Counting Prime Graphs and Point-Determining Graphs
Using Combinatorial Theory of Species

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2007
Dedication

To Kailang Li and Youzhi Jiang.

Lù Màn Màn Qí Xiū Yuǎn Xi,
Wú Jiāng Shàng Xià Eí Qiú Suò.
by: Qū Yuán

The way is long with obstacles,
I’m questing for the truth to and fro.
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Abstract

Counting Prime Graphs and Point-Determining Graphs Using

Combinatorial Theory of Species

A dissertation presented to the Faculty of the
Graduate School of Arts and Sciences of Brandeis
University, Waltham, Massachusetts

by Ji Li

In this thesis, we enumerate different types of graphs in light of the combinatorial
theory of species initiated by Joyal [13]. The prime graphs with respect to the
Cartesian multiplication is enumerated using the exponential composition of species,
which is constructed based on the arithmetic product of species studied by Maia
and Méndez [18]. The point-determining graphs and bi-point-determining graphs are
enumerated by finding functional equations relating them to the species of graphs.
Contents

List of Figures ix

Chapter 1. Groups Actions and Pólya’s Cycle Index Polynomial 1
  1.1. Symmetric Groups and Group Actions 1
  1.2. Pólya’s Cycle Index Polynomials 5
  1.3. Exponentiation Group 8

Chapter 2. Combinatorial Theory of Species 15
  2.1. Definition of Species 15
  2.2. Species Operations 21
  2.3. Molecular Species 25
  2.4. Compositional Inverse of $E_+$ 31
  2.5. Multisort Species 35
  2.6. Arithmetic Product of Species 38

Chapter 3. Cartesian Product of Graphs and Prime Graphs 48
  3.0. Introduction 48
  3.1. Cartesian Product of Graphs 49
  3.2. Labeled Prime Graphs 54
  3.3. Unlabeled Prime Graphs 61
  3.4. Exponential Composition with a Molecular Species 67
  3.5. Exponential Composition 78
3.6. Cycle Index of Prime Graphs

Chapter 4. Point-Determining Graphs

4.0. Introduction

4.1. Point-Determining Graphs and Co-Point-Determining Graphs

4.2. Connected Point-Determining Graphs and Connected Co-Point-Determining Graphs

4.3. Bi-Point-Determining Graphs

4.4. 2-Colored Graphs and Connected 2-colored Graphs

4.5. Point-Determining 2-Colored Graphs

Appendix A. Index of Species

Appendix B. General Notations

Appendix. Bibliography
List of Figures

1.1 Group action of $A \ast B$. 3
1.2 Group action of $A \times B$. 3
1.3 Group action of $B \wr A$. 4
1.4 Group action of $B^A$. 9
1.5 An element of $B^A$. 10
1.6 Cycle type of an element of $B^A$. 10

2.1 Transport of $G$-structures. 16
2.2 Species associated to a graph. 17
2.3 A linear order and a permutation. 20
2.4 Addition of species. 21
2.5 Multiplication of species. 23
2.6 Composition of species. 23
2.7 The formula $(X^m/A) \cdot (X^n/B) = X^{m+n}/(A \times B)$. 31
2.8 The formula $(X^m/A) \circ (X^n/B) = X^{mn}/(B \wr A)$. 31
2.9 Unlabeled connected graphs. 35
2.10 Multisort species. 37
2.11 The 2-sort species of rooted trees. 38
2.12 A rectangle. 39
2.13 Another rectangle.

2.14 A 3-rectangle.

2.15 Arithmetic product of species.

2.16 Unit of the arithmetic product.

2.17 The species $E_2 \sqcup E_2$.

2.18 The formula \((X^m/A) \sqcup (X^n/B) = X^{mn}/(A \times B)\).

2.19 The $E_2 \sqcup E_2$-structures.

2.20 An element of $A \times B$.

3.1 The Cartesian product of graphs.

3.2 A prime decomposition.

3.3 The automorphism group of a prime power.

3.4 The species $E_2(E_2)$.

3.5 The formula \(((X^n/B)^{\sqcup m})/A = X^{nm}/B^A\).

3.6 Unlabeled prime graphs.

3.7 Unlabeled non-prime graphs.

4.1 Labeled point-determining graphs and co-point-determining graphs.

4.2 Transform a graph into a point-determining graph.

4.3 Unlabeled point-determining graphs.

4.4 Unlabeled connected point-determining graphs and unlabeled connected
    co-point-determining graphs.

4.5 A phylogenetic tree.

4.6 A functional equation for the species of phylogenetic trees.
4.7 Unlabeled phylogenetic trees.

4.8 Unlabeled phylogenetic trees corresponding to the species $X \mathcal{E}_2^2$.

4.9 An alternating phylogenetic tree.

4.10 An illustration of $(g, h)$.

4.11 Operations $O_\mathcal{X}$ and $O_\mathcal{\varphi}$.

4.12 An illustration of $(g', h')$.

4.13 Alternating applications of operations $O_\mathcal{X}$ and $O_\mathcal{\varphi}$.

4.14 Construct a graph from a given triple $(\pi, \varphi, \gamma)$.

4.15 Unlabeled bi-point-determining graphs.

4.16 The 2-sort species of 2-colored graphs.

4.17 Unlabeled 2-colored graphs counted by the number of edges.

4.18 Unlabeled 2-colored graphs.

4.19 Unlabeled connected 2-colored graphs.

4.20 The formula $\mathcal{P}^s(X, Y) = (1 + X)(1 + Y) \mathcal{E}(\mathcal{P}^c_{\geq 2}(X, Y))$.

4.21 The formula $\mathcal{P}(X, Y) = (1 + X + Y) \mathcal{E}(\mathcal{P}^c_{\geq 2}(X, Y))$.

4.22 Unlabeled point-determining 2-colored graphs.

4.23 Unlabeled point-determining 2-colored graphs with 5 vertices.
CHAPTER 1

Groups Actions and Pólya’s Cycle Index Polynomial

1.1. Symmetric Groups and Group Actions

The symmetric group of order \( n \), denoted \( \mathfrak{S}_n \), is the group of permutations of \( [n] = \{1, 2, \ldots, n\} \). Let \( \lambda = (\lambda_1, \lambda_2, \ldots) \), where the \( \lambda_i \) are arranged in weakly decreasing order, be a partition of \( n \), denoted \( \lambda \vdash n \). That is, \(|\lambda| = \sum \lambda_i = n\). Let \( \sigma \) be a permutation of \([n]\). We say \( \lambda \) is the cycle type of \( \sigma \), denoted by \( \lambda = c.t.(\sigma) \), if the \( \lambda_i \) are the lengths of the cycles in the decomposition of \( \sigma \) into disjoint cycles in weakly decreasing order. Sometimes we write \( \lambda = (1^{c_1(\lambda)}, 2^{c_2(\lambda)}, \ldots) \), where \( c_k(\lambda) \) is the number of parts of length \( k \) in \( \lambda \) for \( k \geq 1 \).

Example 1.1.1. Let \( \sigma = (\begin{array}{cccc} 1&2&3&4 \\ 4&2&5&1 \\ 6&5&1&6 \end{array}) = (3, 5, 6)(1, 4)(2) \). Then the cycle type of \( \sigma \) is \((3, 2, 1)\), and \( c_1(\sigma) = c_2(\sigma) = c_3(\sigma) = 1 \).

It is well-known that the number of permutations of \([n]\) of cycle type

\[
\lambda = (1^{c_1}, 2^{c_2}, \ldots, k^{c_k})
\]

is

\[
d_\lambda := \frac{n!}{c_1! c_2! c_3! \cdots c_k! k^{c_k}} ,
\]

in which the denominator

\[
z_\lambda := c_1! c_2! c_3! \cdots c_k! k^{c_k}
\]
is the number of permutations in $\mathfrak{S}_n$ that commute with a permutation of cycle type $\lambda$.

**Definition 1.1.2.** An action of a group $A$ on a set $S$ is a function

$$\rho : A \times S \to S,$$

where for $x \in A$ and $s \in S$, $\rho(x, s)$ is written $x \cdot s$. We say this action is *natural* if both of the following conditions are satisfied:

$$x \cdot (y \cdot s) = (xy) \cdot s, \quad \text{id}_A \cdot s = s,$$

for any $x, y \in A$ and $s \in S$.

Let $A$ be a subgroup of $\mathfrak{S}_m$, and let $B$ be a subgroup of $\mathfrak{S}_n$. We construct new groups as described below.

**Definition 1.1.3.** We define two groups $A \ltimes B$ and $A \times B$ both isomorphic to the product of $A$ and $B$, where $A \ltimes B$ is a subgroup of $\mathfrak{S}_{m+n}$ and $A \times B$ is a subgroup of $\mathfrak{S}_{mn}$.

The elements of the product groups are of the form $(a, b)$, where $a \in A$ and $b \in B$. The group operation is defined by

$$(a_1, b_1) \cdot (a_2, b_2) = (a_1a_2, b_1b_2),$$

where $a_1$ and $a_2$ are elements of $A$, and $b_1$ and $b_2$ are elements of $B$.

The group $A \ltimes B$ acts on the set $[m+n]$ by

$$(a, b)(i) = \begin{cases} a(i), & \text{if } i \in \{1, 2, \ldots, m\}, \\ b(i - m) + m, & \text{if } i \in \{m+1, m+2, \ldots, m+n\}. \end{cases}$$
Figure 1.1 illustrates the action of an element \((a, b)\) of the group \(A \rtimes B\).

![Figure 1.1. Group action of \(A \rtimes B\).](image)

The group \(A \times B\) acts on the set \([m] \times [n]\) and may therefore be viewed as a subgroup of \(\mathfrak{S}_{mn}\). The action of an element of \(A \times B\) on an element of \([m] \times [n]\) is given by

\[(a, b)(i, j) = (a(i), b(j)),\]

for all \(i \in [m]\) and \(j \in [n]\).

Figure 1.2 illustrates the action of an element \((a, b)\) of the group \(A \times B\).

![Figure 1.2. Group action of \(A \times B\).](image)

**Definition 1.1.4.** The **wreath product** of \(A\) and \(B\), denoted \(B \wr A\) is the group in which the elements are ordered pairs \((\alpha, \tau)\), where \(\alpha\) is a permutation in \(A\) and \(\tau\) is
a function from $[m]$ to $B$. An element $(\alpha, \tau)$ of $B \wr A$ acts on the set $[m] \times [n]$ by

$$(\alpha, \tau)(i, j) = (\alpha i, \tau(i)j),$$

for all $i \in [m]$ and $j \in [n]$.

Figure 1.3 illustrates the action of an element $(\alpha, \tau)$ of the group $B \wr A$.

![Figure 1.3. Group action of $B \wr A$.](image)

The composition of two elements $(\alpha, \tau)$ and $(\beta, \eta)$ of $B \wr A$ is given by

$$(\alpha, \tau)(\beta, \eta) = (\alpha \beta, (\tau \circ \beta)\eta),$$

where $\beta \in A$ is viewed as a function from $[m]$ to $[m]$, and $(\tau \circ \beta)\eta$ denotes the point-wise multiplication of $\tau \circ \beta$ and $\eta$, both functions from $[m]$ to $B$.

Again $B \wr A$ can be identified with a subgroup of $\mathfrak{S}_{mn}$. Note that the order of $B \wr A$ is

$$|B \wr A| = |A| \cdot |B|^m.$$ 

**Example 1.1.5.** Let $A$ be the symmetric group of order 2, and let $B$ be the cyclic group of order 3. The element $(\alpha, \tau)$ in $B \wr A$, where $\alpha = (1, 2)$, $\tau(1) = \text{id}$ and $\tau(2) = (1, 2, 3)$, acts on the set $[2] \times [3]$ by

- $(1, 1) \mapsto (2, 1)$
- $(2, 1) \mapsto (1, 2)$
- $(1, 2) \mapsto (2, 2)$
- $(2, 2) \mapsto (1, 3)$
- $(1, 3) \mapsto (2, 3)$
- $(2, 3) \mapsto (1, 1)$
Therefore, the element \((\alpha, \tau)\) of \(B \wr A\) is a 6-cycle.

The following Theorem is a generalization of the Cauchy-Frobenius Theorem, alias Burnside’s Lemma. For the proof of a more general result, with applications and further references, see Robinson [25]. Another application is given in [6].

**Theorem 1.1.6.** (Cauchy-Frobenius) *Suppose that a finite group \(M \times N\) acts on a set \(S\). The groups \(M\) and \(N\), considered as subgroups of \(M \times N\), also act on \(S\). The group \(N\) acts on the set of \(M\)-orbits. Then for any \(g \in N\), the number of \(M\)-orbits fixed by \(g\) is given by*

\[
\frac{1}{|M|} \sum_{f \in M} \text{fix}(f, g),
\]

*where \(\text{fix}(f, g)\) denotes the number of elements in \(S\) that are fixed by \((f, g) \in M \times N\).*

**1.2. Pólya’s Cycle Index Polynomials**

**Definition 1.2.1.** Let \(\lambda\) be a partition of \(n\). The *power sum* symmetric function in the variables \(x_1, x_2, \ldots\) [27, p. 297] indexed by \(\lambda\), denoted \(p_\lambda\), is defined by

\[
p_n = p_n[x] = \sum_i x_i^n, \quad n \geq 1
\]

\[
p_\lambda = p_\lambda[x] = p_{\lambda_1} p_{\lambda_2} \cdots \prod_{k \geq 1} p_k^{c_k(\lambda)}, \text{ if } \lambda = (\lambda_1, \lambda_2, \ldots) = (1^{c_1(\lambda)}, 2^{c_2(\lambda)}, \ldots).
\]

The \(p_\lambda\) form a basis for the ring of symmetric functions in the variables \(x_1, x_2, \ldots\). We can also define power sum symmetric functions in the variables \(y_1, y_2, y_3, \ldots\), written as \(p_\lambda[y]\), in a similar fashion.

**Definition 1.2.2.** The operation called *plethysm* on the ring of symmetric functions (see Stanley [27, p. 447]) is defined to be such that if \(f\) is a symmetric function in the variables \(x_1, x_2, \ldots\), then the plethysm \(f \circ p_n\) is obtained from the expression for
f in terms of the $x_i$’s by replacing each $x_i$ with $x_i^n$. More generally, if $f$ and $g$ are arbitrary symmetric functions, where $g$ is expressed as a function of the power sum symmetric functions, i.e., $g = g(p_1, p_2, \ldots)$, then $f \circ g$ is the polynomial obtained from $f$ by replacing each variable $p_k$ by $g(p_k, p_{2k}, \ldots)$.

It follows immediately that $p_m \circ p_n = p_{mn}$ for all positive integers $m, n$.

Next, we introduce an operation $\boxtimes$ on power sum symmetric functions that was studied by Harary [10], and by Maia and Méndez [18].

**Definition 1.2.3.** We define an operation $\boxtimes$ on the symmetric functions by letting

$$p_\nu := p_\lambda \boxtimes p_\mu,$$

where

$$c_k(\nu) = \sum_{\text{lcm}(i,j)=k} \text{gcd}(i,j) c_i(\lambda) c_j(\mu),$$

in which $\text{lcm}(i,j)$ denotes the least common multiple of $i$ and $j$, and $\text{gcd}(i,j)$ denotes the greatest common divisor of $i$ and $j$, and then extending it to all symmetric functions through bilinearity.

**Proposition 1.2.4.** The operation $\boxtimes$ as defined by Definition 1.2.3 is commutative and associative. That is, for any partitions $\lambda, \mu$ and $\nu$,

(commutativity) \hspace{1cm} p_\lambda \boxtimes p_\mu = p_\mu \boxtimes p_\lambda,

(associativity) \hspace{1cm} (p_\lambda \boxtimes p_\mu) \boxtimes p_\nu = p_\lambda \boxtimes (p_\mu \boxtimes p_\nu).

**Proof.** The commutativity is clear.

For the associativity, we write

$$(p_\lambda \boxtimes p_\mu) \boxtimes p_\nu = p_\alpha,$$
$p_\lambda \boxtimes (p_\mu \boxtimes p_\nu) = p_\beta.$

Using the fact that for any positive integers $i$ and $j$,

$$ij = \text{lcm}(i,j) \text{ gcd}(i,j),$$

we calculate the number of cycles of length $l$, for any integer $l$, in the partition $\alpha$ as follows:

$$c_l(\alpha) = \sum_{\text{lcm}(i,j,k)=l} \gcd(i,j) \gcd(\text{lcm}(i,j),k) c_i(\lambda) c_j(\mu) c_k(\nu)$$

$$= \sum_{\text{lcm}(i,j,k)=l} \frac{ij \text{lcm}(i,j,k)}{i j k} \text{lcm}(\text{lcm}(i,j),k) c_i(\lambda) c_j(\mu) c_k(\nu)$$

$$= \sum_{\text{lcm}(i,j,k)=l} \frac{ijk}{i j k} c_i(\lambda) c_j(\mu) c_k(\nu)$$

$$= \sum_{\text{lcm}(i,j,k)=l} \frac{ijk}{i j k} c_i(\lambda) c_j(\mu) c_k(\nu).$$

The calculation for the partition $\beta$ is similar. □

The properties of $\boxtimes$ allow us to talk about the $\boxtimes$ operation on a set of partitions. Let $\lambda^{(i)}$, $i = 1, 2, \ldots, l$, be partitions of $n_1, n_2, \ldots, n_l$, respectively. We have

$$p_{\lambda^{(1)}} \boxtimes p_{\lambda^{(2)}} \boxtimes \cdots \boxtimes p_{\lambda^{(l)}} = p_\nu,$$

where $\nu$ is a partition of $N = n_1 n_2 \cdots n_l$. It is easy to verify that

$$c_k(\nu) = \sum_{\text{lcm}(j_1, j_2, \ldots, j_l)=k} \frac{\prod_{r=1}^{l} j_r}{k} \prod_{i=1}^{l} c_{j_i}(\lambda^{(i)}).$$
Definition 1.2.5. Let $\sigma \in \mathfrak{S}_n$. The cycle type monomial of $\sigma$, denoted $Z(\sigma)$, is the monomial in the variables $p_1, p_2, \ldots, p_n$ defined by

$$Z(\sigma) = \prod_{k=1}^{n} p_{c_k(\sigma)}^{c_k(\sigma)} = p_{\text{c.t.}(\sigma)}.$$  

In other words, the cycle type monomial of $\sigma$ is the power sum symmetric function indexed by the cycle type of $\sigma$.

Let $A$ be a subgroup of $\mathfrak{S}_n$. The cycle index polynomial of $A$, defined by Pólya [22, pp. 64–65], is

$$Z(A) = Z(A; p_1, p_2, \ldots, p_n) = \frac{1}{|A|} \sum_{\sigma \in A} Z(\sigma).$$

Pólya [21] (translated in [22]) gave the cycle index polynomials of the product and the wreath product of two permutation groups.

**Theorem 1.2.6.** (Pólya) Let $A$ and $B$ be permutation groups on $[m]$ and $[n]$, respectively. Let $A \ast B$ be the product of $A$ and $B$ acting on $[m+n]$, and let $B \wr A$ be the wreath product of $A$ and $B$ acting on $[mn]$. Then the cycle index polynomials of $A \ast B$ and $B \wr A$ are

$$Z(A \ast B) = Z(A)Z(B),$$

$$Z(B \wr A) = Z(A) \circ Z(B),$$

where $Z(A) \circ Z(B)$ denotes the plethysm of $Z(A)$ with $Z(B)$.

### 1.3. Exponentiation Group

Let $A$ be a subgroup of $\mathfrak{S}_m$, and let $B$ be a subgroup of $\mathfrak{S}_n$. We introduce in the following another representation of the wreath product (Definition 1.1.4).
**Definition 1.3.1.** The exponentiation group $B^A$, studied by Palmer [19], is isomorphic to the wreath product $B \wr A$. That means, the set of elements of $B^A$ is the same as the set of elements of $B \wr A$, and hence the order of $B^A$ is the same as the order of $B \wr A$, i.e.,

$$|B^A| = |A| \cdot |B|^m.$$ 

However the exponentiation group $B^A$ acts on $[n]^m$, identified with the set of functions from $[m]$ to $[n]$, instead of $[m] \times [n]$. Given any $\alpha \in A$ and $\tau \in B^m$, the element $(\alpha, \tau) \in B^A$ sends each element $f \in [n]^m$ to the element $g \in [n]^m$ defined by

$$(\alpha, \tau)(f)(i) = g(i) = \tau(i)(f(\alpha^{-1}i)),$$

for any $i \in [m]$. Therefore, $B^A$ can be identified with a subgroup of $\mathfrak{S}_{n^m}$.

Figure 1.4 illustrates the action of an element $(\alpha, \tau)$ of the group $B^A$.

