} = 1$, this implies that $x^{(2)} = 1$ also.

We conclude that the pair (f, g) is fpf.

Example 3.3. Take $n = 3$ and let $f, g \in \mathrm{End}(G)$ be such that

$$f(x^{(1)}, x^{(2)}, x^{(3)}) = (\varphi_{f,1}(x^{(0)}), \varphi_{f,2}(x^{(2)}), \varphi_{f,3}(x^{(2)})),$$
$$g(x^{(1)}, x^{(2)}, x^{(3)}) = (\varphi_{g,1}(x^{(1)}), \varphi_{g,2}(x^{(3)}), \varphi_{g,3}(x^{(3)})).$$

The associated graph $\Gamma_{\{f,g\}}$ is given by

and is not a tree. The cycle $2 - 3 - 2$ may be thought of as representing

$$\varphi_{f,3}^{-1} \circ \varphi_{g,3} \circ \varphi_{g,2}^{-1} \circ \varphi_{f,2} \in \mathrm{Aut}(T^{(2)})$$

or its inverse. It is a consequence of CFSG that T has no fpf automorphism, whence there exists $\sigma^{(2)} \in T^{(2)}$ with $\sigma^{(2)} \neq 1$ such that

$$(\varphi_{f,3}^{-1} \circ \varphi_{g,3} \circ \varphi_{g,2}^{-1} \circ \varphi_{f,2})(\sigma^{(2)}) = \sigma^{(2)}.$$

We then see that (f, g) has a fixed point other than the identity, namely

$$(x^{(1)}, x^{(2)}, x^{(3)}) = (1, \sigma^{(2)}, (\varphi_{g,2}^{-1} \circ \varphi_{f,2})(\sigma^{(2)})).$$

We conclude that the pair (f, g) is not fpf.

In general, we have the following criterion.

Proposition 3.4. *A pair (f, g), with $f, g \in \mathrm{End}(G)$, is fpf if and only if the graph $\Gamma_{\{f,g\}}$ is a tree.*

Proof. See [15, Propositions 2.5 and 2.9]. □

Combining (3.3) and Proposition 3.4, we obtain

$$\mathcal{R}(G,G) = \{\mathcal{G}_{(f,g)} : f, g \in \mathrm{End}(G) \text{ such that } \Gamma_{\{f,g\}} \text{ is tree}\}. \tag{3.6}$$

We remark that the proof of Theorem 1.3 given in [15] uses this characterization of $\mathcal{R}(G,G)$ and the formula (1.1) with 0 as the specified vertex.

4. Counting orbits of regular subgroups

In this section, we shall prove Theorem 1.5. To do so, we need to consider the conjugation action of $\mathrm{Aut}(G)$ on elements of $\mathcal{R}(G,G)$, and we shall again use graph theory. Let us first refine Definition 3.1 as follows.

Definition 4.1. Given any $f, g \in \mathrm{End}(G)$, define $\Gamma_{(f,g),\to}$ to be the directed multigraph obtained from $\Gamma_{\{f,g\}}$ by replacing the edge $\mathfrak{e}_i$ with an arrow from $\theta_f(i)$ to $\theta_g(i)$ for each $i \in \mathbb{N}_{0,n}$. The arrow $\to$ in the subscript indicates that the orientation is chosen to go from $\theta_f(\cdot)$ to $\theta_g(\cdot)$.

Recall the definition in (3.2) and also the equivalence relation $\sim$ on the set $\mathcal{T}(n)$ in Definition 1.4. The key is the next theorem.

Theorem 4.2. *Let (f,g) and (f',g'), with $f,g,f',g' \in \mathrm{End}(G)$, be such that the graphs $\Gamma_{\{f,g\}}$ and $\Gamma_{\{f',g'\}}$ are trees. Then, the subgroups $\mathcal{G}_{(f,g)}$ and $\mathcal{G}_{(f',g')}$ are $\mathrm{Aut}(G)$-conjugates exactly when $\Gamma_{(f,g),\to} \sim \Gamma_{(f',g'),\to}$.*

From (3.6) and Theorem 4.2, we see that $(f,g) \mapsto \Gamma_{(f,g),\to}$, induces a well-defined injection

$$\{\mathrm{Aut}(G)\text{-orbits of } \mathcal{R}(G,G)\} \longrightarrow \{\text{equivalence classes of} \sim \text{on } \mathcal{T}(n)\}.$$

This map is also surjective. Indeed, given any Γ in $\mathcal{T}(n)$, label the n arrows in Γ as $\mathfrak{a}_1, \dots, \mathfrak{a}_n$, where the numbering may be randomly chosen. For each $i \in \mathbb{N}_n$, simply define $\theta_f(i)$ to be the tail and $\theta_g(i)$ to be the head of $\mathfrak{a}_i$. Then, clearly $\Gamma = \Gamma_{(f,g),\to}$ for $f, g \in \mathrm{End}(G)$ given by

$$f(x^{(1)}, \dots, x^{(n)}) = (x^{(\theta_f(1))}, \dots, x^{(\theta_f(n))}),$$
$$g(x^{(1)}, \dots, x^{(n)}) = (x^{(\theta_g(1))}, \dots, x^{(\theta_g(n))}).$$

Theorem 1.5 now follows from Proposition 1.1.

In the next two subsections, we shall prove Theorem 4.2, from which Theorem 1.5 would follow. Before we proceed, let us make two observations.