![Figure 1.4. Group action of $B^A$.](image)

**Example 1.3.2.** Let $A$, $B$, $\alpha$ and $\tau$ be the same as in Example 1.1.5.
Let \( f : [2] \rightarrow [3] \) be such that \( f(1) = 1 \) and \( f(2) = 3 \). We see that the image of \( f \) under the action of \( (\alpha, \tau) \in B^A \) is the function \( g : [2] \rightarrow [3] \) such that \( g(1) = 3 \) and \( g(2) = 2 \), as shown in Figure 1.5.

\[
\begin{align*}
  f(1) &= 1 \\
  f(2) &= 3 \\
  g(1) &= 3 \\
  g(2) &= 2
\end{align*}
\]

Figure 1.5. The element \((\alpha, \tau)\) of \( B^A \) sends \( f \) to \( g \).

The action of \((\alpha, \tau)\) on the set of functions from \([2]\) to \([3]\) is illustrated in Figure 1.6. Hence the cycle type of \((\alpha, \tau)\) is \((6, 3)\).

Figure 1.6. The cycle type of \((\alpha, \tau)\) is \((6, 3)\).

The cycle index polynomial of the exponentiation group was given by Palmer and Robinson [20]. They defined the following operators \( I_k \) for positive integers \( k \).

Let \( \mathfrak{R} = \mathbb{Q}[p_1, p_2, \ldots] \) be the ring of polynomials with the operation \( \boxtimes \) as defined by Definition 1.2.3. Palmer and Robinson defined for positive integers \( k \) the \( \mathbb{Q} \)-linear operators \( I_k \) on \( \mathfrak{R} \) as follows:
Let \( \lambda = (\lambda_1, \lambda_2, \ldots) \) be a partition of \( n \). The action of \( I_k \) on the monomial \( p_\lambda \) is given by

\[
I_k(p_\lambda) = p_\gamma,
\]

where \( \gamma = (\gamma_1, \gamma_2, \ldots) \) is the partition of \( n^k \) with

\[
c_j(\gamma) = \frac{1}{j} \sum_{l|j} \mu\left(\frac{j}{l}\right) \left( \sum_{i|l/\gcd(k,l)} ic_i(\lambda) \right)^{\gcd(k,l)}.
\]

Furthermore, \( \{I_k\} \) generates a \( \mathbb{Q} \)-algebra \( \Omega \) of \( \mathbb{Q} \)-linear operators on \( \mathfrak{R} \). For any elements \( I, J \in \Omega \), any \( r \in \mathfrak{R} \) and \( a \in \mathbb{Q} \), we set

\[
(aI)(r) = a(I(r)),
\]

\[
(I + J)(r) = I(r) + J(r),
\]

\[
(IJ)(r) = I(r) \boxtimes J(r).
\]

**Remark 1.3.3.** As discussed in Palmer and Robinson’s proof of Theorem 1.3.6, if \( I_m(p_\mu) = p_\nu \), then \( \nu \) is the cycle type of an element \( (\alpha, \tau) \) of the exponentiation group \( B^A \) acting on \( [n]^m \), where \( \alpha \) is a permutation in \( A \) with a single \( m \)-cycle, and \( \tau \in B^m \) is such that

\[
c. t. (\tau(m)\tau(m-1) \cdots \tau(2)\tau(1)) = \mu.
\]

**Example 1.3.4.** We take the same \( A, B, \alpha \) and \( \tau \) from Examples 1.1.5. That is, \( A = \mathfrak{S}_2, B = C_3, \alpha = (1, 2) \) and \( \tau(1) = \text{id}, \tau(2) = (1, 2, 3) \). Then the cycle type of \( \alpha \) is \( \lambda = (2) \), and the cycle type of \( \tau(2)\tau(1) \) is \( \mu = (3) \). The cycle type of \( (\alpha, \tau) \) acting on the set \( [3]^2 \) is \( \nu = (6, 3) \), as shown in Figure 1.6, hence

\[
I_2(p_3) = p_5p_6.
\]
**Definition 1.3.5.** Let \( f_1 \) and \( f_2 \) be elements of the ring \( \mathcal{R} = \mathbb{Q}[p_1, p_2, \ldots] \). We define the *exponential composition* of \( f_1 \) and \( f_2 \), denoted \( f_1 \ast f_2 \), to be the image of \( f_2 \) under the operator obtained by substituting the operator \( I_r \) for the variables \( p_r \) in \( f_1 \).

Note that the operation \( \ast \) is linear in the left parameters, but not on the right parameters. We call this the *partial linearity* of the operation \( \ast \).

Let \( A \) be a subgroup of \( \mathfrak{S}_m \), and let \( B \) be a subgroup of \( \mathfrak{S}_n \). Palmer and Robinson proved the following formula [20, pp. 128–131] for computing the cycle index polynomial of the exponentiation group \( B^A \) in terms of the cycle index polynomials of \( A \) and \( B \).

**Theorem 1.3.6.** (Palmer and Robinson) Let \( A \) and \( B \) be as described in above. Then the cycle index polynomial of \( B^A \) is the exponential composition of \( Z(A) \) with \( Z(B) \). That is,

\[
Z(B^A) = Z(A) \ast Z(B).
\]

**Example 1.3.7.** Continuing Example 1.3.4, we apply Theorem 1.3.6 to compute the cycle index of the group \( B^A \), where \( A = \mathfrak{S}_2 \) and \( B = C_3 \). Note that the order of \( B^A \) is

\[
|B^A| = |A| \cdot |B|^2 = 18.
\]

We get the cycle index polynomial of \( B^A \)

\[
Z(B^A) = Z(A) \ast Z(B) = \left[ \frac{1}{2} (p_1^2 + p_2) \right] \ast \left[ \frac{1}{3} (p_1^3 + 2p_3) \right]
\]
The cycle index polynomial $Z(B^A)$ tells the structure of the group $B^A$. For example, the coefficient 6 for the term $p_3p_6$ tells that there are 6 elements in $B^A$ with cycle type $(6, 3)$. These elements are precisely those $(\alpha, \tau)$, where $\alpha$ is the 2-cycle in group $A$, and $\tau : [2] \to B$ is such that $\tau(1)\tau(2)$ is a 3-cycle in group $B$. Moreover, we observe that the term $p_3^3$ in $Z(B^A)$ with coefficient 8 is contributed in two ways. One is from those $(\alpha, \tau)$ such that $\alpha$ is the identity element of $A$, and $\tau(1)$ and $\tau(2)$ are 3-cycles in $B$, each having two choices; the other is from those $(\alpha, \tau)$ such that $\alpha$ is the identity element of $A$, one of $\tau(1)$ and $\tau(2)$ is the identity of $B$, and the other is a 3-cycle in $B$, which gives rise to 4 possibilities.

**Remark 1.3.8.** Let $A$ and $B$ be the same as in Theorem 1.3.6. Let $(\alpha, \tau)$ be an element of $B^A$, where

$$
c. t.(\alpha) = \lambda = (\lambda_1, \lambda_2, \ldots),
$$

and $\tau \in B^m$ is such that the cycle type of $\tau$ restricted on each $\lambda_i$-cycle of $\alpha$ is $\mu^{(i)}$, i.e., if the $i$-th cycle of $\alpha$ is written as

$$(a_1, a_2, \ldots, a_{\lambda_i}),$$
then $\mu^{(i)}$ is the cycle type of the permutation

$$\tau(a_1)\tau(a_2)\cdots\tau(a_{\lambda_i}).$$

Then the cycle type of $(\alpha, \tau)$, as an element of the group $B^A$ acting on the set of functions from $[m]$ to $[n]$, is $\nu$ for which

$$p_\nu = I_{\lambda_1}(p_{\mu^{(1)}}) \boxtimes I_{\lambda_2}(p_{\mu^{(2)}}) \boxtimes \cdots.$$ 

In such cases, for simplicity and without ambiguity, we write

$$p_\nu = I(\lambda; \mu^{(1)}, \mu^{(2)}, \ldots).$$
CHAPTER 2

Combinatorial Theory of Species

2.1. Definition of Species

The combinatorial theory of species was initiated by Joyal [13, 12]. In short, species are classes of “labeled structures”. A formal definition (see Bergeron, Labelle, and Leroux [2, pp. 1–11]) is given in the following.

Definition 2.1.1. Let $\mathbb{B}$ be the category of finite sets with bijections. A species (of structures) is a functor from $\mathbb{B}$ to itself, i.e.,

$$F : \mathbb{B} \to \mathbb{B}.$$

Given a species $F$, we obtain for each finite set $U$ a finite set $F[U]$, which is called the set of $F$-structures on $U$, and for each bijection $\sigma : U \to V$ a bijection

$$F[\sigma] : F[U] \to F[V],$$

which is called the transport of $F$-structures along $\sigma$.

We denote by $F[n] = F[\{1, 2, \ldots, n\}]$ the set of $F$-structures on $[n]$. The symmetric group $\mathfrak{S}_n$ acts on the set $F[n]$ by transport of structures. The $\mathfrak{S}_n$-orbits under this action are called unlabeled $F$-structures of order $n$.

Example 2.1.2. The species of graphs is denoted by $\mathcal{G}$. Note that by graphs we mean simple graphs, that is, graphs without loops or multiple edges. Thus defined,
we mean by $G[U]$ the set of graphs with vertex set $U$, and by a $G$-structure on $U$ a graph with vertex set $U$. More formally, the species of structures $G$ generates

- for any finite set $U$, a set of graphs with vertex set $U$;
- for any bijection $\sigma : U \to V$, a bijection $G[\sigma] : G[U] \to G[V]$.

![Diagram](image)

Figure 2.1. A bijection $\sigma$ from $U$ to $V$ induces a bijection $G[\sigma]$, the transport of $G$-structures along $\sigma$, sending a graph with vertex set $U$ to a graph with vertex set $V$.

Example 2.1.3. We give a list of examples of species.

- The *empty* species $0$ is defined by setting $0[U] = \emptyset$ for all $U$.
- The *singleton set* species $1$ is defined by setting

$$1[U] = \begin{cases} \{U\}, & \text{if } U = \emptyset, \\ \emptyset, & \text{otherwise.} \end{cases}$$

- The species of *singletons* $X$ is defined by setting

$$X[U] = \begin{cases} \{U\}, & \text{if } |U| = 1, \\ \emptyset, & \text{otherwise.} \end{cases}$$

- The species of *sets* $\mathcal{E}$ is defined by setting $\mathcal{E}[U] = \{U\}$ for each finite set $U$. 


The species of linear orders $L$. In particular, the species of linear orders on $n$-element sets is denoted by $X^n$.

- The species of connected graphs $G^c$.
- The species of complete graphs $K$.
- The species of permutations $\Phi$.

**Example 2.1.4.** For any graph $G$, we define the *species associated to $G$*, denoted $O_G$, to be such that

a) for each finite set $U$, $O_G[U]$ is the set of graphs isomorphic to $G$ with vertex set $U$. Note that $L(G) = |O_G[n]|$.

b) for each bijection $\sigma: U \to V$, where $|U| = |V|$, $O_G[\sigma]$ is a bijection from $O_G[U]$ to $O_G[V]$, sending a graph $H$ isomorphic to $G$ with vertex set $U$ to a graph $O_G[\sigma](H)$ whose vertex labeling is obtained from the vertex labeling of $H$ by replacing each label $u \in U$ with $\sigma(u)$.

It is straightforward to see that the bijections $O_G[\sigma]$ further satisfy

i. for all bijections $\sigma: U \to V$ and $\tau: V \to W$, $O_G[\tau \sigma] = O_G[\tau]O_G[\sigma]$.

ii. if $U = V$ and $\sigma$ is the identity map on $U$, then $O_G[\sigma]$ is also the identity map on $O_G[U]$.

![Figure 2.2.](image) The 5 $O_G$-structures on the vertex set $\{a, b, c, d, e\}$ for a given graph $G$. 

17
Definition 2.1.5. Each species $F$ is associated with three generating series. First, the exponential generating series of the species $F$, given by

$$F(x) = \sum_{n \geq 0} |F[n]| \frac{x^n}{n!},$$

counts labeled $F$-structures.

Second, the type generating series of the species $F$, given by

$$\tilde{F}(x) = \sum_{n \geq 0} f_n x^n,$$

where $f_n$ is the number of unlabeled $F$-structures of order $n$, counts unlabeled $F$-structures.

The last, but also the most important, associated series is called the cycle index of the species $F$:

$$Z_F = Z_F(p_1, p_2, \ldots) = \sum_{n \geq 0} \left( \sum_{\lambda \vdash n} \text{fix } F[\lambda] \frac{p_\lambda}{z_\lambda} \right).$$

In this definition, $\text{fix } F[\lambda]$ denotes the number of $F$-structures on $[n]$ fixed by $F[\sigma]$, where $\sigma$ is a permutation of $[n]$ with cycle type $\lambda$, and $p_\lambda$ is the power sum symmetric function indexed by the partitions $\lambda$ of $n$.

The following theorem (see [2]) illustrates the importance of the cycle index in the theory of species.

Theorem 2.1.6. (Bergeron, Labelle and Leroux) For any species of structures $F$, we have

$$F(x) = Z_F(x, 0, 0, \ldots),$$

$$\tilde{F}(x) = Z_F(x, x^2, x^3, \ldots).$$
Remark 2.1.7. Consider the functorial aspects of the species of sets $\mathcal{E}$ and the species of complete graphs $\mathcal{K}$. We see that there is a natural transformation $\alpha$ that produces for every finite set $U$ a bijection between $\mathcal{E}[U]$ and $\mathcal{K}[U]$, namely, sending the set $U$ to the complete graph with vertex set $U$. Furthermore, the following diagram commutes for any finite sets $U, V$ and any bijection $\sigma : U \to V$:

$$
\begin{array}{ccc}
\mathcal{E}[U] & \xrightarrow{\mathcal{E}[\sigma]} & \mathcal{E}[V] \\
\downarrow{\alpha} & & \downarrow{\alpha} \\
\mathcal{K}[U] & \xrightarrow{\mathcal{K}[\sigma]} & \mathcal{K}[V]
\end{array}
$$

In this case we call these two species isomorphic to each other, denoted $\mathcal{E} = \mathcal{K}$. The general definition of two species being isomorphic to each other is similar. As pointed out on [2, p. 21], the concept of isomorphism is compatible with the transition to series. Therefore, we do not make distinctions between isomorphic species during calculations.

Example 2.1.8. For $\Phi$ and $\mathcal{L}$ the species of permutations and the species of linear orders, we notice that their exponential generating series are identical:

$$
\Phi(x) = \mathcal{L}(x) = \frac{1}{1 - x},
$$

while their type generating series and cycle indices differ:

$$
\tilde{\Phi}(x) = \prod_{k \geq 1} \frac{1}{1 - x^k}, \quad \tilde{\mathcal{L}}(x) = \frac{1}{1 - x},
$$

$$
Z_\Phi = \prod_{k \geq 1} \frac{1}{1 - p_k}, \quad Z_{\mathcal{L}} = \frac{1}{1 - p_1}.
$$

This is because that although there are same number of permutations and linear orders on a given finite set $U$, the permutations and linear orders are not transported
in the same manner along bijections. In fact, a linear order admits only a single automorphism, while a permutation admits many automorphisms in general.

![Figure 2.3.](image)

**Example 2.1.9.** Let $\mathcal{G}$ be the species of graphs. It is well-known that the exponential generating series of $\mathcal{G}$ is given by

$$\mathcal{G}(x) = \sum_{n \geq 0} 2^{\binom{n}{2}} \frac{x^n}{n!}.$$

The cycle index of $\mathcal{G}$ was given on [2, p. 76]:

$$Z_{\mathcal{G}} = \sum_{n \geq 0} \left( \sum_{\lambda \vdash n} \text{fix } \mathcal{G}[\lambda] \frac{p_{\lambda}}{z_{\lambda}} \right),$$

where

$$\text{fix } \mathcal{G}[\lambda] = 2^{\frac{1}{2} \sum_{i,j \geq 1} \gcd(i,j) c_i(\lambda)c_j(\lambda) - \frac{1}{2} \sum_{k \geq 1} (k \mod 2) c_k(\lambda)},$$

in which $c_i(\lambda)$ denotes the number of parts of length $i$ in $\lambda$.

The above formulas permit us to write out the first several terms of the associated series of $\mathcal{G}$ using Maple:

$$\mathcal{G}(x) = 1 + \frac{x}{1!} + 2 \frac{x^2}{2!} + 8 \frac{x^3}{3!} + 64 \frac{x^4}{4!} + 1024 \frac{x^5}{5!} + 32768 \frac{x^6}{6!} + 2097152 \frac{x^7}{7!} + 68435456 \frac{x^8}{8!} + 68719476736 \frac{x^9}{9!} + \cdots,$$

$$\tilde{\mathcal{G}}(x) = 1 + x + 2x^2 + 4x^3 + 11x^4 + 34x^5 + 156x^6 + 1044x^7 + 12346x^8 + \cdots,$$
\[ Z_{z} = 1 + p_1 + (p_1^2 + p_2) + \left( \frac{4}{3} p_1^3 + 2p_1p_2 + \frac{2}{3} p_3 \right) + \left( \frac{8}{3} p_1^4 + 4p_1^2p_2 + 2p_2^2 + \frac{4}{3} p_1p_3 + p_4 \right) + \left( \frac{128}{15} p_1^5 + \frac{32}{3} p_1^3p_2 + 8p_1p_2^2 + \frac{8}{3} p_1^2p_3 + \frac{4}{3} p_2p_3 + 2p_1p_4 + \frac{4}{5} p_5 \right) + \cdots , \]

2.2. Species Operations

We describe in this section some frequently used operations on species, namely, the sum, product, and substitution of species. Readers are referred to [2, pp. 1–58] for more detailed definitions of \( F_1 + F_2, F_1F_2, F_1(F_2), F_1 \times F_2, F_1^*, F_1' \) for arbitrary species \( F_1 \) and \( F_2 \).

**Definition 2.2.1.** The sum of \( F_1 \) and \( F_2 \) is denoted by \( F_1 + F_2 \). An \( F_1 + F_2 \)-structure on a finite set \( U \) is either an \( F_1 \)-structure on \( U \) or an \( F_2 \)-structure on \( U \).

![Figure 2.4. Addition of species \( F_1 + F_2 \).](image)

The formulae for \( F_1 + F_2 \) are given by

\[
(F_1 + F_2)(x) = F_1(x) + F_2(x),
\]

\[
(F_1 + F_2^*)(x) = F_1^*(x) + F_2^*(x),
\]

\[
Z_{F_1+F_2} = Z_{F_1} + Z_{F_2}.
\]
Each species $F$ gives rise to a *canonical decomposition*

$$F = F_0 + F_1 + F_2 + \cdots + F_n + \cdots,$$

where \(\{F_n\}_{n \geq 0}\) is the family of species defined by setting, for each $n$,

$$F_n[U] = \begin{cases} F[U], & \text{if } |U| = n, \\ \emptyset, & \text{otherwise}. \end{cases}$$

If $F = F_n$, then we say the species $F$ is *concentrated* on the cardinality $n$. We denote by $F_+$ the species of nonempty $F$-structures:

$$F_+ = F_1 + F_2 + \cdots + F_n + \cdots,$$

$$F_+[U] = \begin{cases} F[U], & \text{if } |U| \geq 1, \\ \emptyset, & \text{if } |U| = 0. \end{cases}$$

**Example 2.2.2.** The species of sets $\mathcal{E}$ and the species of linear orders $\mathcal{L}$ can be decomposed as

$$\mathcal{E} = \mathcal{E}_0 + \mathcal{E}_1 + \mathcal{E}_2 + \cdots = 1 + X + \mathcal{E}_2 + \cdots.$$

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1 + \mathcal{L}_2 + \cdots = 1 + X + X^2 + \cdots.$$

**Definition 2.2.3.** The *product* of $F_1$ and $F_2$ is denoted by $F_1 \cdot F_2$. An $F_1F_2$-structure on a finite set $U$ is of the form $(\pi; f_1, f_2)$, where $\pi$ is an ordered partition of $U$ with two blocks $U_1$ and $U_2$, $U_i$ possibly empty, and $f_i$ is an $F_i$-structure on $U_i$ for each $i$.

The formulae for the associated series of $F_1F_2$ are given by

$$(F_1F_2)(x) = F_1(x)F_2(x),$$

$$(\widetilde{F_1F_2})(x) = \widetilde{F_1}(x)\widetilde{F_2}(x),$$

22
\[ Z_{F_1F_2} = Z_{F_1}Z_{F_2}. \]

**Figure 2.5.** Multiplication of species \( F_1 \cdot F_2 \).

**Definition 2.2.4.** The *composition* of \( F_1 \) and \( F_2 \) is denoted by \( F_1 \circ F_2 \), or equivalently, \( F_1(F_2) \). An \( F_1(F_2) \)-structure on a finite set \( U \) is a tuple of the form \((\pi, f, \gamma)\), where \( \pi \) is a partition of \( U \), \( f \) is an \( F_1 \)-structure on \( \pi \), and \( \gamma \) is a set of \( F_2 \)-structures on the blocks of \( \pi \).

**Figure 2.6.** Composition of species \( F_1 \circ F_2 \).

The formulae for the associated series of \( F_1(F_2) \) are given by

\[
(F_1(F_2))(x) = F_1(F_2(x)),
\]

\[
(\tilde{F}_1(F_2))(x) = Z_{F_1}(\tilde{F}_2(x), \tilde{F}_2(x^2), \ldots),
\]

23
\[ Z_{F_1(F_2)} = Z_{F_1} \circ Z_{F_2}, \]

where \( \circ \) is the operation of plethysm on symmetric functions defined by Definition 1.2.2.

**Definition 2.2.5.** A group \( A \) is said to *act naturally* on a species \( F \) if, for any finite set \( U \), there is an \( A \)-action

\[ \rho_U : A \times F[U] \to F[U] \]

so that for each bijection \( \sigma : U \to V \), the following diagram commutes:

\[
\begin{array}{ccc}
A \times F[U] & \xrightarrow{\rho_U} & F[U] \\
\downarrow{id_A \times F[\sigma]} & & \downarrow F[\sigma] \\
A \times F[V] & \xrightarrow{\rho_V} & F[V]
\end{array}
\]

**Definition 2.2.6.** The *quotient species* (see Bergeron, Labelle, and Leroux [2, p. 159]) of \( F \) by \( A \), denoted \( F/A \), is defined based on a group \( A \) acting naturally on a species \( F \) such that

a) for each finite set \( U \), the set of \( F/A \)-structures on \( U \) is the set of \( A \)-orbits of \( F \)-structures on \( U \), i.e.,

\[ (F/A)[U] = F[U]/A, \]

b) for each bijection \( \sigma : U \to V \), the transport of structures

\[ (F/A)[\sigma] : F[U]/A \to F[V]/A \]

is induced from the bijection \( F[\sigma] \) that sends each orbit of the action of \( A \) on \( F[U] \) to an orbit of the action of \( A \) on \( F[V] \).
The bijections \((F/A)[\sigma]\) satisfy the functorial properties
\[
(F/A)[\tau \sigma] = (F/A)[\tau] (F/A)[\sigma], \quad (F/A)[\id_U] = \id_{(F/A)[U]},
\]
because of the functoriality of the species \(F\).

The notion of quotient species appeared in \([8]\) and \([3]\) as an important tool in combinatorial enumeration.

**Example 2.2.7.** Let \(\mathcal{E}_+\) be the species of nonempty sets. Then an \((\mathcal{E}_+ \cdot \mathcal{E}_+)\)-structure on a finite set \(U\) is an ordered pair of nonempty subsets \((U_1, U_2)\) whose union equals \(U\). The symmetric group \(\mathfrak{S}_2\) acts naturally on the subscripts of \(U_i\) for \(i = 1, 2\), with orbits unordered pairs of such \((U_1, U_2)\). Thus we get a quotient species \((\mathcal{E}_+ \cdot \mathcal{E}_+)/\mathfrak{S}_2\), the species of *partitions* into two blocks, denoted \(\Psi^{(2)}\).

**Proposition 2.2.8.** Let \(F_1\) and \(F_2\) be two species. Let \(A\) be a group acting naturally on both \(F_1\) and \(F_2\). Then
\[
(F_1 + F_2)/A = F_1/A + F_2/A.
\]

**Proof.** An \((F_1 + F_2)\)-structure on a finite set \(U\) is either an \(F_1\)-structure on \(U\) or an \(F_2\)-structure on \(U\). It follows immediately that an orbit of \(A\) acting on the set of \((F_1 + F_2)\)-structures on \(U\) is either an orbit of \(A\) acting on the set \(F_1[U]\) or an orbit of \(A\) acting on the set \(F_2[U]\). \(\square\)

### 2.3. Molecular Species

**Definition 2.3.1.** A species of structures \(M\) is said to be *molecular* \([31, 30]\) if there is only one isomorphism class of \(M\)-structures, i.e., if two arbitrary \(M\)-structures are isomorphic.
In other words, the species $M$ is molecular if and only if $M \neq 0$, $M$ is concentrated on $n$, and any element in the set $M[n]$ can be sent through some transport of structures to any other element in $M[n]$.

We introduce in the following a construction of, for any subgroup $A$ of $\mathfrak{S}_n$, a molecular species $X^n/A$ (see Bergeron, Labelle, and Leroux [2, p. 144]). These species satisfy that $X^n/A = X^n/B$ if and only if $A$ and $B$ are conjugates in $\mathfrak{S}_n$. In fact, if $M$ is any molecular species concentrated on the cardinality $n$, and $s$ is any $M$-structure, then $M$ is the same as the species $X^n/A$, as defined in below, for some $A$ that is the automorphism group of $s$.

**Definition 2.3.2.** Let $n$ be a non-negative integer, $A$ a subgroup of $\mathfrak{S}_n$, $U$ and $V$ finite sets of cardinality $n$, and $\tau : U \rightarrow V$ a bijection. Define a species $X^n/A$ to be such that

a) the set of $X^n/A$-structures on $U$ is the set of (left) cosets with respect to $A$ of bijections $[n] \rightarrow U$. That is,

$$(X^n/A)[U] = \{ \sigma A \mid \sigma : [n] \rightarrow U \},$$

where $\sigma A = \{ \sigma \circ a \mid a \in A \}$.

b) the transport

$$(X^n/A)[\tau] : (X^n/A)[U] \rightarrow (X^n/A)[V]$$

is defined by setting

$$(X^n/A)[\tau](\sigma A) = (\tau \sigma)A.$$

**Example 2.3.3.** a) There is only one element in the set $\mathcal{E}_n[n]$, so that the condition “any two elements in $\mathcal{E}_n[n]$ are isomorphic” is automatically true. Hence the species
\( \mathcal{E}_n \) is a molecular species, and

\[
\mathcal{E}_n = \frac{X^n}{\mathfrak{S}_n}.
\]

b) We denote by \( \mathcal{C}_n \) the species of oriented cycles of length \( n \). We see that \( \mathcal{C}_n \) is a molecular species, and

\[
\mathcal{C}_n = \frac{X^n}{C_n},
\]

where \( C_n \) is the cyclic group of order \( n \), i.e., \( C_n \) is the subgroup of \( \mathfrak{S}_n \) in which all elements are \( n \)-cycles.

**Remark 2.3.4.** Let \( U \) be a finite set of cardinality \( n \), and let \( A \) be a subgroup of \( \mathfrak{S}_n \). Then \( A \) acts naturally on the set of linear orders on \( U \). If we call the orbit of a linear order \( s \) on \( U \) under this \( A \)-action the \( A \)-orbit of \( s \), then the \( X^n/A \)-structures on \( U \) is just the set of \( A \)-orbits of the action of \( A \) on the set of linear orders on \( U \), which is also, as pointed out on [2, p. 160], the quotient species of \( X^n \) by \( A \).

The following proposition (see [15, p. 117] Example 7.4) illustrates the close connection between Pólya’s cycle index polynomial and the cycle index of a species.

**Proposition 2.3.5.** Let \( A \) be a subgroup of \( \mathfrak{S}_n \). Then

\[
Z(A) = Z_{X^n/A}.
\]

**Proof.** Recall that the set \( (X^n/A)[n] \) is the set of cosets of \( A \) in \( \mathfrak{S}_n \). We set

\[
(X^n/A)[n] = \{g_1A, g_2A, \ldots, g_kA\},
\]

where \( g_1, g_2, \ldots, g_k \) are coset representatives. Then according to the definition of cycle index series, we have

\[
Z_{X^n/A} = \frac{1}{n!} \sum_{\tau \in \mathfrak{S}_n} \text{fix} \left( \frac{X^n}{A} \right)[\tau] Z(\tau),
\]
where $Z(\tau)$ is the cycle type polynomial of $\tau$, and the number of elements in $(X^n/A)[n]$ fixed by $\tau$ is

$$\text{fix} \frac{X^n}{A} [\tau] = |\{ i \in [k] : \tau g_i A = g_i A \}| = |\{ i \in [k] : g_i^{-1} \tau g_i \in A \}|.$$  

We notice that if for some $i$, $g_i^{-1} \tau g_i \in A$, then every element $g$ in the coset represented by $g_i A$ satisfies $g^{-1} \tau g \in A$. We notice also that each coset $g_i A$ contains exactly $|A|$ elements.

Hence we get

$$\text{fix} \frac{X^n}{A} [\tau] = \frac{1}{|A|} |\{ g \in \mathfrak{S}_n : g^{-1} \tau g \in A \}|.$$  

Therefore,

$$Z_{X^n/A} = \frac{1}{n!} \frac{1}{|A|} \sum_{\tau \in \mathfrak{S}_n} |\{ g \in \mathfrak{S}_n : g^{-1} \tau g \in A \}| Z(\tau)$$

$$= \frac{1}{n!} \frac{1}{|A|} \sum_{\tau, g \in \mathfrak{S}_n, g^{-1} \tau g \in A} Z(\tau) = \frac{1}{|A|} \sum_{\sigma \in A} Z(\sigma) = \frac{1}{|A|} \sum_{\sigma \in A} Z(\sigma) = Z(A).$$

Each subgroup $A$ of $\mathfrak{S}_n$ corresponds to a molecular species concentrated on the cardinality $n$, namely, $X^n/A$. Proposition 2.3.5 says that Pólya’s cycle index polynomial of $A$ is the same as the cycle index of the species $X^n/A$, hence these two definitions are equivalent in the case of molecular species.

**Example 2.3.6.** There are $d_{\lambda} = n!/z_\lambda$ permutations with cycle type $\lambda$ in $\mathfrak{S}_n$. Thus the cycle index polynomial of $\mathfrak{S}_n$, which is the same as the cycle index of the species
\[ Z_{\mathcal{E}_n} = Z(\mathfrak{S}_n) = \frac{1}{n!} \sum_{\lambda \vdash n} d_{\lambda} p_{\lambda} = \sum_{\lambda \vdash n} \frac{P_{\lambda}}{z_{\lambda}}. \]

**Example 2.3.7.** Recall for any graph \( G \), \( \mathcal{E}_G \) is the species associated to \( G \). We observe that \( \mathcal{E}_G \) is indeed the molecular species \( X^n/\text{aut}(G) \), where \( n \) is the number of vertices in \( G \), and \( \text{aut}(G) \) is the automorphism group of \( G \). It follows from Proposition 2.3.5 that the cycle index of \( \mathcal{E}_G \) is the cycle index polynomial of the automorphism group of \( G \). That is,

\[ Z_{\mathcal{E}_G} = Z(\text{aut}(G)). \]

For example, the cycle index of the graph \( G \) in Figure 2.2 is

\[ Z_{\mathcal{E}_G} = Z(A), \]

where \( A \) is the automorphism group of \( G \), which is the subgroup of \( \mathfrak{S}_5 \) isomorphic to \( \mathfrak{S}_4 \). To be more precise,

\[ Z_{\mathcal{E}_G} = \frac{1}{24} \left( p_1^5 + 6p_1^3p_2 + 8p_1^2p_3 + 3p_1p_2^2 + 6p_1p_4 \right). \]

We see from Definition 2.3.1 that molecular species are indecomposable under addition. This observation leads to a **molecular decomposition** of any species [2, p. 141]:

**Proposition 2.3.8.** Every species of structures \( F \) is the sum of its molecular subspecies:

\[ F = \sum_{\substack{M \subseteq F \subseteq \mathfrak{S} \text{ molecular}}} M. \]
Example 2.3.9. The molecular decomposition of the species of graphs $G$ is given on [2, p. 421]:

$$G = 1 + X + 2E + (2E^2 + 2X^2E) + (2E^3 + 2XE^2 + 2E^2 + 2X^2E) + \cdots$$

Consider the molecular species $X^m/A$ and $X^n/B$. That means $A$ is subgroup of $S_m$ and $B$ is a subgroup of $S_n$. Yeh [31, 30] proved the following theorem for molecular species.

**Theorem 2.3.10.** (Yeh) Let $A$ be a subgroup of $S_m$, and $B$ a subgroup of $S_n$ with $n \geq 1$. We have

$$\frac{X^m}{A} \cdot \frac{X^n}{B} = \frac{X^{m+n}}{A \ast B},$$

$$\frac{X^m}{A} \circ \frac{X^n}{B} = \frac{X^{mn}}{B \wr A},$$

where the product group $A \ast B$ acts on the set $[m+n]$, and the wreath product group $B \wr A$, as defined by Definition 1.1.4, acts on the set $[mn]$.

Note that Yeh’s results agree with Pólya’s Theorem 1.2.6 for the cycle index polynomials of $A \ast B$ and $B \wr A$.

In fact, as mentioned in Remark 2.3.4, we think of an $X^m/A$-structure on the set $U_1$ with $|U_1| = m$ as an $A$-orbit of linear orders on $U_1$, and an $X^n/B$-structure on the set $U_2$ with $|U_2| = n$ as a $B$-orbit of linear orders on $U_2$. Then an $(X^m/A) \cdot (X^n/B)$-structure on $U = U_1 \lor U_2$, where $\lor$ denotes the disjoint union admits an automorphism group isomorphic to the product group $A \ast B$, as shown in Figure 2.7.

We also observe that an $(X^m/A) \circ (X^n/B)$-structure is an $X^m/A$-structure on a set of $X^n/B$-structures, which is the same as a set of $B$-orbits of linear orders on $[n]$,
as shown in Figure 2.8, and hence admits an automorphism group isomorphic to the wreath product $B \wr A$.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure2.8.png}
\caption{(\(X^m/A\)) \circ (\(X^n/B\)) = X^{mn}/(B \wr A).}
\end{figure}

\section*{2.4. Compositional Inverse of \(E_+\)}

The species \(1 + X\) is the sum of the singleton set species 1 and the species of singletons \(X\). A \(1 + X\)-structure on \([n]\) is

\[
(1 + X)[n] = \begin{cases} 
\{\emptyset\}, & \text{if } n = 0, \\
\{1\}, & \text{if } n = 1, \\
\emptyset, & \text{otherwise.}
\end{cases}
\]
The associated series of $1 + X$ are

$$(1 + X)(x) = 1 + x,$$

$$(\tilde{1} + X)(x) = 1 + x,$$

$$Z_{(1+X)} = 1 + p_1.$$

A virtual species is, roughly speaking, the formal difference of species [2, p. 121]. Since the species $1 + X$ satisfies $(1 + X)(0) = 1$, Proposition 18 of [2, p. 129] gives that there exists a unique virtual species $\Gamma$, so-called “connected $(1 + X)$-structures” as defined on [2, p. 121], with

$$(2.4.1) \quad 1 + X = \mathcal{E}(\Gamma).$$

In fact, Equation (2.4.1) leads to

$$X = \mathcal{E}^+_+(\Gamma),$$

which implies that $\Gamma$ is the compositional inverse of $\mathcal{E}^+_+$, written as

$$\Gamma = \mathcal{E}^+_+(-1)(X).$$

The associated series of $\Gamma$ are given by [2, p. 131]:

$$\Gamma(x) = \log(1 + X)(x) = \log(1 + x),$$

$$\tilde{\Gamma}(x) = \sum_{k \geq 1} \frac{\mu(k)}{k} \log (1 + X)(x^k) = \sum_{k \geq 1} \frac{\mu(k)}{k} \log(1 + x^k),$$

$$Z_{\Gamma} = \sum_{k \geq 1} \frac{\mu(k)}{k} \log Z_{(1+X)} \circ p_k = \sum_{k \geq 1} \frac{\mu(k)}{k} \log(1 + p_k),$$

32
where \( \mu \) denotes the M"obius function, defined by

\[
\mu(k) = \begin{cases} 
0, & \text{if } n \text{ has one or more repeated prime factors,} \\
1, & \text{if } n = 1, \\
(-1)^j, & \text{if } n \text{ is a product of } j \text{ distinct primes.}
\end{cases}
\]

In fact, we can compute the first several terms of the associated series of \( \Gamma \):

\[
\Gamma(x) = \frac{x}{1!} - \frac{x^2}{2!} + 2 \frac{x^3}{3!} - 6 \frac{x^4}{4!} + 24 \frac{x^5}{5!} - 120 \frac{x^6}{6!} + 720 \frac{x^7}{7!} - \ldots,
\]

(2.4.2)

\[
\tilde{\Gamma}(x) = x - x^2,
\]

\[
Z_{\Gamma} = p_1 - \left( \frac{1}{2} p_1^2 + \frac{1}{2} p_2 \right) + \left( \frac{1}{3} p_1^3 - \frac{1}{3} p_3 \right) - \left( \frac{1}{4} p_1^4 - \frac{1}{4} p_2^2 \right) + \left( \frac{1}{5} p_1^5 - \frac{1}{5} p_5 \right) + \cdots.
\]

Read [23, p. 4] derived identity (2.4.2) as the type generating series of the compositional inverse of the species \( E_+ \).

**Example 2.4.1.** Let \( G^c \) be the species of connected graphs, and \( E \) the species of sets. The observation that every graph is a set of connected graphs gives rise to the following species identity:

\[
(2.4.3) \quad G = E(G^c),
\]

which can be read as “a graph is a set of connected graphs”, and gives rise to the identity

\[
G^c = \Gamma(G_+),
\]

which leads to the enumeration of connected graphs:

\[
G^c(x) = \log(G(x)),
\]
\[ \widetilde{G}^c(x) = \sum_{k \geq 1} \frac{\mu(k)}{k} \log(\widetilde{G}(x^k)), \]

\[ Z_{G^c} = \sum_{k \geq 1} \frac{\mu(k)}{k} \log(Z_G \circ p_k - p_k + 1). \]

Using Maple, we can compute the first several terms of the associated series of \( G^c \):

\[ (2.4.4) \quad G^c(x) = \frac{x}{1!} + \frac{x^2}{2!} + 4 \frac{x^3}{3!} + 38 \frac{x^4}{4!} + 728 \frac{x^5}{5!} + 26704 \frac{x^6}{6!} + 1866256 \frac{x^7}{7!} + 251548592 \frac{x^8}{8!} + 66296291072 \frac{x^9}{9!} + \ldots, \]

\[ (2.4.5) \quad \widetilde{G}^c(x) = x + x^2 + 2x^3 + 6x^4 + 21x^5 + 112x^6 + 853x^7 + 11117x^8 + \ldots, \]

\[ Z_{G^c} = p_1 + \left( \frac{1}{2} p_1^2 + \frac{1}{2} p_2 \right) + \left( \frac{1}{3} p_3 + \frac{2}{3} p_1^3 + p_1 p_2 \right) + \left( \frac{19}{12} p_1^4 + 2 p_1^2 p_2 + \frac{5}{4} p_2^2 + \frac{2}{3} p_1 p_3 + \frac{1}{2} p_4 \right) + \left( \frac{193}{15} p_1^5 + 5 p_1 p_2 + 4 \frac{p_1^2 p_3}{3} + \frac{3}{5} p_5 + p_1 p_4 \right) + \left( \frac{1669}{45} p_1^6 + \frac{91}{3} p_1^4 p_2 + \frac{38}{9} p_1^3 p_3 + \frac{43}{2} p_1^2 p_2^2 + 2 p_1^2 p_4 + \frac{8}{3} p_1 p_2 p_3 \right) + \left( \frac{4}{5} p_1 p_5 + \frac{26}{3} p_2^3 + \frac{5}{2} p_2 p_4 + \frac{25}{18} p_3^2 + \frac{5}{6} p_6 \right) + \ldots. \]

Recall Proposition 2.3.8 that states that there is a molecular decomposition of any species up to isomorphism. We can often identify a given species in terms of molecular species using combinatorial operators. Figure 2.9 shows unlabeled connected graphs on no more than 4 vertices.
In this way, the molecular decomposition of the species of connected graphs $\mathcal{G}^c$ takes the form

$$\mathcal{G}^c = X + \mathcal{E}_2 + \left( X^2 \mathcal{E}_2 + \mathcal{E}_3 \right) + \left( \mathcal{E}_2 \circ X^2 + X \mathcal{E}_3 + X^2 \mathcal{E}_2 + \mathcal{E}_2 \mathcal{E}_2 + \mathcal{E}_4 + \mathcal{D}_4 \right) + \cdots,$$

where $\mathcal{D}_4$ is the molecular species corresponding to the dihedral group $D_4$ of order 4, that is, $\mathcal{D}_4 = X^4/D_4$, and

$$Z_{\mathcal{D}_4} = Z(D_4) = \frac{1}{8} \left( p_1^4 + 2p_1^2p_2 + 3p_2^2 + 2p_4 \right).$$

### 2.5. Multisort Species

The theory of multisort species [2, p. 100] is analogous to multivariate functions.

**Definition 2.5.1.** A $k$-set $U$ is a $k$-tuple of sets

$$U = (U_1, U_2, \ldots, U_k).$$

A *multifunction* $f$ from $(U_1, U_2, \ldots, U_k)$ to $(V_1, V_2, \ldots, V_k)$, denoted

$$f : (U_1, U_2, \ldots, U_k) \rightarrow (V_1, V_2, \ldots, V_k),$$
is a \(k\)-tuple of functions \(f = (f_1, f_2, \ldots, f_k)\) such that \(f_i : U_i \to V_i\) for \(i = 1, \ldots, k\). Such \(f\) is called bijective if each \(f_i\) is a bijection.