Lemma 4.3. *Let* (f, g) *and* (f', g')*, with* $f, g \in \mathrm{End}(G)$*, be such that* $\Gamma_{\{f,g\}}$ *and* $\Gamma_{\{f',g'\}}$ *are trees. Then* $\mathcal{G}_{(f,g)}$ *and* $\mathcal{G}_{(f',g')}$ *are* $\mathrm{Aut}(G)$*-conjugates precisely when there exist* $\psi, \pi \in \mathrm{Aut}(G)$ *such that*

$$(f', g') = (\psi \circ f \circ \pi, \psi \circ g \circ \pi). \tag{4.1}$$

Proof. It is clear that $\mathcal{G}_{(f,g)}$ and $\mathcal{G}_{(f',g')}$ are $\mathrm{Aut}(G)$-conjugates if and only if there exist $\psi \in \mathrm{Aut}(G)$ and $\pi \in \mathrm{Perm}(G)$ such that for all $x \in G$, we have

$$\begin{aligned} \rho(g'(x)) \cdot \lambda(f'(x)) &= \psi\rho(g(\pi(x)))\psi^{-1} \cdot \psi\lambda(f(\pi(x)))\psi^{-1} \\ &= \rho((\psi \circ g \circ \pi)(x)) \cdot \lambda((\psi \circ f \circ \pi)(x)), \end{aligned} \tag{4.2}$$

where the second equality follows from a simple calculation. Note that $\lambda(G)$ and $\rho(G)$ intersect trivially because G has trivial center. This then implies that the equation (4.2) holds for all $x \in G$ exactly when (4.1) is satisfied. It thus remains to prove that π must be a homomorphism in this case. Since $\psi \in \mathrm{Aut}(G)$, from (4.1) we see that $f \circ \pi$ and $g \circ \pi$ are homomorphisms, so for all $x, y \in G$, we have

$$\pi(xy) \equiv \pi(x)\pi(y) \pmod{\ker(f) \cap \ker(g)}.$$

But (f, g) is fpf by Proposition 3.4, whence $\ker(f)$ and $\ker(g)$ intersect trivially. We see that π is indeed a homomorphism. □

Lemma 4.4. *Let* $f \in \mathrm{End}(G)$ *and* $\psi, \pi \in \mathrm{Aut}(G)$*. Then, we have*

$$\theta_{\psi\circ f\circ\pi} = \theta_\pi \circ \theta_f \circ \theta_\psi \text{ in } \mathrm{Map}(\mathbb{N}_{0,n}, \mathbb{N}_{0,n}),$$

and for each $i \in \mathbb{N}_n$*, we also have*

$$\varphi_{\psi\circ f\circ\pi,i} = \varphi_{\psi,i} \circ \varphi_{f,\theta_\psi(i)} \circ \varphi_{\pi,(\theta_f\circ\theta_\psi)(i)}.$$

Here the notation is as in Definition 2.2.

Proof. We compute that

$$(x^{(1)}, \dots, x^{(n)}) \overset{\pi}{\longmapsto} (\dots, \varphi_{\pi,i}(x^{(\theta_\pi(i))}), \dots)$$

$$\stackrel{f}{\longmapsto} (\ldots, (\varphi_{f,i} \circ \varphi_{\pi,\theta_f(i)})(x^{((\theta_\pi \circ \theta_f)(i))}), \ldots)$$
$$\stackrel{\psi}{\longmapsto} (\ldots, (\varphi_{\psi,i} \circ \varphi_{f,\theta_\psi(i)} \circ \varphi_{\pi,(\theta_f \circ \theta_\psi)(i)})(x^{((\theta_\pi \circ \theta_f \circ \theta_\psi)(i))}), \ldots),$$

and from here, the claims are clear once we verify the condition (2.1). More precisely, we need to check that for each $i \in \mathbb{N}_n$, we have

$$\varphi_{\psi,i} \circ \varphi_{f,\theta_\psi(i)} \circ \varphi_{\pi,(\theta_f \circ \theta_\psi)(i)} \text{ is non-trivial when } (\theta_\pi \circ \theta_f \circ \theta_\psi)(i) \neq 0. \tag{4.3}$$

Since $\psi, \pi \in \mathrm{Aut}(G)$, the maps θ_π and $\varphi_{\psi,i}$ are bijections, and $\varphi_{\pi,(\theta_f \circ \theta_\psi)(i)}$ is a bijection when $(\theta_f \circ \theta_\psi)(i) \neq 0$. It follows that (4.3) is equivalent to

$$\varphi_{f,\theta_\psi(i)} \text{ is non-trivial when } \theta_f(\theta_\psi(i)) \neq 0,$$

and this indeed holds by (2.1). □

In what follows, let us fix (f, g) and (f', g'), with $f, g, f', g' \in \mathrm{End}(G)$, to be such that $\Gamma_{\{f,g\}}$ and $\Gamma_{\{f',g'\}}$ are trees.