Let \(\mathbb{B}^k\) be the category of \(k\)-sets with bijective multifunctions.

**Definition 2.5.2.** A species of \(k\) sorts, where \(k \geq 1\), is a functor from the category of finite \(k\)-sets \(\mathbb{B}^k\) to the category of finite sets \(\mathbb{B}\), i.e.,

\[
F : \mathbb{B}^k \to \mathbb{B}.
\]

A \(k\)-sort species \(F\) gives rise for each \(k\)-set

\[
U = (U_1, U_2, \ldots, U_k)
\]

a finite set \(F[U_1, U_2, \ldots, U_k]\), and for each bijective multifunction

\[
\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_k) : (U_1, U_2, \ldots, U_k) \to (V_1, V_2, \ldots, V_k)
\]

a bijection

\[
F[\sigma] = F[\sigma_1, \sigma_2, \ldots, \sigma_k] : F[U_1, U_2, \ldots, U_k] \to F[V_1, V_2, \ldots, V_k]
\]

that is called the transport of \(F\)-structures along \(\sigma\).

We denote by \(F(X, Y)\) a 2-sort species \(F\). We use the notation \([m, n]\), where \(m\) and \(n\) are positive integers, to denote the 2-set \((\{1, 2, 3, \ldots, m\}, \{1, 2, 3, \ldots, n\})\).

The exponential generating series of \(F(X, Y)\) is

\[
F(x, y) = \sum_{m,n \geq 0} |F[m, n]| \frac{x^m}{m!} \frac{y^n}{n!},
\]

where \(F[m, n] = F[\{1, 2, \ldots, m\}, \{1, 2, \ldots, n\}]\) is the number of labeled \(F\)-structures on the 2-set \([m, n]\).
The type generating series of \( F(X, Y) \) is

\[
\tilde{F}(x, y) = \sum_{m,n \geq 0} f_{m,n} x^m y^n,
\]

where \( f_{m,n} \) is the number of unlabeled \( F \)-structures in which the cardinality of the first sort set is \( m \) and the cardinality of the second sort set is \( n \).

The cycle index of \( F(X, Y) \) is

\[
Z_{F(X,Y)} = \sum_{m,n \geq 0} \left( \sum_{\lambda \vdash m, \mu \vdash n} \text{fix } F[\lambda, \mu] \frac{p_{\lambda}[x]}{z_{\lambda}} \frac{p_{\mu}[y]}{z_{\mu}} \right),
\]

where \( p_{\lambda}[x] \) and \( p_{\lambda}[y] \) are power sum symmetric functions in variable sets \( x_1, x_2, \ldots \) and \( y_1, y_2, \ldots \), respectively, \( \text{fix } F[\lambda, \mu] \) denotes the number of \( F \)-structures on \( [m, n] \) fixed by \( F[\sigma, \pi] \), where \( \sigma \) is a permutation of \( [m] \) with cycle type \( \lambda \) and \( \pi \) is a permutation of \( [n] \) with cycle type \( \mu \).

**Example 2.5.3.** Let \( \mathcal{A}(X, Y) \) be the 2-sort species of rooted trees whose internal vertices are of sort \( X \) and whose leaves are of sort \( Y \). Figure 2.11 shows the transport
of structures of two $\mathcal{A}(X, Y)$-structures under a bijective multifunction

$$\sigma = \begin{pmatrix} 2 & 3 & 4 & 5 & 7 & 8 & 9 & 12 \\ j & a & g & m & f & e & d & n \end{pmatrix} \quad \begin{pmatrix} 1 & 6 & 10 & 11 & 13 & 14 \\ l & k & h & b & i & c \end{pmatrix};$$

![Figure 2.11](image)

**Figure 2.11.** The transport of structures $\mathcal{A}[\sigma]$ sends an element of $\mathcal{A}[U_1, U_2]$ to an element of $\mathcal{A}[V_1, V_2]$, where

$U_1 = \{2, 3, 4, 5, 7, 8, 9, 12\}$, $U_2 = \{1, 6, 10, 11, 13, 14\}$,

$V_1 = \{j, a, g, m, f, e, d, n\}$, $V_2 = \{l, k, h, b, i, c\}$.

### 2.6. Arithmetic Product of Species

The arithmetic product was studied by Manuel Maia and Miguel Méndez [18]. They developed a decomposition of a set, called a *rectangle*, which, as we shall see, is essentially an equivalence class of high dimensional linear orders.

**Definition 2.6.1.** Let $U$ be a finite set. Suppose $|U| = ab$. A *rectangle* on $U$ of *height* $a$ is a pair $(\pi_1, \pi_2)$ such that $\pi_1$ is a partition of $U$ with $a$ blocks, each of size $b$, and $\pi_2$ is a partition of $U$ with $b$ blocks, each of size $a$, and if $B$ is a block of $\pi_1$ and $B'$ is a block of $\pi_2$ then $|B \cap B'| = 1$. 

38
Figure 2.12 shows two representations of a rectangle on \([12]\) of height 3. They both represent the rectangle \((\pi_1, \pi_2)\).

\[
\pi_1 = \{\{1, 3, 4, 9\}, \{2, 5, 8, 10\}, \{6, 7, 11, 12\}\}, \\
\pi_2 = \{\{1, 8, 12\}, \{3, 5, 6\}, \{2, 4, 11\}, \{7, 9, 10\}\}.
\]

![Figure 2.12. A rectangle on \([12]\) of height 3.](image)

Equivalently we can represent a rectangle as a bipartite graph. A rectangle which is the same as in Figure 2.12 is shown by Figure 2.13, where the labels are on the edges, and the vertex sets on the left and on the right represent partitions \(\pi_1\) and \(\pi_2\). More precisely, each edge \(x\) in the bipartite graph corresponds to exactly one pair of vertices \((A_i, B_j)\) with \(A_i \in \pi_1\) and \(B_j \in \pi_2\), and this can be interpreted as \(x\) being the only element in the intersection of \(A_i\) and \(B_j\).

\[
\pi_1 = \{A_1, A_2, A_3\} \\
\pi_2 = \{B_1, B_2, B_3, B_4\}
\]

![Figure 2.13. A rectangle on \([12]\) of height 3.](image)
Definition 2.6.2. Let \( U \) be a finite set. A \( k \)-rectangle on \( U \) is a \( k \)-tuple of partitions \((\pi_1, \pi_2, \ldots, \pi_k)\) such that

a) for each \( i \in [k] \), \( \pi_i \) has \( a_i \) blocks, each of size \( |U|/a_i \), where \( |U| = \prod_{i=1}^{k} a_i \).

b) for any \( k \)-tuple \((B_1, B_2, \ldots, B_k)\), where \( B_i \) is a block of \( \pi_i \) for each \( i \in [k] \), we have \(|B_1 \cap B_2 \cap \cdots \cap B_k| = 1\).

Figure 2.14 shows a 3-rectangle \((\pi_1, \pi_2, \pi_3)\), represented by a 3-partite graph, and labeled are on the triangles.

We denote by \( \mathcal{N} \) the species of rectangles, and by \( \mathcal{N}^{(k)} \) the species of \( k \)-rectangles.

Let \( n = \prod_{i=1}^{k} a_i \), and let \( \Delta \) be the set of bijections of the form

\[ \delta : [a_1] \times [a_2] \times \cdots \times [a_k] \to [n], \]

Note that the cardinality of the set \( \Delta \) is \( n! \). The group

\[ \prod_{i=1}^{k} \mathfrak{S}_{a_i} = \{ \sigma = (\sigma_1, \sigma_2, \ldots, \sigma_k) : \sigma_i \in \mathfrak{S}_{a_i} \} \]

acts on the set \( \Delta \) by setting

\[ (\sigma \cdot \delta)(i_1, i_2, \ldots, i_k) = \delta(\sigma_1(i_1), \sigma_2(i_2), \ldots, \sigma_k(i_k)), \]

Figure 2.14. A 3-rectangle labeled on the triangles.
for each \((i_1, i_2, \ldots, i_k) \in [a_1] \times [a_2] \times \cdots \times [a_k]\). We observe that this group action result in a set of \(\prod_{i=1}^{k} \mathfrak{S}_{a_i}\)-orbits, and that each orbit consists of exactly \(a_1!a_2! \cdots a_k!\) elements of \(\Delta\). Observe further that there is a one-to-one correspondence between the set of \(\prod_{i=1}^{k} \mathfrak{S}_{a_i}\)-orbits on the set \(\Delta\) and the set of \(k\)-rectangles of the form \((\pi_1, \ldots, \pi_k)\), where each \(\pi_i\) has \(a_i\) blocks. Therefore, the number of such \(k\)-rectangles is

\[
\{ \frac{n}{a_1, a_2, \ldots, a_k} \} := \frac{n!}{a_1!a_2! \cdots a_k!}.
\]

**Definition 2.6.3.** Let \(F_1\) and \(F_2\) be species of structures with \(F_1[\emptyset] = F_2[\emptyset] = \emptyset\). The **arithmetic product** of \(F_1\) and \(F_2\), denoted \(F_1 \Box F_2\), is defined by setting for each finite set \(U\),

\[
(F_1 \Box F_2)[U] = \sum_{(\pi_1, \pi_2) \in \mathcal{N}[U]} F_1[\pi_1] \times F_2[\pi_2],
\]

where the sum represents the disjoint union. In other words, an \(F_1 \Box F_2\)-structure on a finite set \(U\) is a tuple of the form \(((\pi_1, f_1), (\pi_2, f_2))\), where \(f_i\) is an \(F_i\)-structure on the blocks of \(\pi_i\) for each \(i\).

A bijection \(\sigma : U \to V\) sends a partition \(\pi\) of \(U\) to a partition \(\pi'\) of \(V\), namely, \(\sigma(\pi) = \pi' = \{\sigma(B) : B\) is a block of \(\pi\}\). Thus \(\sigma\) induces a bijection \(\sigma_{\pi} : \pi \to \pi'\), sending each block of \(\pi\) to a block of \(\pi'\).

The transport of structures for any bijection \(\sigma : U \to V\) is defined by

\[
(F_1 \Box F_2)[\sigma]((\pi_1, f_1), (\pi_2, f_2)) = ((\pi'_1, F_1[\sigma_{\pi_1}](f_1)), (\pi'_2, F_2[\sigma_{\pi_2}](f_2))).
\]

The arithmetic product on species satisfies the following properties. They are straightforward to check using the definition.
Figure 2.15. Arithmetic product $F_1 \boxtimes F_2$.

**Proposition 2.6.4.** (Maia and Méndez) Let $F_1, F_2$ and $F_3$ be species of structures with $F_i[\emptyset] = \emptyset$ for $i = 1, 2, 3$, and let $X$ be the species of singleton sets. Then we have

- **(commutativity)** $F_1 \boxtimes F_2 = F_2 \boxtimes F_1$,
- **(associativity)** $F_1 \boxtimes (F_2 \boxtimes F_3) = (F_1 \boxtimes F_2) \boxtimes F_3$,
- **(distributivity)** $F_1 \boxtimes (F_2 + F_3) = F_1 \boxtimes F_2 + F_1 \boxtimes F_3$,
- **(unit)** $F_1 \boxtimes X = X \boxtimes F_1 = F_1$.

Figure 2.16. $X$ is the unit of the arithmetic product: $F \boxtimes X = F$.

The following proposition about the arithmetic product of two molecular species could be taken as an alternative definition of the arithmetic product.

**Proposition 2.6.5.** Let $X^m/A$ and $X^n/B$ be two molecular species. That is, $A$ is a subgroup of $\mathfrak{S}_m$, and $B$ is a subgroup of $\mathfrak{S}_n$. Then

$$\frac{X^m}{A} \boxtimes \frac{X^n}{B} = \frac{X^{mn}}{A \times B},$$
where $A \times B$ is the product group acting on the set $[mn]$ as defined by Definition 1.1.3.

**Example 2.6.6.** Recall that the molecular species $E_2$ is the same as the species $X^2/S_2$. The arithmetic product of the species $E_2$ with itself is a species concentrated on the cardinality 4. To be more precise, the set of $E_2 \bowtie E_2$-structures on a set $U$ with $|U| = 4$ are obtained by taking the $S_2 \times S_2$-orbits of 2 by 2 squares filled with elements of $U$, where the group $S_2 \times S_2$ acts by switching the rows and the columns. In other words, $E_2 \bowtie E_2 = X^4/(S_2 \times S_2)$.

![Diagram](image)

**Figure 2.17.** The species $E_2 \bowtie E_2$ is isomorphic to the species $X^4/(S_2 \times S_2)$.

We can quickly verify Proposition 2.6.5 by observing that the $X^m/A$-structures are $A$-orbits of linear orders on $[m]$, and the $X^n/B$-structures are $B$-orbits of linear orders on $[n]$, and hence an $(X^m/A) \bowtie (X^n/B)$-structure on $[mn]$ is just a matrix whose rows and columns are $A$-orbits of linear orders on $[m]$ and $B$-orbits of linear orders on $[n]$, respectively. The automorphism group of such an $(X^m/A) \bowtie (X^n/B)$-structure is therefore isomorphic to the product group $A \times B$.

The associativity of the arithmetic product allows us to talk about the arithmetic product of a set of species.
Definition 2.6.7. The arithmetic product of species $F_1, F_2, \ldots, F_k$ with $F_i(\emptyset) = \emptyset$ for all $i$ is defined by setting

$$\bigboxtimes_{i=1}^{k} F_i = F_1 \boxtimes F_2 \boxtimes \cdots \boxtimes F_k,$$

which sends each finite set $U$ to the set

$$\bigboxtimes_{i=1}^{k} F_i[U] = \sum F_1[\pi_1] \times F_2[\pi_2] \times \cdots \times F_k[\pi_k],$$

where the sum is taken over all $k$-rectangles $(\pi_1, \pi_2, \ldots, \pi_k)$ of $U$, and represents the disjoint union. We denote by $F^{\boxtimes k}$ the arithmetic product of $k$ copies of $F$.

For each bijection $\sigma : U \rightarrow V$, the transport of structures of $\bigboxtimes_{i=1}^{k} F_i$ along $\sigma$ sends an $\bigboxtimes_{i=1}^{k} F_i$-structure on $U$ of the form

$$((\pi_1, f_1), (\pi_2, f_2), \ldots, (\pi_k, f_k))$$

to and $\bigboxtimes_{i=1}^{k} F_i$-structure on $V$ of the form

$$((\pi'_1, F_1[\sigma_{\pi_1}]f_1), (\pi'_2, F_2[\sigma_{\pi_2}]f_2), \ldots, (\pi'_k, F_k[\sigma_{\pi_k}]f_k)),$$
where $\sigma_{\pi_i}$ is the bijection induced by $\sigma$ sending blocks of $\pi_i$ to blocks of $\pi'_i$.

**Proposition 2.6.8.** (Maia and Méndez) *We have the following identities for the species of $k$-rectangles.*

\[
\mathcal{N} = \mathcal{E}_+ \boxtimes \mathcal{E}_+,
\]
\[
\mathcal{N}^{(k)} = \mathcal{E}_+ \boxtimes \mathcal{E}_k,
\]
\[
\mathcal{N}^{(i+j)} = \mathcal{N}^{(i)} \boxtimes \mathcal{N}^{(j)}.
\]

**Proof.** These identities follow straightforwardly from the definitions of rectangle and arithmetic product of species. \qed

Figures 2.17 and 2.19 show that the set $\mathcal{E}_2 \boxtimes \mathcal{E}_2[4]$ is the same as the set of rectangles on $[4]$ of height 2.

![Image of E2 boxtimes E2 structures on [4]](image)

**Figure 2.19.** The $\mathcal{E}_2 \boxtimes \mathcal{E}_2$-structures on the set $[4]$.

Maria and Méndez [18] gave the formula for the cycle index of the arithmetic product.
Theorem 2.6.9. (Maria and Méndez) Let species $F_1$ and $F_2$ satisfy

$$F_1[\emptyset] = F_2[\emptyset] = \emptyset.$$ 

Then we have

(2.6.1) 

$$Z_{F_1 \boxplus F_2} = Z_{F_1} \boxtimes Z_{F_2},$$

where the operation $\boxtimes$ on the power sum symmetric functions on the right-hand side of the equation is given by Definition 1.2.3.

We notice that due to the linearities of both the arithmetic product of species and the operation $\boxtimes$ on power sum symmetric functions, identity (2.6.1) reduces to the case when $F_1$ and $F_2$ are both molecular species.

Suppose, say, $F_1 = X^m/A$ and $F_2 = X^n/B$ for some integers $m, n$, and some $A$ and $B$ subgroups of $\mathfrak{S}_m$ and $\mathfrak{S}_n$, respectively. We apply Proposition 2.6.5 and Proposition 2.3.5 to translate the formula

$$Z_{(X^m/A) \boxplus (X^n/B)} = Z_{X^m/A} \boxtimes Z_{X^n/B}$$

into

(2.6.2) 

$$Z(A \times B) = Z(A) \boxtimes Z(B).$$

Identity (2.6.2) can be roughly verified by observing that if $a$ is an element of $A$ and $b$ is an element of $B$, then the cycle type of $(a, b)$ in the group $A \times B$ satisfies

$$p_{c.t.((a, b))} = p_{c.t.(a)} \boxtimes p_{c.t.(b)}.$$
This is because each pair of a $k$-cycle in $a$ and an $l$-cycle in $b$ generates cycles of length $\text{lcm}(k, l)$ in the group $A \times B$ with multiplicity $\gcd(k, l)$, and that the formula for such pairs of $k$-cycles in $a$ and $l$-cycles in $b$ is

$$p_k^{i_k} \boxtimes p_l^{i_l} = p_{\text{lcm}(k, l)}^{\gcd(k, l)i_k,i_l}.$$ 

Figure 2.20 gives an illustration of $p_3 \boxtimes p_4 = p_{12}$.

FIGURE 2.20. A 3-cycle in the group $A$ and a 4-cycle in the group $B$ generates a 12-cycle in the group $A \times B$.

Summing up on all different cycle lengths of $a$ and $b$, we get the desired result.
CHAPTER 3

Cartesian Product of Graphs and Prime Graphs

3.0. Introduction

In this chapter, we look at the well-known operation of Cartesian product (Definition 3.1.1) on graphs, and the notion of prime graphs (Definition 3.1.3) with respect to Cartesian multiplication. Our goal is to find the cycle index of the species of prime graphs.

First, we get a relation (Proposition 3.1.8) between the Cartesian product of graphs and the arithmetic product of species (Definition 2.6.3). We then use the tool of Dirichlet exponential generating series (Definition 3.2.3) to get a formula (Theorem 3.2.9) expressing the number of labeled prime graphs in terms of the number of labeled connected graphs. Furthermore, we see that the unique factorization of a nontrivial connected graph into the product of powers of prime graphs (Sabidussi [26]) gives a free commutative monoid structure on the set of unlabeled connected graphs, and leads to a formula (Theorem 3.3.10) that counts unlabeled prime graphs in terms of unlabeled connected graphs.

In terms of species, the arithmetic product of species studied by Maia and Méndez [18] comes back into play. As it turns out, we need a stronger notion than arithmetic product in order to express the species of connected graphs in terms of the species of prime graphs. We therefore define a new operation, the exponential composition of species (Definition 3.5.1), which is related to the arithmetic product of species as
the composition of species is related to the multiplication of species, and get a formula (Theorem 3.6.2) expressing the species of connected graphs as the exponential composition of the species of prime graphs. An explicit formula for the inverse of exponential composition would be nice to find, but that problem remains open.

The enumeration of the species of prime graphs is therefore complete by applying the enumeration theorem (Theorem 3.4.4) for the exponential composition of species, which is a generalization of the enumeration theorem by Palmer and Robinson about the cycle index polynomial of the exponentiation group (Theorem 1.3.6).

### 3.1. Cartesian Product of Graphs

For any graph $G$, we let $V(G)$ be the vertex set of $G$, $E(G)$ the edge set of $G$, and $l(G) = |V(G)|$ the number of vertices in $G$. Two graphs $G$ and $H$ with the same number of vertices are said to be isomorphic, denoted $G \cong H$, if there exists a bijection from $V(G)$ to $V(H)$ that preserves adjacency. Such a bijection is called an isomorphism from $G$ to $H$. In the case when $G$ and $H$ are identical, this bijection is called an automorphism of $G$. The collection of all automorphisms of $G$, denoted $\text{aut}(G)$, constitutes a group called the automorphism group of $G$.

We call the isomorphism classes of graphs unlabeled graphs. If $G$ is a graph with $n$ vertices, $L(G)$ is the number of graphs isomorphic to $G$ with vertex set $[n]$. It is well-known that

$$L(G) = \frac{l(G)!}{|\text{aut}(G)|}.$$  

We use the notation $\sum_{i=1}^{n} G_i = G_1 + G_2 + \cdots + G_n$ to mean the disjoint union of a set of graphs $\{G_i\}_{i=1,\ldots,n}$.