4.1. **Proof of Theorem 4.2: forward implication.** This direction is easy to prove. Suppose that $\mathcal{G}_{(f,g)}$ and $\mathcal{G}_{(f',g')}$ are $\mathrm{Aut}(G)$-conjugates. Then

$$(\theta_{f'}, \theta_{g'}) = (\theta_\pi \circ \theta_f \circ \theta_\psi, \theta_\pi \circ \theta_g \circ \theta_\psi) \text{ for some } \psi, \pi \in \mathrm{Aut}(G)$$

by Lemmas 4.3 and 4.4. Since $\psi, \pi \in \mathrm{Aut}(G)$, the maps

$$\theta_\psi, \theta_\pi : \mathbb{N}_{0,n} \longrightarrow \mathbb{N}_{0,n} \text{ are bijections, with } \theta_\psi(0) = 0 = \theta_\pi(0)$$

by definition. For any $v, v' \in \mathbb{N}_{0,n}$, we then see that

$$\begin{aligned}
& \text{there is an arrow } v \longrightarrow v' \text{ in } \Gamma_{(f,g),\to} \\
\Longleftrightarrow\ & (v, v') = (\theta_f(i), \theta_g(i)) \text{ for some } i \in \mathbb{N}_n \\
\Longleftrightarrow\ & (v, v') = (\theta_f(\theta_\psi(j)), \theta_g(\theta_\psi(j))) \text{ for some } j \in \mathbb{N}_n \\
\Longleftrightarrow\ & (\theta_\pi(v), \theta_\pi(v')) = ((\theta_\pi \circ \theta_f \circ \theta_\psi)(j), (\theta_\pi \circ \theta_g \circ \theta_\psi)(j)) \text{ for some } j \in \mathbb{N}_n \\
\Longleftrightarrow\ & (\theta_\pi(v), \theta_\pi(v')) = (\theta_{f'}(j), \theta_{f'}(j)) \text{ for some } j \in \mathbb{N}_n \\
\Longleftrightarrow\ & \text{there is an arrow } \theta_\pi(v) \longrightarrow \theta_\pi(v') \text{ in } \Gamma_{(f',g'),\to}.
\end{aligned}$$

It thus follows that $\Gamma_{(f,g),\to}$ and $\Gamma_{(f',g'),\to}$ are equivalent via θ_π. This proves the forward implication of Theorem 4.2.

4.2. **Proof of Theorem 4.2: backward implication.** This direction is a lot harder to prove. Suppose that $\Gamma_{(f,g),\rightarrow}$ and $\Gamma_{(f',g'),\rightarrow}$ are equivalent, which means that there exists a bijection

$$\xi \in \mathrm{Map}(\mathbb{N}_{0,n}, \mathbb{N}_{0,n}) \text{ with } \xi(0) = 0$$

such that for any $v, v' \in \mathbb{N}_{0,n}$, there is an arrow $v \longrightarrow v'$ in $\Gamma_{(f,g),\rightarrow}$ precisely when there is an arrow $\xi(v) \longrightarrow \xi(v')$ in $\Gamma_{(f',g'),\rightarrow}$. By Lemmas 4.3 and 4.4, we need to show that there exist $\psi, \pi \in \mathrm{Aut}(G)$ such that

$$(\theta_{f'}, \theta_{g'}) = (\theta_\pi \circ \theta_f \circ \theta_\psi, \theta_\pi \circ \theta_g \circ \theta_\psi), \tag{4.4}$$

and for each $i \in \mathbb{N}_n$, we have the equalities

$$\varphi_{f',i} = \varphi_{\psi,i} \circ \varphi_{f,\theta_\psi(i)} \circ \varphi_{\pi,(\theta_f\circ\theta_\psi)(i)}, \quad \varphi_{g',i} = \varphi_{\psi,i} \circ \varphi_{g,\theta_\psi(i)} \circ \varphi_{\pi,(\theta_g\circ\theta_\psi)(i)}. \tag{4.5}$$

In other words, we need to find bijections

$$\theta_\psi, \theta_\pi \in \mathrm{Map}(\mathbb{N}_{0,n}, \mathbb{N}_{0,n}) \text{ with } \theta_\psi(0) = 0 = \theta_\pi(0)$$

satisfying (4.4), as well as isomorphisms

$$\varphi_{\psi,i} \in \mathrm{Iso}(T^{(\theta_\psi(i))}, T^{(i)}),\ \varphi_{\pi,i} \in \mathrm{Iso}(T^{(\theta_\pi(i))}, T^{(i)}) \text{ for } i \in \mathbb{N}_n \tag{4.6}$$

satisfying both equations in (4.5).

First, we consider condition (4.4). Let us take $\theta_\pi = \xi$, and we shall define θ_ψ via the next proposition. It shall be helpful to recall Definition 4.1.

Proposition 4.5. *For each $i \in \mathbb{N}_n$, there is a unique $\theta_\psi(i) \in \mathbb{N}_n$ such that*

$$(\theta_\pi^{-1}(\theta_{f'}(i)), \theta_\pi^{-1}(\theta_{g'}(i))) = (\theta_f(\theta_\psi(i)), \theta_g(\theta_\psi(i))).$$

Moreover, the map

$$\theta_\psi \in \mathrm{Map}(\mathbb{N}_{0,n}, \mathbb{N}_{0,n}), \text{ where we define } \theta_\psi(0) = 0,$$

is a bijection.

Proof. Note that there is an arrow $\theta_{f'}(i) \longrightarrow \theta_{g'}(i)$ in $\Gamma_{(f',g'),\rightarrow}$ by definition, so there is an arrow $\theta_\pi^{-1}(\theta_{f'}(i)) \longrightarrow \theta_\pi^{-1}(\theta_{g'}(i))$ in $\Gamma_{(f,g),\rightarrow}$. This means that

$$(\theta_\pi^{-1}(\theta_{f'}(i)), \theta_\pi^{-1}(\theta_{g'}(i))) = (\theta_f(j_i), \theta_g(j_i))$$

for some $j_i \in \mathbb{N}_n$, which is unique, for otherwise there would be two distinct edges joining $\theta_\pi^{-1}(\theta_{f'}(i))$ and $\theta_\pi^{-1}(\theta_{g'}(i))$ in $\Gamma_{\{f,g\}}$, and $\Gamma_{\{f,g\}}$ would not be a tree. Similarly distinct i give rise to distinct j_i because $\Gamma_{\{f',g'\}}$ is a tree. The claims are then clear. □

We have thus chosen bijections θ_ψ and θ_π such that (4.4) is satisfied. Now, we also need to show that the equations (4.5), for i ranging over $\mathbb{N}_n$, have a common solution (4.6). Let us put

$$\mathbb{N}_{n,\mathbf{f}} = \{i \in \mathbb{N}_n : \theta_{f'}(i) = 0\} = \{i \in \mathbb{N}_n : \theta_f(\theta_\psi(i)) = 0\},$$
$$\mathbb{N}_{n,\mathbf{g}} = \{i \in \mathbb{N}_n : \theta_{g'}(i) = 0\} = \{i \in \mathbb{N}_n : \theta_g(\theta_\psi(i)) = 0\},$$

where the latter equalities hold by (4.4) and the fact that θ_π is bijection. By Definition 2.2, we have

$$\begin{cases} \varphi_{f',i} \in \mathrm{Hom}(T^{(\theta_{f'}(i))}, T^{(i)}), & \varphi_{f,\theta_\psi(i)} \in \mathrm{Hom}(T^{(\theta_f(\theta_\psi(i)))}, T^{(i)}), \\ \varphi_{g',i} \in \mathrm{Hom}(T^{(\theta_{g'}(i))}, T^{(i)}), & \varphi_{g,\theta_\psi(i)} \in \mathrm{Hom}(T^{(\theta_g(\theta_\psi(i)))}, T^{(i)}). \end{cases}$$

Hence, the first and second equations in (4.5), respectively, are trivially satisfied when $i \in \mathbb{N}_{n,\mathbf{f}}$ and $i \in \mathbb{N}_{i,\mathbf{g}}$. So we only need to solve

$$\varphi_{f',i} = \varphi_{\psi,i} \circ \varphi_{f,\theta_\psi(i)} \circ \varphi_{\pi,(\theta_f \circ \theta_\psi)(i)} \text{ for } i \in \mathbb{N}_n \setminus \mathbb{N}_{n,\mathbf{f}}, \tag{4.7}$$

$$\varphi_{g',i} = \varphi_{\psi,i} \circ \varphi_{g,\theta_\psi(i)} \circ \varphi_{\pi,(\theta_g \circ \theta_\psi)(i)} \text{ for } i \in \mathbb{N}_n \setminus \mathbb{N}_{n,\mathbf{g}}. \tag{4.8}$$

We are in a situation very similar to (3.4). Again, we shall use graph theory and represent these equations as edges on a graph, as follows.

Definition 4.6. Let us put

$$\Psi = \{1_\psi, \dots, n_\psi\} \text{ and } \Pi = \{1_\pi, \dots, n_\pi\}.$$

Define $\Gamma_{\Psi,\Pi}$ to be the undirected simple graph with vertex set $\Psi \sqcup \Pi$, and we draw one edge $\mathfrak{e}_{i,\mathbf{f}}$ between i_ψ and $(\theta_f \circ \theta_\psi)(i)_\pi$ for each $i \in \mathbb{N}_n \setminus \mathbb{N}_{n,\mathbf{f}}$, as well as one edge $\mathfrak{e}_{i,\mathbf{g}}$ between i_ψ and $(\theta_g \circ \theta_\psi)(i)_\pi$ for each $i \in \mathbb{N}_n \setminus \mathbb{N}_{n,\mathbf{g}}$. We note that $(\theta_f \circ \theta_\psi)(i) \neq (\theta_g \circ \theta_\psi)(i)$ for all $i \in \mathbb{N}_n$ because $\Gamma_{\{f,g\}}$ is a tree, and this implies that $\Gamma_{\Psi,\Pi}$ is indeed a simple graph. Also $\Gamma_{\Psi,\Pi}$ is a bipartite graph, with parts Ψ and Π.

Definition 4.7. For each $i \in \mathbb{N}_n$, define

$$\begin{cases} \Phi_{i,\mathbf{f}} : \mathrm{Iso}(T^{(\theta_\psi(i))}, T^{(i)}) \longrightarrow \mathrm{Iso}(T^{(\theta_{f'}(i))}, T^{((\theta_f \circ \theta_\psi)(i))}) & \text{when } i \notin \mathbb{N}_{n,\mathbf{f}}, \\ \Phi_{i,\mathbf{g}} : \mathrm{Iso}(T^{(\theta_\psi(i))}, T^{(i)}) \longrightarrow \mathrm{Iso}(T^{(\theta_{g'}(i))}, T^{((\theta_g \circ \theta_\psi)(i))}) & \text{when } i \notin \mathbb{N}_{n,\mathbf{g}}, \end{cases}$$

respectively, by setting

$$\begin{cases} \Phi_{i,\mathbf{f}}(\varphi) = \varphi_{f,\theta_\psi(i)}^{-1} \circ \varphi^{-1} \circ \varphi_{f',i} & \text{when } i \notin \mathbb{N}_{n,\mathbf{f}}, \\ \Phi_{i,\mathbf{g}}(\varphi) = \varphi_{g,\theta_\psi(i)}^{-1} \circ \varphi^{-1} \circ \varphi_{g',i} & \text{when } i \notin \mathbb{N}_{n,\mathbf{g}}. \end{cases}$$

Note that these $\Phi_{i,\mathbf{f}}$ and $\Phi_{i,\mathbf{g}}$ are well-defined bijections by (2.1).