**Definition 3.1.1.** The Cartesian product of graphs $G_1$ and $G_2$, denoted $G_1 \odot G_2$, as defined by Sabidussi [26] under the name the weak Cartesian product, is the graph
whose vertex set is

\[ V(G_1 \odot G_2) = V(G_1) \times V(G_2) = \{(u, v) : u \in V(G_1), v \in V(G_2)\}, \]

in which \((u, v)\) is adjacent to \((w, z)\) if

either \(u = w\) and \(\{v, z\} \in E(G_2)\) or \(v = z\) and \(\{u, w\} \in E(G_1)\).

For simplicity and without ambiguity, we call \(G_1 \odot G_2\) the product of \(G_1\) and \(G_2\).

The following properties of the Cartesian multiplication can be verified straightforwardly.

**Proposition 3.1.2.** Let \(G_1, G_2\) and \(G_3\) be graphs. Then

\[
\begin{align*}
\text{(commutativity)} & \quad G_1 \odot G_2 \cong G_2 \odot G_1, \\
\text{(associativity)} & \quad (G_1 \odot G_2) \odot G_3 \cong G_1 \odot (G_2 \odot G_3).
\end{align*}
\]
These properties allow us to talk about the Cartesian product of a set of graphs \( \{G_i\}_{i \in I} \), denoted \( \circ \bigcirc G_i \). We denote by \( G^n \) the Cartesian product of \( n \) copies of \( G \).

**Definition 3.1.3.** A graph \( G \) is *prime* with respect to Cartesian multiplication if \( G \) is a connected graph with more than one vertex such that \( G \cong H_1 \circ H_2 \) implies that either \( H_1 \) or \( H_2 \) is a singleton vertex.

Two graphs \( G \) and \( H \) are called *relatively prime* with respect to Cartesian multiplication, if and only if \( G \cong G_1 \circ J \) and \( H \cong H_1 \circ J \) imply that \( J \) is a singleton vertex.

We denote by \( \mathcal{P} \) the species of prime graphs. We also denote by \( \mathbb{C} \) the set of unlabeled connected graphs, and by \( \mathbb{P} \) the set of unlabeled prime graphs.

If \( G \) is a connected graph, then \( G \) can be decomposed into prime factors, that is, there is a set \( \{P_i\}_{i \in I} \) of prime graphs such that \( G \cong \bigcirc P_i \). In Figure 3.2, a connected graph \( G \) with 24 vertices is decomposed into the product of prime graphs \( P_1, P_2, P_3 \) with 3, 2 and 4 vertices, respectively.

\[ \text{Figure 3.2. The decomposition of a connected graph into prime graphs.} \]

Furthermore, we have the following theorem given by Sabidussi [26].

**Theorem 3.1.4.** (Sabidussi) For any non-trivial connected graph \( G \), the factorization of \( G \) into the Cartesian product of prime powers is unique up to isomorphism.
The automorphism groups of the Cartesian product of a set of graphs was studied by Sabidussi [26] and Palmer [19].

**Theorem 3.1.5.** (Sabidussi) Let \( \{G_i\}_{i=1,...,n} \) be a set of graphs. Then the automorphism group of the Cartesian product of \( \{G_i\}_{i=1,...,n} \) is isomorphic to the automorphism group of the sum of \( \{G_i\}_{i=1,...,n} \). That is,

\[
\text{aut} \left( \bigodot_{i=1}^{n} G_i \right) \cong \text{aut} \left( \sum_{i=1}^{n} G_i \right).
\]

**Theorem 3.1.6.** (Sabidussi) Let \( G_1, G_2, \ldots, G_n \) be connected graphs which are pairwise relatively prime with respect to Cartesian multiplication. Then the automorphism group of the Cartesian product of \( \{G_i\}_{i=1,...,n} \) is isomorphic to the product of each of the automorphism groups of \( \{G_i\}_{i=1,...,n} \). That is,

\[
\text{aut} \left( \bigodot_{i=1}^{n} G_i \right) \cong \prod_{i=1}^{n} \text{aut}(G_i).
\]

**Example 3.1.7.** The prime graphs \( P_1, P_2 \) and \( P_3 \) in Figure 3.2 are pairwise relatively prime, so the automorphism group of \( G \) is

\[
\text{aut}(G) = \text{aut}(P_1) \times \text{aut}(P_2) \times \text{aut}(P_3) = S_2 \times S_2 \times V_4,
\]

where \( V_4 \cong S_2 \times S_2 \).

Recall the arithmetic product of species defined by Definition 2.6.3 and the species associated to a graph defined in Example 2.1.4. We present in the following the close connection between the arithmetic product and the Cartesian product.
Proposition 3.1.8. Let $G_1$ and $G_2$ be two graphs that are relatively prime to each other. Then the species associated to the Cartesian product of $G_1$ and $G_2$ is equivalent to the arithmetic product of the species associated to $G_1$ and the species associated to $G_2$. That is,

$$\mathcal{O}_{G_1 \odot G_2} = \mathcal{O}_{G_1} \boxtimes \mathcal{O}_{G_2}$$

Proof. Let $l(G_1) = m$ and $l(G_2) = n$. Then $l(G_1 \odot G_2) = mn$.

Since $G_1$ and $G_2$ are relatively prime, applying Theorem 3.1.6 we get

$$\text{aut}(G_1 \odot G_2) = \text{aut}(G_1) \times \text{aut}(G_2).$$

Therefore,

$$\mathcal{O}_{G_1 \odot G_2} = \frac{X^{l(G_1 \odot G_2)}}{\text{aut}(G_1 \odot G_2)} = \frac{X^{mn}}{\text{aut}(G_1) \times \text{aut}(G_2)} = \frac{X^m}{\text{aut}(G_1)} \boxtimes \frac{X^n}{\text{aut}(G_2)} = \mathcal{O}_{G_1} \boxtimes \mathcal{O}_{G_2}.$$ 

Note that if $G_1$ and $G_2$ are not relatively prime to each other, then the species associated to the Cartesian product of $G_1$ and $G_2$ is generally different from the arithmetic product of $\mathcal{O}_{G_1}$ and $\mathcal{O}_{G_2}$. This is because that the automorphism group of the product of the graphs is no longer the product of the automorphism groups of the graphs. For example, we will see in Remark 3.2.2 that for any prime graph $P$,

$$\text{aut}(P \odot P) = \text{aut}(P)^{\mathfrak{S}_2},$$

and $\text{aut}(P)^{\mathfrak{S}_2}$ is generally much larger than $\text{aut}(P)^2$. 

53
3.2. Labeled Prime Graphs

We introduce in the following an important theorem by Sabidussi about the automorphism group of a connected graph using its prime factorization.

**Theorem 3.2.1.** (Sabidussi) Let $G$ be a connected graph with prime factorization

$$G \cong P_{s_1}^1 \odot P_{s_2}^2 \odot \cdots \odot P_{s_k}^k,$$

where for $r = 1, 2, \ldots, k$, all $P_r$ are distinct prime graphs, and all $s_r$ are positive integers. Then we have

$$\text{aut}(G) \cong \prod_{r=1}^{k} \text{aut}(P_{s_r}^r) \cong \prod_{r=1}^{k} \text{aut}(P_r)^{s_r}.$$

In other words, the automorphism group of $G$ is generated by the automorphism groups of the factors and the transpositions of isomorphic factors.

**Remark 3.2.2.** (A quick verification of Theorem 3.2.1, and more.) Note that the $P_{s_r}^r$, for $r = 1, 2, \ldots, k$, are pairwise relatively prime. With Theorem 3.1.6 handy, we see that Theorem 3.2.1 is equivalent to the following special case:

If $P$ is any prime graph and $k$ is a nonnegative integer, then the automorphism group of $P^k$ is the exponentiation group $\text{aut}(P)^{\mathfrak{S}_k}$, i.e.,

$$\text{aut}(P^k) = \text{aut}(P)^{\mathfrak{S}_k}.$$

In fact, we quickly observe that $\text{aut}(P)^{\mathfrak{S}_k}$ is a subgroup of $\text{aut}(P^k)$, since every element

$$(\alpha, \tau) = (\alpha; \tau(1), \tau(2), \ldots, \tau(k)) \in \text{aut}(P)^{\mathfrak{S}_k}$$

54
with $\alpha \in \mathfrak{S}_k$ and $\tau(i) \in \text{aut}(P)$, for all $i$, gives rise to an automorphism of the product graph $P^k$ by letting each $\tau(i)$ act on a copy of $P$ in $P^k$ and letting $\alpha$ act on the $k$ copies of $P$ in $P^k$. More precisely, since each of the vertices of $P^k$ is a $k$-vector where the $i$-th coordinate is contributed by a vertex in the $i$-th copy of $P$, the permutation $\alpha$ acts on $P^k$ by permuting the coordinates of the vertices of $P^k$. Therefore, the exponentiation group $\text{aut}(P)^{\mathfrak{S}_k}$ is a subgroup of the automorphism group of $P^k$.

Hence what Sabidussi’s theorem really says is that the automorphism group of $P^k$ is no bigger than the exponentiation group $\text{aut}(P)^{\mathfrak{S}_k}$. Therefore, Theorem 3.2.1 can be verified by showing that these two groups contain the same number of elements. That is, it remains to show that

$$\text{aut}(P^k) = |\text{aut}(P)^{\mathfrak{S}_k}|.$$ 

Recall that for any graph $G$, $kG$ is the sum of $k$ copies of $G$. By Theorem 3.1.5, we have

$$|\text{aut}(P^k)| = |\text{aut}(kP)|.$$ 

Therefore, it suffices for us to show that

$$|\text{aut}(kP)| = k! |\text{aut}(P)|^k,$$

where the right-hand side is the same as the order of the exponentiation group $\text{aut}(P)^{\mathfrak{S}_k}$.

Note that $kP$ has $k$ connected components, each of which is a copy of $P$. Let $\alpha$ be an automorphism of $kP$, and let $v_1, v_2$ be vertices of $kP$ that are in the same connected component. Since automorphisms preserve adjacency, $\alpha(v_1)$ and $\alpha(v_2)$ are in the same connected component of $\alpha(kP) = kP$. Therefore, $\alpha$ sends one connected component of $kP$ to another connected component of $kP$, possibly the same one.
Let us assume, say, that $\alpha(P_1) = P_2$, where $P_1$ and $P_2$ are two arbitrary connected components of $kP$, possibly the same one. This means that $P_1$ and $P_2$ are both copies of $P$. Let $\alpha_1$ be the action of $\alpha$ restricted to $P_1$. Then there is some $\sigma : P_2 \to P_1$ such that $\sigma \alpha_1$ is an automorphism of $P$. Therefore, such an $\alpha$ can be obtained by taking an automorphism of each connected component of $kP$, separately, followed by putting a permutation on $[k]$ over the $k$ copies of $P$. In the meanwhile, the above argument also implies that this is the only way to construct an automorphism of $kP$. Thus we see from Definition 1.1.4 that the automorphism group of $kP$ is the wreath product group $\text{aut}(P) \wr \mathfrak{S}_k$, i.e.,

$$\text{aut}(kP) = \text{aut}(P) \wr \mathfrak{S}_k,$$

which gives that

$$|\text{aut}(kP)| = |\text{aut}(P) \wr \mathfrak{S}_k| = k! |\text{aut}(P)|^k.$$

In what follows in this section all graphs considered are connected.

**Definition 3.2.3.** The *Dirichlet exponential generating series* for a sequence of numbers $\{a_n\}_{n \in \mathbb{N}}$ is defined by $\sum_{n \geq 1} a_n/n! n^s$. 

56
Multiplication of Dirichlet exponential generating series is given by

\[
(\sum_{n \geq 1} \frac{a_n}{n! n^s})(\sum_{n \geq 1} \frac{b_n}{n! n^s}) = \sum_{n \geq 1} \frac{c_n}{n! n^s},
\]

where

\[
c_n = \sum_{k \mid n} \binom{n}{k} a_k b_{n/k} = \sum_{k \mid n} \frac{n!}{k! (n/k)!} a_k b_{n/k}.
\]

The Dirichlet exponential generating function for a species \( F \) with the restriction \( F[\emptyset] = \emptyset \) is defined by

\[
\mathcal{D}(F) = \sum_{n \geq 1} \frac{|F[n]|}{n! n^s}.
\]

**Example 3.2.4.** Recall that for any graph \( G \), \( \mathcal{O}_G \) is the species associated to \( G \). We denote by \( \mathcal{D}(G) \) the Dirichlet exponential generating function for the species \( \mathcal{O}_G \). More explicitly,

\[
\mathcal{D}(G) = \mathcal{D}(\mathcal{O}_G) = \frac{L(G)}{l(G)! l(G)^s}.
\]

It is illustrated by the following proposition that the Dirichlet exponential generating functions are useful for enumeration involving the arithmetic product of species.

**Proposition 3.2.5.** (Maia and Méndez) Let \( F_1 \) and \( F_2 \) be species with \( F_i[\emptyset] = \emptyset \) for \( i = 1, 2 \). Then

\[
\mathcal{D}(F_1 \boxtimes F_2) = \mathcal{D}(F_1) \mathcal{D}(F_2).
\]

**Proof.** This proof was given by Maia and Méndez [18, p. 6]. We calculate the number of \( F_1 \boxtimes F_2 \)-structures on the set \([n]\):

\[
|F_1 \boxtimes F_2[n]| = \sum_{(\pi_1, \pi_2) \in \mathcal{N}[n]} |F_1[\pi_1]| |F_2[\pi_2]|
\]
\[ \sum_{a|n} \sum_{\pi_1, \pi_2 \in \pi \leftarrow [n]} |F_1[a]| |F_2[n/a]| \]

\[ = \sum_{a|n} \left\{ \frac{n}{a} \right\} |F_1[a]| |F_2[n/a]|. \]

Equation (3.2.2) follows from the multiplication rule of Dirichlet exponential generating functions given by Equation (3.2.1).

\[ \square \]

**Lemma 3.2.6.** Let \( G_1 \) and \( G_2 \) be relatively prime graphs. Then

\[ \mathcal{D}(G_1 \odot G_2) = \mathcal{D}(G_1) \mathcal{D}(G_2) \]

**Proof.** Applying Proposition 3.1.8 and Proposition 3.2.5, we get

\[ \mathcal{D}(G_1 \odot G_2) = \mathcal{D}(\mathcal{O}_{G_1 \odot G_2}) = \mathcal{D}(\mathcal{O}_{G_1} \square \mathcal{O}_{G_2}) = \mathcal{D}(\mathcal{O}_{G_1}) \mathcal{D}(\mathcal{O}_{G_2}) = \mathcal{D}(G_1) \mathcal{D}(G_2). \]

\[ \square \]

**Lemma 3.2.7.** Let \( P \) be any prime graph. Let \( T \) be the sum of all nonnegative integer powers of \( P \), i.e., \( T = \sum_{k \geq 0} P^k \). Then the Dirichlet exponential generating functions for \( T \) and \( P \) are related by

\[ \mathcal{D}(T) = \exp(\mathcal{D}(P)). \]

**Proof.** For any graph \( G \), we have

\[ L(G) = \frac{l(G)!}{|\text{aut}(G)|}, \]

and

\[ \mathcal{D}(G) = \frac{L(G)}{l(G)! \cdot l(G)^s} = \frac{1}{|\text{aut}(G)| \cdot l(G)^s}. \]

58
Now it follows from Remark 3.2.2 that

\[ |\text{aut}(P^k)| = |\text{aut}(P)^k| = k! \cdot |\text{aut}(P)|^k, \]

which gives that

\[ L(P^k) = \frac{l(P^k)!}{|\text{aut}(P^k)|} = \frac{l(P^k)!}{k! \cdot |\text{aut}(P)|^k}. \]

Hence we get

\[ \mathcal{D}(P^k) = \frac{L(P^k)}{l(P^k)! \cdot l(P)^k} = \frac{1}{k! \cdot |\text{aut}(P)|} \cdot \frac{l(P)^k}{l(P)^k} = \frac{\mathcal{D}(P)^k}{k!}. \]

Summing up on \( k \), we get

\[ \mathcal{D}(T) = \sum_{k \geq 0} \frac{\mathcal{D}(P)^k}{k!} = \exp(\mathcal{D}(P)). \]

\[ \square \]

**Example 3.2.8.** Let \( \mathcal{P} \) be the species of prime graphs, and \( \mathcal{G}^c \) the species of connected graphs. Then \( \mathcal{D}(\mathcal{G}^c) \) and \( \mathcal{D}(\mathcal{P}) \) are the Dirichlet exponential generating functions for these two species, respectively:

\[ \mathcal{D}(\mathcal{G}^c) = \sum_{n \geq 1} \frac{|\mathcal{G}^c[n]|}{n! n^s} = \sum_{G \in \mathcal{C}} \mathcal{D}(G), \quad \mathcal{D}(\mathcal{P}) = \sum_{n \geq 1} \frac{|\mathcal{P}[n]|}{n! n^s} = \sum_{P \in \mathcal{P}} \mathcal{D}(P), \]

where \( \mathcal{C} \) is the set of unlabeled connected graphs and \( \mathcal{P} \) is the set of unlabeled prime graphs.

**Theorem 3.2.9.** Let \( \mathcal{G}^c \) be the species of connected graphs, and let \( \mathcal{P} \) be the species of prime graphs. We have

\[ \mathcal{D}(\mathcal{G}^c) = \exp(\mathcal{D}(\mathcal{P})). \]
CHAPTER 3. PRIME GRAPHS

Proof. Lemma 3.2.6 gives that the Dirichlet exponential generating function of a product of two relatively prime graphs is the product of the Dirichlet exponential generating functions of the two graphs. Note that according to Proposition 3.1.2, the operation of Cartesian product on graphs is associative up to isomorphism. Then it follows that if we have a set of pairwise relatively prime graphs \( \{G_i\}_{i=1}^{r} \), and let \( G = \bigodot_{i=1}^{r} G_i \), then

\[
\mathcal{D}(G) = \prod_{i=1}^{r} \mathcal{D}(G_i).
\]

Now according to the definition of the Dirichlet exponential generating function for graphs, we get

\[
\mathcal{D}(G^c) = \sum_{G \in \mathcal{C}} \mathcal{D}(G) = \prod_{P \in \mathcal{P}} \mathcal{D} \left( \sum_{k \geq 0} P^k \right) = \prod_{P \in \mathcal{P}} \exp(\mathcal{D}(P)) = \exp \left( \sum_{P \in \mathcal{P}} \mathcal{D}(P) \right) = \exp(\mathcal{D}(\mathcal{P})).
\]

\[\square\]

Recall the exponential generating series of \( G^c \) given by (2.4.5):

\[
G^c(x) = \frac{x}{1!} + \frac{x^2}{2!} + 4 \frac{x^3}{3!} + 38 \frac{x^4}{4!} + 728 \frac{x^5}{5!} + 26704 \frac{x^6}{6!} + 1866256 \frac{x^7}{7!} + 251548592 \frac{x^8}{8!} + 66296291072 \frac{x^9}{9!} + \ldots,
\]

We obtain \( \mathcal{D}(G^c) \) by replacing \( x^n \) with \( n^{-s} \) for each \( n \) in the above expression:

\[
\mathcal{D}(G^c) = \sum_{n \geq 1} |g^c[n]| \frac{1}{n! n^s} = \frac{1}{1! 1^s} + \frac{1}{2! 2^s} + 4 \frac{1}{3! 3^s} + 38 \frac{1}{4! 4^s} + 728 \frac{1}{5! 5^s} + 26704 \frac{1}{6! 6^s} + 1866256 \frac{1}{7! 7^s} + 251548592 \frac{1}{8! 8^s} + 66296291072 \frac{1}{9! 9^s} + \ldots.
\]
CHAPTER 3. PRIME GRAPHS

Theorem 3.2.9 gives a way of counting labeled prime graphs by writing

\[ \mathcal{D}(\mathcal{P}) = \log \mathcal{D}(\mathcal{P}^c). \]

For example, we write down the first terms of \( \mathcal{D}(\mathcal{P}) \) as follows:

\[
\mathcal{D}(\mathcal{P}) = \frac{1}{1! 1^s} + \frac{1}{2! 2^s} + 4 \frac{1}{3! 3^s} + 35 \frac{1}{4! 4^s} + 728 \frac{1}{5! 5^s} + 26464 \frac{1}{6! 6^s} + 1866256 \frac{1}{7! 7^s} \\
+ 251518352 \frac{1}{8! 8^s} + 66296210432 \frac{1}{9! 9^s} + \ldots.
\]

Let \( p_n^r \) and \( c_n \) be the number of labeled prime graphs and the number of labeled connected graphs, respectively. We obtain the following table.

**Table 1.** Values of \( p_n^r \) and \( c_n \), for \( n \leq 12 \).

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<th>( p_n^r )</th>
<th>( c_n )</th>
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3.3. Unlabeled Prime Graphs

In this section all graphs considered are unlabeled and connected.