The vertices in Ψ and Π, respectively, should be viewed as the variables

$$\varphi_{\psi,1}, \dots, \varphi_{\psi,n} \text{ and } \varphi_{\pi,1}, \dots, \varphi_{\pi,n}$$

which we wish to solve. For each $i \in \mathbb{N}_n$, the edges $\mathfrak{e}_{i,\mathbf{f}}$ and $\mathfrak{e}_{i,\mathbf{g}}$, respectively, represent (4.7) and (4.8) when $i \notin \mathbb{N}_{n,\mathbf{f}}$ and $i \notin \mathbb{N}_{n,\mathbf{g}}$. Observe that:

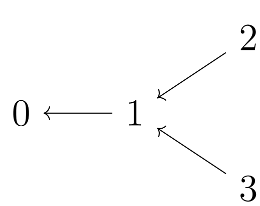
$$\begin{cases} (4.7) \text{ is equivalent to } \varphi_{\pi,(\theta_f \circ \theta_\psi)(i)} = \Phi_{i,\mathbf{f}}(\varphi_{\psi,i}) & \text{for } i \notin \mathbb{N}_{n,\mathbf{f}}, \\ (4.8) \text{ is equivalent to } \varphi_{\pi,(\theta_g \circ \theta_\psi)(i)} = \Phi_{i,\mathbf{g}}(\varphi_{\psi,i}) & \text{for } i \notin \mathbb{N}_{n,\mathbf{g}}. \end{cases} \tag{4.9}$$

Therefore, analogous to the case of (3.4), we may solve the equations (4.7) and (4.8) by "following the edges" in the graph $\Gamma_{\Psi,\Pi}$. Let us first consider an explicit example to illustrate the idea.

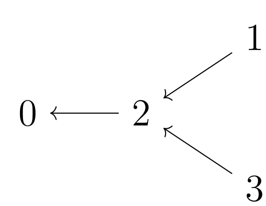
Example 4.8. Take $n = 3$ and suppose that

$$\begin{aligned} f(x^{(1)}, x^{(2)}, x^{(3)}) &= (\varphi_{f,1}(x^{(1)}), \varphi_{f,2}(x^{(3)}), \varphi_{f,3}(x^{(2)})), \\ g(x^{(1)}, x^{(2)}, x^{(3)}) &= (\varphi_{g,1}(x^{(0)}), \varphi_{g,2}(x^{(1)}), \varphi_{g,3}(x^{(1)})), \\ f'(x^{(1)}, x^{(2)}, x^{(3)}) &= (\varphi_{f',1}(x^{(1)}), \varphi_{f',2}(x^{(2)}), \varphi_{f',3}(x^{(3)})), \\ g'(x^{(1)}, x^{(2)}, x^{(3)}) &= (\varphi_{g',1}(x^{(2)}), \varphi_{g',2}(x^{(0)}), \varphi_{g',3}(x^{(2)})). \end{aligned}$$

The graphs $\Gamma_{(f,g),\rightarrow}$ and $\Gamma_{(f',g'),\rightarrow}$, respectively, are equal to



and



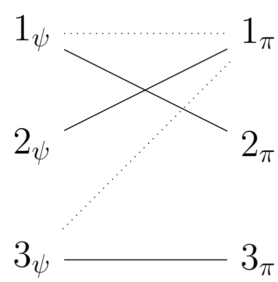
according to Definition 4.1. We may take $\theta_\pi = \xi$ to be the bijection

$$\theta_\pi(0) = 0,\ \ \theta_\pi(1) = 2,\ \ \theta_\pi(2) = 1,\ \ \theta_\pi(3) = 3,$$

and following Proposition 4.5, we see that θ_ψ in turn is given by

$$\theta_\psi(0) = 0,\ \ \theta_\psi(1) = 3,\ \ \theta_\psi(2) = 1,\ \ \theta_\psi(3) = 2.$$

Then, the graph $\Gamma_{\Psi,\Pi}$ is equal to



where we have used solid and dotted lines, respectively, to denote the edges $\mathfrak{e}_{i,\mathbf{f}}$ and $\mathfrak{e}_{i,\mathbf{g}}$. To get a solution to (4.7) and (4.8), we first pick

$$\varphi_{\psi,1} \in \mathrm{Iso}(T^{(\theta_\psi(1))}, T^{(1)})$$

to be any isomorphism. Then, we "follow the edges" in $\Gamma_{\Psi,\Pi}$ and define

$$\begin{cases} \varphi_{\pi,1} = \Phi_{1,\mathbf{g}}(\varphi_{\psi,1}),\ \ \varphi_{\pi,2} = \Phi_{1,\mathbf{f}}(\varphi_{\psi,1}). \\ \varphi_{\psi,2} = \Phi_{2,\mathbf{f}}^{-1}(\varphi_{\pi,1}),\ \ \varphi_{\psi,3} = \Phi_{3,\mathbf{g}}^{-1}(\varphi_{\pi,1}), \\ \varphi_{\pi,3} = \Phi_{3,\mathbf{f}}(\varphi_{\psi,3}), \end{cases}$$

recursively. The equations (4.7) and (4.8) are then all satisfied by (4.9). We have thus obtained a common solution (4.6) to the equations (4.5).

The idea of Example 4.8 is somewhat similar to that of Example 3.2. But unlike Proposition 3.4, in this case we do not need $\Gamma_{\Psi,\Pi}$ to be a tree for the idea to work in general. Indeed, in the special case that

$$f' = f = \mathrm{Id}_G,\ \ g' = g = \text{the trivial map},\ \theta_\pi = \mathrm{Id}_{\mathbb{N}_{0,n}} = \theta_\psi,$$

the graph $\Gamma_{\Psi,\Pi}$ has exactly n edges, namely

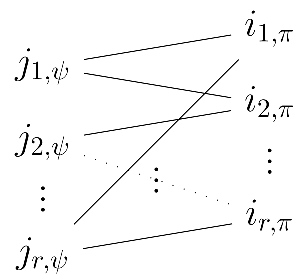
$$i_\psi \overset{\mathfrak{e}_{i,\mathbf{f}}}{\rule[0.5ex]{4em}{0.4pt}} i_\pi \quad \text{for } i \in \mathbb{N}_n,$$

which is not a tree, but certainly (4.5) has a solution (4.6) corresponding to $\psi = \mathrm{Id}_G = \pi$. Nevertheless, we do need $\Gamma_{\Psi,\Pi}$ to have no cycle.

Proposition 4.9. *There is no cycle in $\Gamma_{\Psi,\Pi}$.*

Proof. Suppose for contradiction that $\Gamma_{\Psi,\Pi}$ has a cycle $\mathfrak{c}$, whose length must be even, say $2r$ with $r \in \mathbb{N}$, because $\Gamma_{\Psi,\Pi}$ is bipartite. Then $\mathfrak{c}$ has the shape

$$\mathfrak{c}:\ i_{1,\pi} - j_{1,\psi} - i_{2,\pi} - j_{2,\psi} - \cdots$$
$$\cdots - i_{r,\pi} - j_{r,\psi} - i_{1,\pi}$$



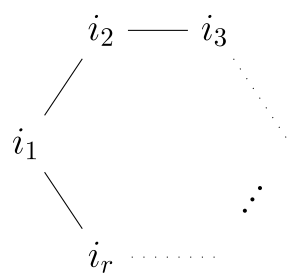
where $i_1, \dots, i_r, j_1, \dots, j_r \in \mathbb{N}_n$. For each $1 \leq s \leq r$, by Definition 4.6, there are at most two edges in $\Gamma_{\Psi,\Pi}$ with $j_{s,\psi}$ as an endpoint, namely

$$\begin{cases} \mathfrak{e}_{j_s,\mathbf{f}}:\ j_{s,\psi} - (\theta_f \circ \theta_\psi)(j_s)_\pi & \text{defined when } (\theta_f \circ \theta_\psi)(j_s) \neq 0, \\ \mathfrak{e}_{j_s,\mathbf{g}}:\ j_{s,\psi} - (\theta_g \circ \theta_\psi)(j_s)_\pi & \text{defined when } (\theta_g \circ \theta_\psi)(j_s) \neq 0. \end{cases}$$

Thus, putting $i_{r+1} = i_1$ when $s = r$, we see that necessarily

$$\{\theta_f(\theta_\psi(j_s)), \theta_g(\theta_\psi(j_s))\} = \{i_s, i_{s+1}\}.$$

But then by Definition 3.1, this means that there is an edge joining i_s and i_{s+1} in $\Gamma_{\{f,g\}}$, so we have a cycle



in $\Gamma_{\{f,g\}}$, which is impossible because $\Gamma_{\{f,g\}}$ is a tree. □

For convenience, let us refine Definition 4.6 as follows.

Definition 4.10. Define $\Gamma_{\Psi,\Pi,\leftrightarrow}$ to be the symmetric directed graph that is obtained from $\Gamma_{\Psi,\Pi}$ by replacing every edge by a pair of arrows going in the opposite directions. In other words, for each $i \in \mathbb{N}_n$, we have the arrows

$$i_\psi \underset{\mathfrak{a}_{i,\mathbf{f}}}{\overset{\mathfrak{a}_{i,\mathbf{f}}^{-1}}{\rightleftarrows}} (\theta_f \circ \theta_\psi)(i)_\pi \qquad \text{and} \qquad i_\psi \underset{\mathfrak{a}_{i,\mathbf{g}}}{\overset{\mathfrak{a}_{i,\mathbf{g}}^{-1}}{\rightleftarrows}} (\theta_g \circ \theta_\psi)(i)_\pi$$

in $\Gamma_{\Psi,\Pi,\leftrightarrow}$ when $i \notin \mathbb{N}_{n,\mathbf{f}}$ and $i \notin \mathbb{N}_{n,\mathbf{g}}$, respectively.

The next lemma is not necessary, but it makes the proof slightly cleaner.

Lemma 4.11. *There is no vertex in $\Gamma_{\Psi,\Pi}$ which has degree 0.*

Proof. Let $i, j \in \mathbb{N}_n$ be arbitrary. Notice that $\theta_f(\theta_\psi(i))$ and $\theta_g(\theta_\psi(i))$ are not both 0 because $\Gamma_{\{f,g\}}$ has no loop, so plainly vertices i_ψ in Ψ have degree at least one. Now, consider the equations

$$\theta_f(\theta_\psi(i)) = j \text{ and } \theta_g(\theta_\psi(i)) = j.$$

By (4.4), they may be rewritten as

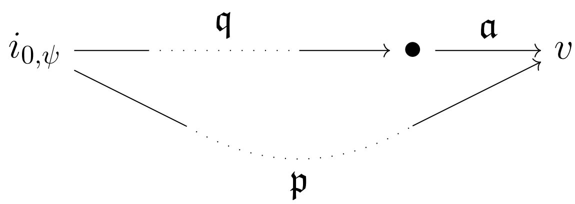
$$\theta_{f'}(i) = \theta_\pi(j) \text{ and } \theta_{g'}(i) = \theta_\pi(j).$$