**Definition 3.3.1.** The (formal) Dirichlet series of a sequence \( \{a_n\}_{n=1,2,\ldots,\infty} \) is defined to be \( \sum_{n=1}^{\infty} a_n/n^s \).
The multiplication of Dirichlet series is given by
\[
\sum_{n \geq 1} a_n \cdot \sum_{m \geq 1} b_m \cdot n^s = \sum_{n \geq 1} \left( \sum_{k | n} a_k b_{n/k} \right) \frac{1}{n^s}.
\]

**Definition 3.3.2.** A monoid is a semigroup with a unit. A free commutative monoid is a commutative monoid \(M\) with a set of primes \(P \subseteq M\) such that each element \(m \in M\) can be uniquely decomposed into a product of elements in \(P\) up to rearrangement.

Let \(M\) be a free commutative monoid. We get a monoid algebra \(CM\), in which the elements are all formal sums \(\sum_{m \in M} c_m m\), where \(c_m \in \mathbb{C}\), with addition and multiplication defined naturally.

For each \(m \in M\), we associate a length \(l(m)\) that is compatible with the multiplication in \(M\). That is, for any \(m_1, m_2 \in M\), we have \(l(m_1)l(m_2) = l(m_1m_2)\).

It is well-known that the monoid algebra yields the following identity:

**Proposition 3.3.3.** Let \(M\) be a free commutative monoid with prime set \(P\). The following identity holds in the monoid algebra \(CM\):
\[
\sum_{m \in M} m = \prod_{p \in P} \frac{1}{1 - p^{-1}}.
\]
Furthermore, we can define a homomorphism from \(M\) to the ring of Dirichlet series under which each \(m \in M\) is sent to \(1/l(m)^s\), where \(l\) is a length function of \(M\). Therefore,
\[
\sum_{m \in M} \frac{1}{l(m)^s} = \prod_{p \in P} \frac{1}{1 - l(p)^{-s}}.
\]

**Example 3.3.4.** Let \(\mathbb{N}\) denote the set of all natural numbers, and let \(\mathbb{P}\) denote the set of all prime numbers. Then \(\mathbb{N}\) is a free commutative monoid with prime set \(\mathbb{P}\), and the length function is given by \(l(n) = n\) for all \(n \in \mathbb{N}\). As an application of Proposition 3.3.3, we have the following well-known identity for expressing the zeta
function:
\[ \zeta(s) = \sum_{n \in \mathbb{N}} \frac{1}{n^s} = \prod_{p \in \mathbb{P}} \frac{1}{1 - p^{-s}}. \]

Recall that \( \mathbb{C} \) is the set of unlabeled connected graphs under the operation of Cartesian product. The unique factorization theorem of Sabidussi gives \( \mathbb{C} \) the structure of a commutative free monoid with a set of primes \( \mathbb{P} \), where \( \mathbb{P} \) is the set of unlabeled prime graphs. This is saying that every element of \( \mathbb{C} \) has a unique factorization of the form \( b_1^{e_1} b_2^{e_2} \cdots b_k^{e_k} \), where the \( b_i \) are distinct primes in \( \mathbb{P} \). Let \( l(G) \), the number of vertices in \( G \), be a length function for \( \mathbb{C} \). We have the following proposition.

**Lemma 3.3.5.** Let \( \mathbb{C} \) and \( \mathbb{P} \) be the set of unlabeled connected graphs and the set of unlabeled prime graphs, respectively. We have

\[ \sum_{G \in \mathbb{C}} \frac{1}{l(G)^s} \prod_{P \in \mathbb{P}} \frac{1}{1 - l(P)^{-s}}. \]

The enumeration of prime graphs was studied by Raphaël Bellèc [1]. We use Dirichlet series to count unlabeled connected prime graphs.

**Theorem 3.3.6.** Let \( \tilde{c}_n \) be the number of unlabeled connected graphs on \( n \) vertices, and let \( b_m \) be the number of unlabeled prime graphs on \( m \) vertices. Then we have

\[ \sum_{n \geq 1} \frac{\tilde{c}_n}{n^s} = \prod_{m \geq 2} \frac{1}{(1 - m^{-s})^{b_m}}. \]

Furthermore, if we define numbers \( d_n \) for positive integers \( n \) by

\[ \sum_{n \geq 1} \frac{d_n}{n^s} = \log \sum_{n \geq 1} \frac{\tilde{c}_n}{n^s}, \]

63
then

\[ d_n = \sum_{m^l = n} \frac{b_m}{l}, \]

where the sum is over all pairs \((m, l)\) of positive integers with \(m^l = n\).

**Remark 3.3.7.** A quick observation from Equation (3.3.3) is that \(b_n = d_n\) whenever \(n\) is not of the form \(r^k\) for some \(k > 1\).

In what follows, we introduce an interesting recursive formula for computing \(d_n\). To start with, we differentiate both sides of Equation (3.3.2) with respect to \(s\) and simplify. We get that

\[ \sum_{n \geq 2} \log n \frac{\tilde{c}_n}{n^s} = \left( \sum_{n \geq 1} \frac{\tilde{c}_n}{n^s} \right) \left( \sum_{n \geq 2} \log n \frac{d_n}{n^s} \right), \]

which gives

\[ \tilde{c}_n \log n = \sum_{m^l = n} c_m d_l \log l. \]

Since \(c_1\) is the number of connected graphs on 1 vertex, \(c_1 = 1\). It follows from Equation (3.3.4) easily that \(d_p = c_p\) when \(p\) is a prime number. Therefore, if \(p\) is a prime number, \(b_p = d_p = c_p\). This fact can be seen directly, since a connected graph with a prime number of vertices is a prime graph.

Raphaël Bellec used Equation (3.3.4) to find formulae for \(d_n\) where \(n\) is a product of two different primes or a product of three different primes:

If \(n = pq\) where \(p \neq q\),

\[ d_n = \tilde{c}_n - c_p c_q; \]
If \( n = pqr \) where \( p, q \) and \( r \) are distinct primes,

\[
d_n = \tilde{c}_n + 2c_pc_qc_r - c_pc_qr - c_qc_pr - c_rc_pq.
\]

In fact, Equations (3.3.5) and (3.3.6) are special cases of the following proposition.

**Proposition 3.3.8.** Let \( d_n, \tilde{c}_n \) be defined as above. Then we have

\[
d_n = \tilde{c}_n - \frac{1}{2} \sum_{n_1n_2=n} c_{n_1}c_{n_2} + \frac{1}{3} \sum_{n_1n_2n_3=n} c_{n_1}c_{n_2}c_{n_3} - \ldots.
\]

**Proof.** We can use the identity

\[
\log(1 + x) = x - \frac{1}{2} x^2 + \frac{1}{3} x^3 - \frac{1}{4} x^4 + \ldots
\]

to compute from Equation (3.3.2) that

\[
\sum_{n \geq 1} \frac{d_n}{n^s} = \log \left( 1 + \sum_{n \geq 2} \frac{\tilde{c}_n}{n^s} \right)
= \sum_{n \geq 2} \frac{\tilde{c}_n}{n^s} - \frac{1}{2} \left( \sum_{n \geq 2} \frac{\tilde{c}_n}{n^s} \right)^2 + \frac{1}{3} \left( \sum_{n \geq 2} \frac{\tilde{c}_n}{n^s} \right)^3 - \ldots.
\]

Equating coefficients of \( n^{-s} \) on both sides, we get the desired result. \( \square \)

**Proof of Theorem 3.3.6.** We start with

\[
\sum_m \frac{1}{l(m)^s} = \prod_p \frac{1}{1 - l(p)^{-s}},
\]

where the left-hand side is summed over all connected graphs, and the right-hand side is summed over all prime graphs. Regrouping the summands on the left-hand side with respect to the number of vertices in \( m \), we get the left-hand side of Equation (3.3.1). Regrouping the factors on the right-hand side with respect to the number of vertices in \( p \), we get the right-hand side of Equation (3.3.1).
Taking the logarithm of both sides of Equation (3.3.1), we get
\[
\log \sum_{n \geq 1} \frac{\tilde{c}_n}{n^s} = \log \prod_{m \geq 2} \frac{1}{(1 - m^{-s})^b_m} = \sum_{m \geq 2} b_m \log \frac{1}{1 - m^{-s}}
\]
\[
= \sum_{m \geq 2} \left( b_m \sum_{l \geq 1} \frac{m^{-sl}}{l} \right) = \sum_{m \geq 2, l \geq 1} \frac{b_m}{l} m^{sl},
\]
and Equation (3.3.3) follows immediately. \qed

Next, we will compute the numbers \(b_n\) in terms of the numbers \(d_n\) using the following lemma.

**Lemma 3.3.9.** Let \(\{D_i\}_{i=1,...}\) and \(\{J_i\}_{i=1,...}\) be sequences of numbers satisfying
\[
(3.3.7) \quad D_k = \sum_{l|k} \frac{J_{k/l}}{l},
\]
and let \(\mu\) be the Möbius function. Then we have
\[
J_k = \frac{1}{k} \sum_{l|k} \mu\left(\frac{k}{l}\right) lD_l.
\]

**Proof.** Multiplying by \(k\) on both sides of Equation (3.3.7), we get
\[
kD_k = \sum_{l|k} \frac{k}{l} J_{k/l} = \sum_{l|k} l J_l.
\]
Applying the Möbius inversion formula, we get
\[
kJ_k = \sum_{l|k} \mu\left(\frac{k}{l}\right) lD_l.
\]
Therefore,
\[
J_k = \frac{1}{k} \sum_{l|k} \mu\left(\frac{k}{l}\right) lD_l.
\]
\qed
Given any natural number \( n \), let \( e \) be the largest number such that \( n = r^e \) for some \( r \). Note that \( r \) is not a power of a smaller integer. We let \( D_k = d_{rk}, J_k = b_{rk} \). It follows that Equation (3.3.3) is equivalent to Equation (3.3.7).

**Theorem 3.3.10.** For any natural number \( n \), let \( e, r \) be as described in above. Then we have

\[
b_n = \frac{1}{e} \sum_{l|e} \mu\left(\frac{e}{l}\right) ld_r^e.
\]

**Proof.** The result follows straightforwardly from Lemma 3.3.9. \qed

Table 2 gives the numbers of unlabeled prime graphs \( b_n \) compared with the numbers of unlabeled connected graphs \( \bar{c}_n \) on no more than 12 vertices.

**Table 2.** Values of \( \bar{c}_n \) and \( b_n \), for \( n \leq 12 \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( \bar{c}_n )</th>
<th>( b_n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>6</td>
<td>5</td>
</tr>
<tr>
<td>5</td>
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<td>21</td>
</tr>
<tr>
<td>6</td>
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<td>110</td>
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<tr>
<td>7</td>
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<td>853</td>
</tr>
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<td>8</td>
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<td>11111</td>
</tr>
<tr>
<td>9</td>
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<td>261077</td>
</tr>
<tr>
<td>10</td>
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<td>1171650</td>
</tr>
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<td>1006700565</td>
</tr>
<tr>
<td>12</td>
<td>164059830476</td>
<td>164059830354</td>
</tr>
</tbody>
</table>

### 3.4. Exponential Composition with a Molecular Species

In this section we introduce an operation on species that is equivalent to the exponentiation groups in the case of molecular species. This operation turns out to be useful for finding a functional equation relating the species of connected graphs and the species of prime graphs.
Let $F$ be a species of structures with $F[\emptyset] = \emptyset$, let $k$ be a positive integer, and let $A$ be a subgroup of $\mathfrak{S}_k$. Recall that an $F_{\square_k}$-structure on a finite set $U$ is a tuple of the form
\[
((\pi_1, f_1), (\pi_2, f_2), \ldots, (\pi_k, f_k)),
\]
where $(\pi_1, \pi_2, \ldots, \pi_k)$ is a $k$-rectangle on $U$, and each $f_i$ is an $F$-structure on the blocks of $\pi_i$. The group $A$ acts on the set of $F_{\square_k}$-structures by permuting the subscripts of $\pi_i$ and $f_i$, i.e.,
\[
\alpha((\pi_1, f_1), \ldots, (\pi_k, f_k)) = ((\pi_{\alpha(1)}, f_{\alpha(1)}), \ldots, (\pi_{\alpha(k)}, f_{\alpha(k)})),
\]
where $\alpha$ is an element of $A$, $(\pi_{\alpha_1}, \pi_{\alpha_2}, \ldots, \pi_{\alpha_k})$ is a $k$-rectangle on $U$, and each $f_{\alpha_i}$ is an $F$-structure on the blocks of $\pi_{\alpha_i}$. It is easy to check that this action of $A$ on $F_{\square_k}$-structures is natural, that is, it commutes with any bijection $\sigma : U \to V$. Hence we get a quotient species under this group action.

**Definition 3.4.1.** We define the exponential composition of $F$ with the molecular species $X^k/A$ to be the quotient species, denoted $(X^k/A)\langle F \rangle$, under the group action described in above. That is,
\[
(X^k/A)\langle F \rangle := F_{\square_k}/A.
\]

**Example 3.4.2.** Figure 3.4 illustrates the group action of $\mathfrak{S}_2$ on the set of $\mathfrak{S}_{2_{\square^2}}$-structures on $[4]$, resulting in three orbits.

Let $A$ be a subgroup of $\mathfrak{S}_m$, and let $B$ be a subgroup of $\mathfrak{S}_n$. We have the following formulas from Theorem 2.3.10 and Proposition 2.6.5:
\[
\frac{X^m}{A} \cdot \frac{X^n}{B} = \frac{X^{m+n}}{A \ast B},
\]

68
CHAPTER 3. PRIME GRAPHS

Figure 3.4. There are three elements in the set $\mathcal{E}_2(\mathcal{E}_2)[4]$.

\[
\begin{align*}
X^m \quad & X^n \\
A \quad & B = X^{mn} \\
\quad & B \triangleleft A^1
\end{align*}
\]

\[
\begin{align*}
X^m \\
A \quad & X^n \\
\boxdot & B = X^{mn} \\
A \quad & A \times B
\end{align*}
\]

Now we can add to this list one more formula representing the group action of $B^A$ on the set $N = n^m$ stated in the following theorem.

**Theorem 3.4.3.** Let $A$ and $B$ be groups described in above, let $N = n^m$, and let $B^A$ be the exponetnation group of $A$ with $B$, as defined in Definition 1.3.1. Then we have

\[
\frac{X^m}{A} \langle \frac{X^n}{B} \rangle = \frac{X^N}{B^A}.
\]

Moreover, we get the cycle index of $(X^m/A)(X^n/B)$:

\[
Z_{(X^m/A)(X^n/B)} = Z(A) \ast Z(B),
\]

where the expression $Z(A) \ast Z(B)$ denotes the image of $Z(B)$ under the operator obtained by substituting the operator $I_r$ for the variables $p_r$ in $Z(A)$.
Proof. Proposition 2.6.5 and the associativity of the arithmetic product give that

\[
\left( \frac{X^n}{B} \right)^{\Box m} = \frac{X^N}{B^m},
\]

where \( B^m \) is the product of \( m \) copies of \( B \), acting on the set

\[
\underbrace{[n] \times [n] \times \cdots \times [n]}_{m \text{ copies}}
\]

piecewise, and hence viewed as a subgroup of \( \mathfrak{S}_N \). According to Remark 2.3.4, the set of \((X^n/B)^{\Box m}\)-structures on \([N]\) is then just the set of \( B^m \)-orbits of linear orders on \([N]\).

The group \( A \) acts on these \( B^m \)-orbits of linear orders by permuting the subscripts. This action results in the quotient species

\[
\frac{X^m}{A} \left\langle \frac{X^n}{B} \right\rangle = \left( \frac{X^n}{B} \right)^{\Box m} / A = \left( \frac{X^N}{B^m} \right) / A.
\]

We observe that an \( A \)-orbit of \( B^m \)-orbits of linear orders on \([N]\) admits an automorphism group isomorphic to the exponentiation group \( B^A \), hence the quotient species \((X^N/B^m)/A\) is the same as the molecular species \( X^N/B^A \).

As for the cycle index of \((X^m/A)\langle X^n/B \rangle\), we apply Proposition 2.3.5 and Theorem 1.3.6 to get that

\[
Z_{(X^m/A)\langle X^n/B \rangle} = Z_{X^N/B^A} = Z(B^A) = Z(A) \ast Z(B).
\]

Figure 3.5 illustrates an group action of \( A \) on a set of \((X^n/B)^{\Box m}\)-structures. \( \square \)

Next, we introduce a theorem that is a generalization of Palmer and Robinson’s Theorem 1.3.6.
CHAPTER 3. PRIME GRAPHS

Figure 3.5. \( ((X^n/B)^m)/A = X^n m / B A \).

Theorem 3.4.4. Let \( A \) be a subgroup of \( \mathfrak{S}_k \), and let \( F \) be a species of structures concentrated on the cardinality \( n \). Then the cycle index of the species \( (X^k / A) \langle F \rangle \) is given by

\[
Z_{(X^k / A) \langle F \rangle} = Z(A) \ast Z_F.
\]  

Remark 3.4.5 (Notation and Set-up). We denote by \( \text{Par}_n \) the set of partitions of \( n \), and by \( \text{Par}_n^k \) the set of \( k \)-sequences of partitions of \( n \).

For fixed integers \( n, k, \) and \( N = n^k \), we denote by \( \mathcal{N}_N \) the species of \( k \)-dimensional cubes, or \( k \)-cubes, on \( [N] \), defined by

\[
\mathcal{N}_N = \mathcal{E}_{n}^{\square k}[N].
\]

We also call the elements of the set \( (X^n)^{\square k}[N] \) \( k \)-dimensional ordered cubes on \( [N] \).
Let \( \sigma \) be a permutation on \([k]\) with cycle type
\[
\text{c.t.}(\sigma) = (r_1, r_2, \ldots, r_d).
\]
Then \( \sigma \) acts on the \( F^{\Box k} \)-structures by permuting the subscripts. Let \( \nu \) be a partition of \( N \). Let \( \delta \) be a permutation of \([N]\) with cycle type \( \nu \). Then \( \delta \) acts on the \( F^{\Box k} \)-structures by transport of structures. Recall the notation introduced in Remark 1.3.8:
\[
I(\text{c.t.}(\sigma); \lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(d)}) = I_{r_1}(p_{\lambda^{(1)}}) \boxtimes I_{r_2}(p_{\lambda^{(2)}}) \boxtimes \cdots \boxtimes I_{r_d}(p_{\lambda^{(d)}}).
\]
We denote by \( \text{Rec}_F(\sigma, \nu) \) a function on the pair \((\sigma, \nu)\) defined by
\[
(3.4.2) \quad \text{Rec}_F(\sigma, \nu) := \sum \prod_{i=1}^{d} \text{fix } F[\lambda^{(i)}],
\]
where the summation is over all sequences \((\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(d)})\) in \( \text{Par}_n^d \) with
\[
I(\text{c.t.}(\sigma); \lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(d)}) = p_{\nu}.
\]
We denote by \( \text{fix}_F(\sigma, \delta) \) the number of \( F^{\Box k} \)-structures on the set \([N]\) fixed by the joint action of the pair \((\sigma, \delta)\).

PROOF OF THEOREM 3.4.4. Let \( \nu \) be a partition of \( N \). It suffices to prove that the coefficients of \( p_{\nu} \) on both sides of Equation (3.4.1) are equal.

The right-hand side of Equation (3.4.1) is
\[
Z(A) \ast Z_F = \left( \frac{1}{|A|} \sum_{\sigma \in A} p_{\text{c.t.}(\sigma)} \right) \ast \left( \sum_{\lambda \vdash n} \text{fix } F[\lambda] \frac{p_{\lambda}}{z_{\lambda}} \right)
\]
\[
= \frac{1}{|A|} \sum_{\sigma \in A} I_{\text{c.t.}(\sigma)} \left( \sum_{\lambda \vdash n} \text{fix } F[\lambda] \frac{p_{\lambda}}{z_{\lambda}} \right).
\]
For $\sigma \in A$ with $c.t.(\sigma) = (r_1, r_2, \ldots, r_d)$, we have

$$I_{c.t.}(\sigma) = I_{r_1} \cdots I_{r_d},$$

and

$$I_{c.t.}(\sigma) \left( \sum_{\lambda \vdash n} F[\lambda] \frac{p_{\lambda}}{z_{\lambda}} \right)$$

$$= I_{r_1} \left( \sum_{\lambda \vdash n} F[\lambda] \frac{p_{\lambda}}{z_{\lambda}} \right) \boxtimes I_{r_2} \left( \sum_{\lambda \vdash n} F[\lambda] \frac{p_{\lambda}}{z_{\lambda}} \right) \boxtimes \cdots \boxtimes I_{r_d} \left( \sum_{\lambda \vdash n} F[\lambda] \frac{p_{\lambda}}{z_{\lambda}} \right).$$

Therefore, the coefficient of $p_\nu$ in the expression $Z(A) \ast Z_F$ is

$$\frac{1}{|A|} \sum \prod_{i=1}^d \frac{\text{fix } F[\lambda(i)]}{z_{\lambda_1} \cdots z_{\lambda_d}} = \frac{1}{|A|} \sum_{\sigma \in A} \text{Rec}_F(\sigma, \nu),$$

where the summation on the left-hand side is taken over all sequences $(\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(d)})$ in $\text{Par}^d_n$ for some $d \geq 1$ and all $\sigma \in A$ with $c.t.(\sigma) = (r_1, r_2, \ldots, r_d)$ such that

$$I(\text{c.t.}(\sigma); \lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(d)}) = p_\nu,$$

and $\text{Rec}_F(\sigma, \nu)$ on the right-hand side is as defined by (3.4.2) in Remark 3.4.5.