Since $\Gamma_{\{f',g'\}}$ is connected, there must be an edge containing $\theta_\pi(j)$ in $\Gamma_{\{f',g'\}}$. This implies that for j fixed, one of the two equations above is solvable in i. Hence, the vertices j_π in Π have degree at least one as well. □

We shall now complete the proof of the backward implication of Theorem 4.2. Recall that we have already picked bijections θ_π and θ_ψ for which (4.4) is satisfied. It remains to exhibit a solution (4.6) to the equations (4.7) and (4.8). As illustrated in Example 4.8, we shall do so by "following the edges" in the graph $\Gamma_{\Psi,\Pi}$. More precisely, we shall carry out the following steps for each connected component Γ of $\Gamma_{\Psi,\Pi}$. Note that Γ cannot be a singleton by Lemma 4.11 and so it contains a vertex in Ψ.

1. Fix a vertex $i_{0,\psi}$ in Ψ lying in Γ and pick $\varphi_{\psi,i_0} \in \mathrm{Iso}(T^{(\theta_\psi(i_0))}, T^{(i_0)})$ to be any isomorphism.
2. Let v be any other vertex in Γ. Since the underlying undirected graph of Γ is a tree by Proposition 4.9, there is a unique simple path in Γ joining

$i_{0,\psi}$ and v, which corresponds to a simple directed path $\mathfrak{p}$ in $\Gamma_{\Psi,\Pi,\leftrightarrow}$. Let us write $\mathfrak{p} = \mathfrak{a} \cdot \mathfrak{q}$ as a concatenation, where $\mathfrak{q}$ is a simple directed path starting at $i_{0,\psi}$, and $\mathfrak{a}$ is an arrow ending at v.

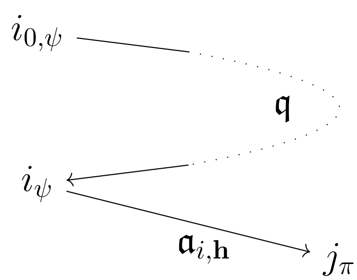


Let $d \in \mathbb{N}$ be the length of $\mathfrak{p}$, and $d-1$ would be the length of $\mathfrak{q}$.

(a) In the case that d is odd, we have

$$v = j_\pi \text{ with } j = (\theta_h \circ \theta_\psi)(i) \text{ and } \mathfrak{a} = \mathfrak{a}_{i,\mathbf{h}}$$

for some $i, j \in \mathbb{N}_n$ and $(h, \mathbf{h}) \in \{(f, \mathbf{f}), (g, \mathbf{g})\}$, as illustrated below.



Assuming that $\varphi_{\psi,i} \in \mathrm{Iso}(T^{(\theta_\psi(i))}, T^{(i)})$ has been chosen, we define

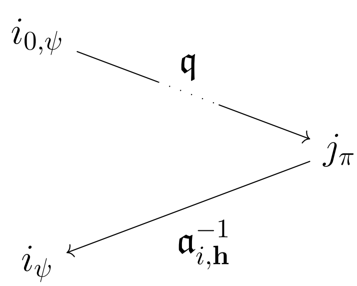
$$\varphi_{\pi,j} = \Phi_{i,\mathbf{h}}(\varphi_{\psi,i}), \text{ so then } \varphi_{h',i} = \varphi_{\psi,i} \circ \varphi_{h,\theta_\psi(i)} \circ \varphi_{\pi,(\theta_h \circ \theta_\psi)(i)}$$

is satisfied, as observed in (4.9).

(b) In the case that d is even, we have

$$v = i_\psi \text{ with } j = (\theta_h \circ \theta_\psi)(i) \text{ and } \mathfrak{a} = \mathfrak{a}_{i,\mathbf{h}}^{-1}$$

for some $i, j \in \mathbb{N}_n$ and $(h, \mathbf{h}) \in \{(f, \mathbf{f}), (g, \mathbf{g})\}$, as illustrated below.



Assuming that $\varphi_{\pi,j} \in \mathrm{Iso}(T^{(\theta_\pi(j))}, T^{(j)})$ has been chosen, we define

$$\varphi_{\psi,i} = \Phi_{i,\mathbf{h}}^{-1}(\varphi_{\pi,j}), \text{ so then } \varphi_{h',i} = \varphi_{\psi,i} \circ \varphi_{h,\theta_\psi(i)} \circ \varphi_{\pi,(\theta_h\circ\theta_\psi)(i)}$$

is satisfied, as observed in (4.9).

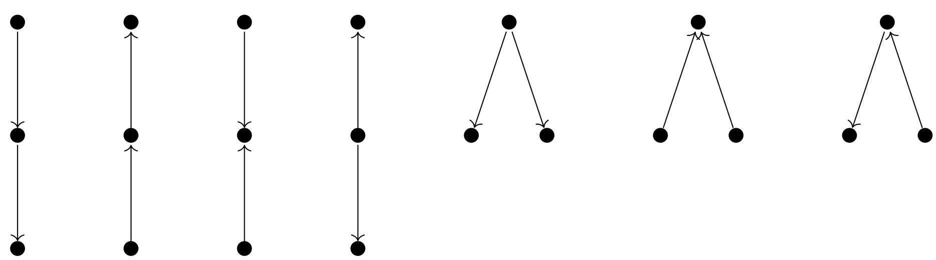
In both cases, the equation (4.7) or (4.8) represented by $\mathfrak{a}$ is satisfied.

Therefore, using induction on d, we may recursively define a solution (4.6) to the equations (4.7) and (4.8). This completes the proof.

5. Counting unlabeled directed trees with a root

Let $\mathcal{T}^\star(n)$ be the set defined as in Remark 1.6 and write $t_n^\star$ for its size. We shall end this paper by briefly discussing the problem of computing the exact value of $t_n^\star$.

Clearly $t_0^\star = 1$ and $t_1^\star = 2$. It is also easy to see that $t_2^\star = 7$, with



as the elements of $\mathcal{T}^\star(2)$, where the root is being placed at the top of graph. For larger values of n, we can somewhat use induction to compute $t_n^\star$, as the next proposition shows.

Definition 5.1. Let Γ be any unlabeled directed tree with a root and write Γ_{un} for its underlying undirected graph. Let 0 denote the root, and let v be any other vertex of Γ.

(1) Let Γ_v be the unlabeled directed tree with root v which is obtained from Γ by removing all the vertices v' such that the unique simple path in Γ_{un} joining 0 and v' does not contain v. We call Γ_v the *subtree* of Γ at v.

(2) The vertex v is a *child* of Γ if the unique simple path in Γ_{un} joining 0 and v has length one. In this case, this path corresponds to an arrow $\mathfrak{a}$ in Γ. We call v an *in-child* if $\mathfrak{a}$ ends at 0, and an *out-child* if $\mathfrak{a}$ starts at 0.

Proposition 5.2. *Suppose that we are given tuples*

$$(n_1, n_2), \ \ (k_{1,1} \ldots, k_{1,n_1}), \ \ (k_{2,1}, \ldots, k_{2,n_2})$$

of non-negative integers such that

$$n = n_1 + n_2, \ \ n_1 = \sum_{s=1}^{n_1} sk_{1,s}, \ \ n_2 = \sum_{s=1}^{n_2} sk_{2,s},$$

where an empty sum represents 0*. Then, the number of* $\Gamma \in \mathcal{T}^\star(n)$ *such that*

(a) *For each* $1 \leq s \leq n_1$*, the number of in-children* v *whose subtrees* Γ_v *have exactly* s *vertices is equal to* $k_{1,s}$*;*

(b) *For each* $1 \leq s \leq n_2$*, the number of out-children* v *whose subtrees* Γ_v *have exactly* s *vertices is equal to* $k_{2,s}$*;*

are both satisfied, is given by

$$\prod_{s=1}^{n_1} \binom{t_{s-1}^\star + k_{1,s} - 1}{k_{1,s}} \cdot \prod_{s=1}^{n_2} \binom{t_{s-1}^\star + k_{2,s} - 1}{k_{2,s}},$$

where an empty product represents 1*.*

Proof. A similar statement is true for unlabeled rooted trees; see [10, p. 386] for example. The only difference is that our trees are directed, which means that the in-children and out-children have to be treated differently.

To count the number of $\Gamma \in \mathcal{T}^\star(n)$ satisfying (a) and (b), note that Γ may be viewed as a collection of subtrees Γ_v at the children v. Also, the subtrees Γ_v at the in-children v are independent from those at the out-children v. For each $\ell = 1, 2$ and $1 \leq s \leq n_\ell$, at the $k_{\ell,s}$ vertices v which are

$$\begin{cases} \text{in-children} & \text{if } \ell = 1 \\ \text{out-children} & \text{if } \ell = 2 \end{cases}$$

and whose subtrees Γ_v are to have exactly s vertices, we can choose any $k_{\ell,s}$ elements of $T^\star(s-1)$ to be these Γ_v with repetition allowed. The number of such choices is known to be equal to

$$\binom{t_{s-1}^\star + k_{\ell,s} - 1}{k_{\ell,s}}.$$

Multiplying over s and ℓ then yields the claim. □

Given any $m \in \mathbb{N}$, let $\mathcal{A}(m)$ be the set of all m-tuples $\mathbf{k} = (k_1, \dots, k_m)$ of non-negative integers such that $m = k_1 + 2k_2 + \cdots + mk_m$, and put

$$P(m; \mathbf{k}) = \prod_{s=1}^{m} \binom{t_{s-1}^{\star} + k_s - 1}{k_s}$$

in this case. From Proposition 5.2, we then deduce that

$$t_n^{\star} = \sum_{m \in \mathbb{N}_{0,n}} \sum_{\mathbf{k}_1 \in \mathcal{A}(m)} \sum_{\mathbf{k}_2 \in \mathcal{A}(n-m)} P(m; \mathbf{k}_1) P(n-m; \mathbf{k}_2). \tag{5.1}$$

This gives us a way to compute $t_n^{\star}$ inductively, but the calculation gets very complicated. The better approach is perhaps to consider the associated generating function given by

$$z \mapsto \sum_{n=0}^{\infty} t_n^{\star} z^n,$$

and then use (5.1) to study its properties. But this is a completely different problem. We shall therefore content ourselves with computing $t_n^{\star}$ for $n \leq 10$ by applying the formula (5.1) directly.

The calculation was done in Magma [1]. The code used gets very slow once $n \geq 10$ and is not an effective way to compute $t_n^{\star}$. It is also a straightforward implementation of (5.1), so we shall not include it here.

n	t_n
1	1
2	7
3	26
4	107
5	458

n	t_n
6	2058
7	9498
8	44947
9	216598
10	1059952

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