The left-hand side of Equation (3.4.1) is

$$Z_{F^{\sqcap k}/A} = \sum_{\nu \vdash N} \text{fix } F^{\sqcap k}_{\nu} \frac{p_\nu}{A \nu},$$

Therefore, the coefficient of $p_\nu$ in the expression $Z_{F^{\sqcap k}/A}$ is

$$\frac{1}{z_\nu} \text{fix } F^{\sqcap k}_{\nu} \frac{p_\nu}{A \nu}.$$
We then apply Theorem 1.1.6 to get that the number of $A$-orbits of $F \Box^k$-structures on $[N]$ fixed by a permutation $\delta \in \mathfrak{S}_N$ of cycle type $\nu$ is

$$\text{fix}_F \frac{F \Box^k}{A} [\nu] = \text{fix}_F \frac{F \Box^k}{A} [\delta] = \frac{1}{|A|} \sum_{\sigma \in A} \text{fix}_F (\sigma, \delta),$$

where fix$_F (\sigma, \delta)$ is as defined in Remark 3.4.5.

Therefore, combining (3.4.4) and (3.4.3), the proof of Equation (3.4.1) is reduced to showing that

$$\text{fix}_F (\sigma, \delta) = z_\nu \text{Rec}_F (\sigma, \nu),$$

for any $\delta, \nu$ and $\sigma$.

To prove (3.4.5), we start with observing that in order for an $F \Box^k$-structure on $[N]$ of the form

$$((\pi_1, f_1), (\pi_2, f_2), \ldots, (\pi_k, f_k))$$

to be fixed by the pair $(\sigma, \delta)$, it is necessary that $(\sigma, \delta)$ fixes the $k$-cube of the form $(\pi_1, \pi_2, \ldots, \pi_k) \in \mathcal{N}_N$. This is equivalent to saying that

$$\mathcal{N}_N[\delta](\pi_1, \pi_2, \ldots, \pi_k) = (\pi_{\sigma(1)}, \pi_{\sigma(2)}, \ldots, \pi_{\sigma(k)}).$$

Suppose (3.4.6) holds for some $k$-cube $(\pi_1, \pi_2, \ldots, \pi_k) \in \mathcal{N}_N$. We let $\beta_i \in \mathfrak{S}_n$ be the induced action of $\delta$ on the blocks of $\pi_i$, for $i = 1, 2, \ldots, k$. That is,

$$\mathcal{N}_N[\delta](\pi_i) = \beta_i(\pi_{\sigma(i)})$$

for all $i \in [k]$.

Now we consider the simpler case when $\sigma$ is a $k$-cycle, say, $\sigma = (1, 2, \ldots, k)$. Then the action of $\delta$ sends $(\pi_1, \pi_2, \ldots, \pi_k)$ to $(\pi_2, \pi_3, \ldots, \pi_1)$. Let $\beta = \beta_1 \beta_2 \cdots \beta_k$. The
above discussion is saying that, according to Remark 1.3.3,

\[ I_k(p_{c.t.}(\beta)) = p_\nu. \]

On the other hand, given a partition \( \lambda \) of \( n \) satisfying \( I_k(p_\lambda) = p_\nu \), there are \( n!/z_\lambda \) permutations in \( \mathfrak{S}_n \) with cycle type \( \lambda \). Let \( \beta \) be one of such. Then the number of sequences \( (\beta_1, \beta_2, \ldots, \beta_k) \) whose product equals \( \beta \) is \( (n!)^{k-1} \), since we can choose \( \beta_1 \) up to \( \beta_{k-1} \) freely, and \( \beta_k \) is therefore determined. All such sequences \( (\beta_1, \beta_2, \ldots, \beta_k) \) will satisfy \( I_k(p_{c.t.}(\beta_1 \cdots \beta_k)) = p_\nu \), thus their action on an arbitrary \( k \)-dimensional ordered cube, combined with the action of \( \sigma \) on the subscripts, would result in a permutation on \([N]\) with cycle type \( \nu \). But there are \( N!/z_\nu \) permutations with cycle type \( \nu \), and only one of them is the \( \delta \) that we started with. Considering that the \( k \)-cubes are just \( \mathfrak{S}_k^k \)-orbits of the \( k \)-dimensional ordered cubes, we count the number of \( k \)-cubes that are fixed by the pair \( (\sigma, \delta) \) with the further condition that the product of the induced permutations on the \( \pi_i \) by \( \delta \) has cycle type \( \lambda \):

\[
\frac{\# \{ (\beta_1, \beta_2, \ldots, \beta_k) \in \mathfrak{S}_n^k \text{ with } c.t.(\beta_1 \cdots \beta_k) = \lambda \} \cdot \# \{ k\text{-dimensional ordered cubes} \}}{\# \{ \text{permutations on } [N] \text{ with cycle type } \nu \} \cdot \# \{ k\text{-dimensional ordered cubes in each equivalence class} \}} = \frac{(n!)^{k-1} \cdot n!/z_\lambda \cdot N!}{N!/z_\nu \cdot (n!)^k} = \frac{z_\nu}{z_\lambda}.
\]

75
Now we try to compute how many $F^{\Box k}$-structures of the form

$$((\pi_1, f_1), (\pi_2, f_2), \ldots, (\pi_k, f_k)),$$

based on a given rectangle $(\pi_1, \pi_2, \ldots, \pi_k)$ that is fixed by the $\beta_i$ with

$$\text{c.t.} \left( \prod_i \beta_i \right) = \lambda,$$

are fixed by the pair $(\sigma, \delta)$. We observe that the action of $(\sigma, \delta)$ determines that

$$f_k = F[\beta_1]f_1$$

and

$$f_i = F[\beta_{i-1}]f_{i-1}$$

for $i = 2, 3, \ldots, k$, and hence

$$f_k = F[\beta_1]F[\beta_2] \cdots F[\beta_k]f_k = F[\beta]f_k = F[\lambda]f_k.$$

In other words,

$$f_k \in \text{Fix } F[\lambda].$$

Hence as long as we choose an $f_k$ from $\text{Fix } F[\lambda]$, then all the other $f_i$ for $i < k$ are determined by our choice of $f_k$. There are $\text{fix } F[\lambda]$ such choices for $f_k$.

Therefore, in the case when $\sigma$ is a $k$-cycle, we get that the number of $F^{\Box k}$-structures on the set $[N]$ fixed by the pair $(\sigma, \delta)$ is

$$\text{fix}_F(\sigma, \delta) = \sum_{\lambda \vdash n \atop l_k(\rho_\lambda) = \rho_\nu} \text{fix } F[\lambda] \frac{z_{\nu}}{z_\lambda} = z_\nu \text{ Rec}_F(\sigma, \nu).$$

Now let us consider the general case when $\sigma$ contains $d$ cycles of lengths $r_1, r_2, \ldots, r_d$. Let $(\pi_1, \pi_2, \ldots, \pi_k)$ be a $k$-cube fixed by the pair $(\sigma, \delta)$. Again we have (3.4.6), and we get an induced $\beta_i$ on the blocks of $\pi_{\sigma^{-1}i}$ for each $i$.

We observe that the action of $\sigma$ on the subscripts of the $k$-cube partitions the list $\pi_1, \pi_2, \ldots, \pi_k$ into $d$ parts, of lengths $r_1, r_2, \ldots, r_d$, within each of which we get a $r_i$-cycle. We group the $\beta_i$ on each of the $d$ parts and get $d$ permutations in the group
\(\mathfrak{S}_n\), whose cycle types are denoted by \(\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(d)}\). This construction gives that such a sequence of partitions \((\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(d)})\) will be those that satisfy

\[
I(\text{c.t.}(\sigma); \lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(d)}) = p_\nu.
\]

Therefore, the number of \(k\)-cubes fixed by \((\sigma, \delta)\) corresponding to such a sequence of partitions \((\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(d)})\) is

\[
\frac{N!}{(n!)^{r_1+\ldots+r_d} z_\nu \lambda^{(1)} \cdots \lambda^{(d)}}.
\]

The number of \(F\)-structures that are assigned to this \(k\)-cube \((\pi_1, \pi_2, \ldots, \pi_k)\) that will be fixed under the action of the pair \((\sigma, \delta)\) corresponding to the sequence of partitions \((\lambda^{(1)}, \lambda^{(2)}, \ldots, \lambda^{(d)})\) is hence

\[
\text{fix } F[\lambda^{(1)}] \cdots \text{fix } F[\lambda^{(d)}],
\]

since, similarly to our previous discussion, within each of the \(d\) parts, we only need to pick an \(F\)-structure that is fixed by a permutation of cycle type \(\lambda^{(i)}\), and all other \(F\)-structures are left determined.

Therefore, we get that for any pair \((\sigma, \delta)\),

\[
\text{fix}_F(\sigma, \delta) = z_\nu \text{Rec}_F(\sigma, \nu),
\]

which concludes our proof.

\[\square\]

**Remark 3.4.6.** We can use the molecular decomposition to define the exponential composition of a species \(F\) with a species \(H\). That is, if the molecular decomposition
CHAPTER 3. PRIME GRAPHS

of $H$ is given by

$$H = \sum_{M \subseteq H} M,$$

then we define $H(F)$ by

$$H(F) = \sum_{M \subseteq H} M(F).$$

The left-linearity of the operation $*$ gives that the cycle index of $H(F)$ is

$$Z_{H(F)} = Z_H * Z_F$$

$$= \left( \sum_{M \subseteq H} Z_M \right) * Z_F$$

$$= \sum_{M \subseteq H} Z_M * Z_F.$$

3.5. Exponential Composition

Let $F$ be a species with $F[\emptyset] = \emptyset$, and let $k$ be a positive integer. We call the quotient species $\mathcal{E}_k(F) = F^{\square_k}/\mathcal{G}_k$ the exponential composition of $F$ of order $k$. We observe that an $\mathcal{E}_k(F)$-structure on a finite set $U$ is a set of the form

$$\{(\pi_1, f_1), (\pi_2, f_2), \ldots, (\pi_k, f_k)\},$$

where $(\pi_1, \pi_2, \ldots, \pi_k)$ is a $k$-rectangle on $U$, and each $f_i$ is an $F$-structure on the blocks of $\pi_i$. We set $\mathcal{E}_0(F) = X$.

**Definition 3.5.1.** Let $F$ be a species with $F[\emptyset] = F[1] = \emptyset$. We define the exponential composition of $F$, denoted $\mathcal{E}(F)$, to be the sum of $\mathcal{E}_k(F)$ on all nonnegative integers $k$, i.e.,

$$\mathcal{E}(F) = \sum_{k \geq 0} \mathcal{E}_k(F).$$
Proposition 3.5.2. Let $F$ be a species with $F[\emptyset] = \emptyset$. Then the cycle index of the exponential composition of $F$ is given by

$$Z_{\mathcal{E}(F)} = p_1 + \sum_{k \geq 1} Z(\mathfrak{S}_k) \ast Z_F.$$ 

Proof. We get from Theorem 3.4.4 that for $k \geq 1$,

$$Z_{\mathcal{E}_k(F)} = Z(\mathfrak{S}_k) \ast Z_F.$$ 

And the rest follows from the partial linearity of the operation $\ast$ on symmetric functions. \hfill \Box

The exponential composition has the following properties.

Theorem 3.5.3. Let $F_1$ and $F_2$ be species with $F_1[\emptyset] = F_2[\emptyset] = \emptyset$, and let $k$ be any nonnegative integer. Then

$$\mathcal{E}_k(F_1 + F_2) = \sum_{i=0}^{k} \mathcal{E}_i(F_1) \boxtimes \mathcal{E}_{k-i}(F_2),$$

(3.5.1) $$\mathcal{E}(F_1 + F_2) = \mathcal{E}(F_1) \boxtimes \mathcal{E}(F_2).$$

We observe that an $(F_1 + F_2)\boxtimes k$-structure on a finite set $U$ is a rectangle on $U$ with each partition in the rectangle enriched with either an $F_1$ or an $F_2$-structure. Taking the $\mathfrak{S}_k$-orbits of these $(F_1 + F_2)\boxtimes k$-structures on $U$ means basically making every partition of the rectangle “indistinguishable”. Hence in each $\mathfrak{S}_k$-orbit, all partitions enriched with an $F_1$-structure are grouped together to give an $\mathfrak{S}_{k_1}$-orbit of $F_1\boxtimes k_1$-structures, and the remaining partitions are grouped together to give an $\mathfrak{S}_{k_2}$-orbit of $F_2\boxtimes k_2$-structures, where $k_1$ and $k_2$ are nonnegative integers whose sum is equal to $k.$
Proof of Theorem 3.5.3. First, we prove that for any nonnegative integer \( k \),

\[
\mathcal{E}_k\langle F_1 + F_2 \rangle = \sum_{i=0}^{k} \mathcal{E}_i\langle F_1 \rangle \boxdot \mathcal{E}_{k-i}\langle F_2 \rangle.
\]

The case when \( k = 0 \) is trivial. Let us consider \( k \) to be a positive integer. Let \( s \) and \( t \) be nonnegative integers whose sum equals \( k \). Let \( U \) be a finite set. To get an \( \mathcal{E}_s\langle F_1 \rangle \boxdot \mathcal{E}_t\langle F_2 \rangle \)-structure on \( U \), we first take a rectangle \((\rho, \tau)\) on \( U \), and then take an ordered pair \((a, b)\), where \( a \) is an \( \mathcal{E}_s\langle F_1 \rangle \)-structure on the blocks of \( \rho \), and \( b \) is an \( \mathcal{E}_t\langle F_2 \rangle \)-structure on the blocks of \( \tau \). That is,

\[
a = \{ (\rho_1, f_1), \ldots, (\rho_s, f_s) \}, \quad b = \{ (\tau_1, g_1), \ldots, (\tau_t, g_t) \},
\]

where \((\rho_1, \ldots, \rho_s)\) is a rectangle on the blocks of \( \rho \), \((\tau_1, \ldots, \tau_t)\) is a rectangle on the blocks of \( \tau \), \( f_i \) is an \( F_1 \)-structure on the blocks of \( \rho_i \), and \( g_j \) is an \( F_2 \)-structure on the blocks of \( \tau_j \).

Recall that Proposition 2.6.8 says for any nonnegative integers \( i, j \),

\[
\mathcal{N}^{(i+j)} = \mathcal{N}^{(i)} \boxdot \mathcal{N}^{(j)}.
\]

It follows that \((\rho_1, \ldots, \rho_s, \tau_1, \ldots, \tau_t)\) is a rectangle on \( U \).

On the other hand, let \( x \) be an \( \mathcal{E}_k\langle F_1 + F_2 \rangle \)-structure on \( U \). We can write \( x \) as a set of the form

\[
x = \{ (\pi_1, f_1), \ldots, (\pi_r, f_r), (\pi_{r+1}, g_{r+1}), \ldots, (\pi_k, g_k) \},
\]

where \((\pi_1, \pi_2, \ldots, \pi_k)\) is a \( k \)-rectangle on \( U \), \( r \) is a nonnegative integer between 0 and \( k \), each \( f_i \) is an \( F_1 \)-structure on \( \pi_i \) for \( i = 1, \ldots, r \), and each \( g_j \) is an \( F_2 \)-structure on \( \pi_j \) for \( j = r + 1, \ldots, k \).
We then write \( x = (x_1, x_2) \), where

\[
x_1 = \{(\pi_1, f_1), \ldots, (\pi_r, f_r)\}, \quad x_2 = \{(\pi_{r+1}, g_{r+1}), \ldots, (\pi_k, g_k)\}.
\]

Hence running through values of \( s \) and \( t \), we get that the set of \( \mathcal{E}_s(F_1) \boxtimes \mathcal{E}_t(F_2) \)-structures on \( U \), written in the form of the pairs \((a, b)\) whose construction we described in above, corresponds naturally to the set of \( \mathcal{E}_k(F_1 + F_2) \)-structures on \( U \).

The proof of

\[
\mathcal{E}(F_1 + F_2) = \mathcal{E}(F_1) \boxtimes \mathcal{E}(F_2).
\]

is straightforward using the properties of the arithmetic product, namely, the commutativity, associativity and distributivity:

\[
\mathcal{E}(F_1 + F_2) = \sum_{k \geq 0} \mathcal{E}_k(F_1 + F_2)
= \sum_{k \geq 0} \left( \sum_{i+j=k} \mathcal{E}_i(F_1) \boxtimes \mathcal{E}_j(F_2) \right)
= \left( \sum_{i \geq 0} \mathcal{E}_i(F_1) \right) \boxtimes \left( \sum_{j \geq 0} \mathcal{E}_j(F_2) \right)
= \mathcal{E}(F_1) \boxtimes \mathcal{E}(F_2).
\]

Note that identity (3.5.1) is analogous to the identity about the composition of a sum of species with the species of sets \( \mathcal{E} \):

\[
\mathcal{E}(F_1 + F_2) = \mathcal{E}(F_1) \mathcal{E}(F_2).
\]

What is more, (3.5.1) illustrates a kind of distributivity of the exponential composition. In fact, if a species of structures \( F \) has its molecular decomposition written in
the form

\[ F = \sum_{M \subseteq P \text{ molecular}} M, \]

then the exponential composition of \( F \) can be written as

\[ \mathcal{E}(F) = \bigoplus_{M \subseteq P \text{ molecular}} \mathcal{E}(M). \]

### 3.6. Cycle Index of Prime Graphs

Now we are ready to come back to the species of prime graphs.

**Lemma 3.6.1.** Let \( P \) be any prime graph, and \( k \) any nonnegative integer. Then the species associated to the \( k \)-th power of \( P \) is the exponential composition of \( \mathcal{O}_P \) of order \( k \). That is,

\[ \mathcal{O}_{P^k} = \mathcal{E}_k(\mathcal{O}_P). \]

**Proof.** We apply Theorem 3.4.3 and get

\[ \mathcal{E}_k(\mathcal{O}_P) = \mathcal{O}_P^{\square k} / \mathfrak{S}_k = \left( \frac{X^n}{\text{aut}(P)} \right)^{\square k} / \mathfrak{S}_k = \frac{X^{nk}}{\text{aut}(P)\mathfrak{S}_k}. \]

It follows from Remark 3.2.2 that

\[ \mathcal{E}_k(\mathcal{O}_P) = \frac{X^{nk}}{\text{aut}(P^k)} = \mathcal{O}_{P^k}. \]

\[ \square \]

We can verify Lemma 3.6.1 in an intuitive way. Note that the set of \( \mathcal{E}_k(\mathcal{O}_P) \)-structures on a finite set \( U \) is the set of \( \mathfrak{S}_k \)-orbits of \( \mathcal{O}_P^{\square k} \)-structures on \( U \), and an element of \( \mathcal{E}_k(\mathcal{O}_P)[U] \) of the form \( \{(\pi_1, f_1), \ldots, (\pi_k, f_k)\} \) is such that \( (\pi_1, \pi_2, \ldots, \pi_k) \) is a \( k \)-rectangle on \( U \), and each \( f_i \) is a graph isomorphic to \( P \) whose vertex set equal to the blocks of \( \pi_i \). Such a set \( \{(\pi_1, f_1), \ldots, (\pi_k, f_k)\} \) corresponds to a graph \( G \)
isomorphic to $P^k$ with vertex set $U$. More precisely, $G$ is the Cartesian product of the $f_i$ in which each vertex $u \in U$ is of the form $u = B_1 \cap B_2 \cap \cdots \cap B_k$, where each $B_i$ is one of the blocks of $\pi_i$. In this way, we get a one-to-one correspondence between the $\mathcal{E}_k(\mathcal{O}_P)$-structures on $U$ and the set of graphs isomorphic to $P^k$ with vertex set $U$.

**Theorem 3.6.2.** The species $\mathcal{G}^c$ of connected graphs and $\mathcal{P}$ of prime graphs satisfy

$$\mathcal{G}^c = \mathcal{E}(\mathcal{P}).$$

**Proof.** In this proof, all graphs considered are unlabeled.

The molecular decomposition of the species of prime graphs is

$$\mathcal{P} = \sum_{P \text{ prime}} \mathcal{O}_P,$$

where each $\mathcal{O}_P$ is a molecular species which is isomorphic to $X_{l(P)}/\text{aut}(P)$.

Let $\{P_1, P_2, \ldots\}$ be the set of unlabeled prime graphs. We have

$$\mathcal{E}(\mathcal{P}) = \mathcal{E}(\mathcal{O}_{P_1} + \mathcal{O}_{P_2} + \cdots)$$

$$= \mathcal{E}(\mathcal{O}_{P_1}) \square \mathcal{E}(\mathcal{O}_{P_2}) \square \cdots$$

$$= (X + \mathcal{O}_{P_1} + \mathcal{O}_{P_2} + \cdots) \square (X + \mathcal{O}_{P_2} + \mathcal{O}_{P_2} + \cdots) \square \cdots$$

$$= \sum_{i_1, i_2, \cdots \geq 0} \mathcal{O}_{P_1^{i_1}} \square \mathcal{O}_{P_2^{i_2}} \square \cdots$$

$$= \sum_{i_1, i_2, \cdots \geq 0} \mathcal{O}_{P_1^{i_1} \square P_2^{i_2} \square \cdots}$$

$$= \sum_{C \text{ connected}} \mathcal{O}_C$$

$$= \mathcal{G}^c.$$
Now we can compute the cycle index of the species of prime graphs recursively using Maple:

\[
Z_{\mathcal{P}} = \left( \frac{1}{2} p_1^2 + \frac{1}{2} p_2 \right) + \left( \frac{2}{3} p_1^3 + p_1p_2 + \frac{1}{3} p_3 \right) + \left( \frac{35}{24} p_1^4 + \frac{7}{4} p_1^2 p_2 + \frac{2}{3} p_1p_3 + \frac{7}{8} p_2^2 + \frac{1}{4} p_4 \right) + \left( \frac{91}{15} p_1^5 + \frac{19}{3} p_1^3 p_2 + \frac{4}{3} p_1^3 p_3 + 5p_1p_2^2 + p_1p_4 + \frac{2}{3} p_2p_3 + \frac{3}{5} p_5 \right) + \left( \frac{1654}{45} p_1^6 + \frac{91}{3} p_1^4 p_2 + \frac{38}{9} p_1^3 p_3 + 21p_1^2 p_2^2 + 2p_1^2 p_4 + \frac{8}{3} p_1 p_2 p_3 \right) + \left( \frac{4}{5} p_1 p_5 + \frac{47}{6} p_2^3 + \frac{5}{2} p_2p_4 + \frac{11}{9} p_3^2 + \frac{2}{3} p_6 \right) + \cdots.
\]

Figure 3.6. Unlabeled prime graphs on \( n \) vertices, \( n \leq 4 \).

We can write down the beginning terms of the molecular decomposition of the species \( \mathcal{P} \):

\[
\mathcal{P} = \mathcal{E}_2 + (X \mathcal{E}_2 + \mathcal{E}_3) + (\mathcal{E}_2 \circ X^2 + X \mathcal{E}_3 + X^2 \mathcal{E}_2 + \mathcal{E}_2^2 + \mathcal{E}_4) + \cdots.
\]

Comparing Figure 3.6 with Figure 2.9, we see that there is only one unlabeled connected graph with 4 vertices that is not prime. In fact, if we compare the first
several terms of $Z_{\gamma c}$, given in (2.4.6), and $Z_\varphi$ of order no more than 6, we get that

$$Z_{\gamma c} - Z_\varphi = p_1 + \frac{1}{8} \left( p_1^4 + 2p_1^2p_2 + 3p_2^2 + 2p_4 \right)$$

$$+ \frac{1}{4} \left( p_1^3 + p_1^2p_2^2 + 2p_2^3 \right) + \frac{1}{12} \left( p_1^6 + 3p_1^2p_2^2 + 4p_2^3 + 2p_3^2 + 2p_6 \right) \cdots ,$$

which is the cycle index of connected non-prime graphs on no more than 6 vertices, as shown in Figure 3.7, which consist of a single vertex, a graph with 4 vertices, and two graphs with 6 vertices.

![Figure 3.7. Unlabeled non-prime graphs on $n$ vertices, $n \leq 6$.](image-url)
CHAPTER 4

Point-Determining Graphs

4.0. Introduction

In this chapter, we examine the species of point-determining graphs (Definition 4.1.1), which are graphs whose vertices all have distinct neighborhoods, the species of co-point-determining graphs (Definition 4.1.2), which are graphs whose complements are point-determining, the species of connected point-determining graphs, and the species of bi-point-determining graphs (Definition 4.3.1), which are graphs that are both point-determining and co-point-determining. Our goal is to find the cycle indices of these species. First, we find a functional equation relating the species of point-determining graphs and the well-known species of graphs (Theorem 4.1.3). At the same time, we find a simple connection between the point-determining graphs and the co-point-determining graphs. The connected cases are similar to the enumeration of connected graphs as shown in Section 2.4. Furthermore, we find a functional equation relating the species of bi-point-determining graphs and the species of graphs.

In addition, we examine the 2-sort species of 2-colored graphs (Definition 4.4.1), which are graphs whose vertices are properly colored with white and black. We develop ways to enumerate the 2-sort species of connected 2-colored graphs and the 2-sort species of point-determining 2-colored graphs.
4.1. Point-Determining Graphs and Co-Point-Determining Graphs

**Definition 4.1.1.** A point-determining graph, previously studied by Sumner [28], also called a mating-type graph by Bull and Pease [4] and Read [23], is a graph $G$ in which any two distinct vertices have distinct neighborhoods, i.e., if $v_1 \neq v_2$, then $N(v_1) \neq N(v_2)$, where $N(v) = \{ w : \overline{vw} \text{ is an edge of } G \}$ is the set of vertices adjacent to $v$.

Note that the neighborhood of an isolated vertex is the empty set. Thus in a point-determining graph, there is at most one isolated vertex.

**Definition 4.1.2.** A graph is called co-point-determining if its complement is point-determining.

In a co-point-determining graph, two non-adjacent distinct vertices have distinct augmented neighborhoods. That is, if $v_1$ and $v_2$ are distinct vertices in this graph, then $N(v_1) \cup \{v_1\} \neq N(v_2) \cup \{v_2\}$.

We denote the species of point-determining graphs by $\mathcal{P}$. Thus in the species language, a point-determining graph is a $\mathcal{P}$-structure. We denote by $\mathcal{Q}$ the species of co-point-determining graphs. We set the number of point-determining graphs and the number of co-point-determining graphs on an empty set of vertices both to be one.

We observe that there is a natural transformation $\alpha$ that produces for every finite set $U$ a bijection between $\mathcal{P}[U]$ and $\mathcal{Q}[U]$, which sends each point-determining graph with vertex set $U$ to its complement, which is a co-point-determining graph with vertex set $U$. Furthermore, the following diagram commutes for any finite sets $U, V$ and any bijection $\sigma : U \to V$: 

87
Hence, according to Remark 2.1.7, the species $\mathcal{P}$ and $\mathcal{Q}$ are isomorphic, and we do not make distinctions between them during calculations.

There are four point-determining graphs and and four co-point-determining graphs labeled on $[3]$, as shown in Figure 4.1, whose first row consists of the point-determining graphs and whose second row consists of the co-point-determining graphs.

![Figure 4.1. Labeled point-determining graphs and co-point-determining graphs with vertex set $[3]$.](image)

The following theorem gives a starting point for counting point-determining graphs.

**Theorem 4.1.3.** Let $\mathcal{G}$ be the species of graphs, $\mathcal{P}$ the species of point-determining graphs, and $\mathcal{E}_+$ the species of nonempty sets. Then we have

\[
\mathcal{G} = \mathcal{P}(\mathcal{E}_+).
\]

**Proof.** Given any graph $G$ with vertex set $V$, we define an equivalence relation on $V$ by setting two elements $v$ and $w$ of $V$ to be equivalent to each other if they
have the same neighborhoods. This gives a partition of \( V \) into \( m \) equivalence classes

\[ \pi = \{ V_1, V_2, \ldots, V_m \}. \]

We then associated to the graph \( G \) the ordered pair \((\pi, G')\), where \( G' \) is the graph whose vertices are the blocks of \( \pi \) in which two vertices \( V_i \) and \( V_j \) in \( G' \) are adjacent if and only if there is an edge in \( G \) connecting a vertex in \( V_i \) with one in \( V_j \). An example of such a transformation from a graph \( G \) to a point-determining graph \( G' \) is illustrated in Figure 4.2. It is straightforward to see that the graph \( G' \) is point-determining, since no two vertices of \( G' \) have the same neighborhoods.

Figure 4.2. A transformation from a graph \( G \) with vertex set \([11]\) to a point-determining graph \( G' \) with vertex set \( \{\{1, 9, 3\}, \{8\}, \{4, 7\}, \{6\}, \{2, 5\}\} \).

On the other hand, we can construct a graph on \( n \) vertices uniquely (up to isomorphism) from an ordered pair consisting of a point-determining graph on \( m \) vertices and a partition of \( n \) vertices into \( m \) blocks by reversing the procedure described in above. This bijection leads to the species equivalence relation (4.1.1).
CHAPTER 4. POINT-DETERMINING GRAPHS

Using the same method we can prove that

\[
G(X) = \mathcal{Q}(\mathcal{K}_+),
\]

where \(\mathcal{K}_+\) is the species of complete graphs with non-empty vertex sets.

Recall \(\Gamma\), the compositional inverse of \(\mathcal{E}_+\) as defined in Section 2.4. Equations (4.1.1) and (4.1.2) can be rewritten as

\[
\mathcal{P} = \mathcal{Q} = G(\Gamma).
\]

This identity gives rise to several identities that can be used to compute the associated series of \(\mathcal{P}\):

\begin{align*}
(4.1.3) & \quad \mathcal{P}(x) = \mathcal{Q}(x) = G(\log(1 + x)), \\
(4.1.4) & \quad \tilde{\mathcal{P}}(x) = \tilde{\mathcal{Q}}(x) = Z_{\mathcal{Q}}(x - x^2, x^2 - x^4, \ldots), \\
& \quad Z_{\mathcal{P}} = Z_{\mathcal{Q}} = Z_{\mathcal{Q}}\left(\sum_{k \geq 1} \frac{\mu(k)}{k} \log(1 + p_k), \sum_{k \geq 1} \frac{\mu(k)}{k} \log(1 + p_{2k}), \ldots\right).
\end{align*}

Read [23] derived formulas (4.1.3) and (4.1.4), and pointed out that identity (4.1.3) gives an explicit expression for the numbers of labeled point-determining graphs with \(k\) vertices \(p_k\):

\[
p_k = \sum_{n \geq 0} 2^{\binom{n}{2}} s(n, k),
\]

where the \(s(n, k)\) denote Stirling numbers of the first kind [29].

Using Maple, we can write down the first several terms of the associated series of \(\mathcal{P}\):

\[
\mathcal{P}(x) = 1 + \frac{x}{1!} + \frac{x^2}{2!} + 4 \frac{x^3}{3!} + 32 \frac{x^4}{4!} + 588 \frac{x^5}{5!} + 21476 \frac{x^6}{6!} + 1551368 \frac{x^7}{7!} + \cdots,
\]

\[
\tilde{\mathcal{P}}(x) = 1 + x + x^2 + 2x^3 + 5x^4 + 16x^5 + 78x^6 + 588x^7 + 8047x^8 + 205914x^9 + \cdots.
\]
Z_{\mathcal{P}} = 1 + p_1 + \left( \frac{1}{2} p_1^2 + \frac{1}{2} p_2 \right) + \left( \frac{1}{3} p_3 + p_1 p_2 + \frac{2}{3} p_1^3 + \frac{3}{2} p_1^2 p_2 \right) \\
+ \left( \frac{1}{2} p_4 + \frac{4}{3} p_1^4 + p_2^2 + \frac{2}{3} p_1 p_3 \right) \\
+ \left( p_1^2 p_3 + \frac{49}{10} p_1^5 + \frac{11}{3} p_1^3 p_2 + \frac{1}{3} p_2 p_3 + \frac{3}{5} p_5 + p_1 p_4 + \frac{9}{2} p_1^2 p_2 \right) + \cdots .

\text{Figure 4.3. Unlabeled point-determining graphs on } n \text{ vertices, } n \leq 4.

In this way, the molecular decomposition of \mathcal{P} takes the form

\mathcal{P} = X + E_2 + \left( X E_2 + E_3 \right) + \left( X^2 E_2 + X E_3 + E_2 \circ E_2 + X^2 E_2 + E_4 \right) + \cdots .

Let \( p_n, c_n \) and \( g_n \) be numbers of labeled point-determining graphs, connected graphs and graphs on \( n \) vertices. We have the following table:

\textbf{4.2. Connected Point-Determining Graphs and Connected Co-Point-Determining Graphs}

A point-determining or a co-point-determining graph is called \textit{connected} if the graph itself is connected. We denote by \( \mathcal{P}^c \) the species of connected point-determining graphs, and by \( \mathcal{Q}^c \) the species of connected co-point-determining graphs.
Table 1. Numbers of labeled point-determining graphs, connected graphs and graphs on \( n \) vertices, \( n \leq 10 \).

<table>
<thead>
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<th>( n )</th>
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<th>( c_n )</th>
<th>( g_n )</th>
</tr>
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**Theorem 4.2.1.** Let \( \mathcal{P} \) be the species of point-determining graphs, and let \( \mathcal{P}^c \) be the species of connected point-determining graphs. We have

\[
\mathcal{P} = (1 + X) \mathcal{E}(\mathcal{P}^c - X).
\]

**Proof.** Since a point-determining graph can have at most one isolated vertex, and the rest of its connected components are connected point-determining graphs with at least two vertices, we have

\[
\mathcal{P} = \mathcal{E}(\mathcal{P}^c - X) + X \mathcal{E}(\mathcal{P}^c - X).
\]

\( \square \)

**Theorem 4.2.2.** For the species \( \mathcal{Q} \) and \( \mathcal{Q}^c \), we have

\[
\mathcal{Q} = \mathcal{E}(\mathcal{Q}^c).
\]

**Proof.** The result follows straightforwardly from the observation that a graph is co-point-determining if and only if all its connected components are. \( \square \)
Since $\mathcal{P}$ and $\mathcal{Q}$ are isomorphic to each other, we get

\[(4.2.1) \quad \mathcal{P} = (1 + X) \mathcal{E}(\mathcal{P}^c - X) = \mathcal{E}(\mathcal{Q}^c).\]

Recall the virtual species $\Gamma$, which is the compositional inverse of $\mathcal{E}_+$ introduced in Section 2.4, we have

$$\mathcal{Q}^c = \Gamma(\mathcal{P}_+),$$

where $\mathcal{P}_+$ is the species of point-determining graphs with nonempty vertex sets. Hence we get to compute the associated series of $\mathcal{Q}^c$:

$$\mathcal{Q}^c(x) = \log(\mathcal{P}(x)),$$

$$\tilde{\mathcal{Q}}^c(x) = \sum_{k \geq 1} \frac{\mu(k)}{k} \log(\tilde{\mathcal{P}}(x^k)),$$

$$Z_{\mathcal{Q}^c} = \sum_{k \geq 1} \frac{\mu(k)}{k} \log(Z_{\mathcal{P}^c} \circ p_k - p_k + 1).$$

We write down the first several terms of the associated series of $\mathcal{Q}^c$ using Maple:

$$\mathcal{Q}^c(x) = x + \frac{x^3}{3!} + 19 \frac{x^4}{4!} + 462 \frac{x^5}{5!} + 18268 \frac{x^6}{6!} + 1410394 \frac{x^7}{7!} + 20667954 \frac{x^8}{8!} + \ldots,$$

$$\tilde{\mathcal{Q}}^c(x) = x + x^3 + 3x^4 + 11x^5 + 61x^6 + 507x^7 + 7442x^8 + 197772x^9 + 9808209x^{10} + \ldots,$$

$$Z_{\mathcal{Q}^c} = p_1 + \left(\frac{1}{2} p_1 p_2 + \frac{1}{2} p_3\right) + \left(\frac{19}{24} p_4 + \frac{3}{4} p_1^2 p_2 + \frac{1}{3} p_1^3 p_3 + \frac{7}{8} p_2^2 + \frac{1}{4} p_4\right) + \ldots.$$

Equation (4.2.1) can be rewritten as

\[(4.2.2) \quad \mathcal{P} = \mathcal{E}(\Gamma + \mathcal{P}^c - X) = \mathcal{E}(\mathcal{Q}^c).\]
As a general fact, if $E(F_1) = E(F_2)$ for any species $F_1$ and $F_2$, then
\[ E_+(F_1) = E_+(F_2). \]

It follows that $\Gamma \circ E_+(F_1) = \Gamma \circ E_+(F_2)$. Since $\Gamma \circ E_+ = X$, we have $F_1 = F_2$.

Therefore, Equation (4.2.2) gives
\[ \Gamma + \mathcal{P}^c - X = \mathcal{Q}^c, \]
or, equivalently,
\[ \Gamma = \mathcal{Q}^c - \mathcal{P}^c_{\geq 2}, \]
which gives an explicit expression for the virtual species $\Gamma$ as the difference of two species.

We also get the functional equations relating the associated series of $\mathcal{P}^c$ and those of $\mathcal{Q}^c$:
\[ \mathcal{P}^c(x) = \mathcal{Q}^c(x) + x - \log(1 + x), \]
\[ \widetilde{\mathcal{P}}^c(x) = \widetilde{\mathcal{Q}}^c(x) + x - (x - x^2), \]
\[ Z_{\mathcal{P}^c} = Z_{\mathcal{Q}^c} + p_1 - \sum_{k \geq 1} \frac{\mu(k)}{k} \log(1 + p_k). \]

Through computation, we get the first several terms of the associated series of $\mathcal{P}^c$:
\[ \mathcal{P}^c(x) = x + \frac{x^2}{2!} + \frac{x^3}{3!} + 25 \frac{x^4}{4!} + 438 \frac{x^5}{5!} + 18388 \frac{x^6}{6!} + 1409674 \frac{x^7}{7!} + 206682994 \frac{x^8}{8!} + \cdots, \]
\[ \widetilde{\mathcal{P}}^c(x) = x + x^2 + x^3 + 3x^4 + 11x^5 + 61x^6 + 507x^7 + 7442x^8 + 197772x^9 + \cdots, \]
\[ Z_{\mathcal{P}^c} = p_1 + \left( \frac{1}{2} p_1^2 + \frac{1}{2} p_2 \right) + \left( \frac{1}{6} p_3 + \frac{1}{3} p_3 + \frac{1}{2} p_1 p_2 \right) \]
Let $p_n^c$ and $q_n^c$ be the numbers of labeled connected point-determining graphs and connected co-point-determining graphs, respectively, so that

\[
\mathcal{P}_n^c(x) = \sum_{n \geq 1} p_n^c \frac{x^n}{n!}, \quad \mathcal{Q}_n^c(x) = \sum_{n \geq 1} q_n^c \frac{x^n}{n!}.
\]

We get from the above species equivalence an identity relating $p_n^c$ and $q_n^c$:

\[
(4.2.3) \quad p_n^c + (-1)^{n-1}(n-1)! = q_n^c, \quad \text{for } n \geq 2.
\]

Figure 4.4 shows the unlabeled connected point-determining graphs and unlabeled connected co-point-determining graphs with 4 vertices.

Figure 4.4. Unlabeled connected point-determining graphs and unlabeled connected co-point-determining graphs on 4 vertices.

We can get the number of labeled connected point-determining graphs and co-point-determining graphs by calculating the number of labeled graphs isomorphic to each $p_i$ and $q_i$:

\[
p_i^c = \left( \frac{24}{\text{aut}(p_1)} + \frac{24}{\text{aut}(p_2)} + \frac{24}{\text{aut}(p_3)} \right) = 12 + 12 + 1 = 25,
\]

\[
q_i^c = \left( \frac{24}{\text{aut}(p_1)} + \frac{24}{\text{aut}(p_2)} + \frac{24}{\text{aut}(p_3)} \right) = 12 + 3 + 4 = 19.
\]
A combinatorial proof of Equation (4.2.3) would be desirable.

Table 2. Values of $p_n^c$ and $q_n^c$, for $n \leq 10$.

<table>
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<tr>
<th>$n$</th>
<th>$p_n^c$</th>
<th>$q_n^c$</th>
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</table>

4.3. Bi-Point-Determining Graphs

Definition 4.3.1. A graph is called *bi-point-determining* if it is both point-determining and co-point-determining.

The enumeration of the bi-point-determining graphs is carried out through the structures called phylogenetic trees.

Definition 4.3.2. A *phylogenetic tree* is a rooted tree with labeled leaves and unlabeled internal vertices in which no vertex has exactly one child.

Figure 4.5. A phylogenetic tree on [6].
**Theorem 4.3.3.** Let $\mathcal{R}$ be the species of bi-point-determining graphs. Let $\mathcal{G}$ and $\mathcal{S}$ be the species of graphs and phylogenetic trees respectively. Then we have

$$\mathcal{G} = \mathcal{R}(2\mathcal{S} - X).$$

The enumeration of phylogenetic trees was studied by Carlitz and Riordan [5], Foulds and Robinson [7], Lomnicki [14], and others.

**Lemma 4.3.4.** Let $\mathcal{S}$ be the species of phylogenetic trees, and let $\mathcal{E}_{\geq 2}$ be the species of sets with no less than two elements. We have

$$(4.3.1) \quad \mathcal{S} = X + \mathcal{E}_{\geq 2}(\mathcal{S}).$$

**Proof.** A phylogenetic tree is either a singleton vertex, which contributes to the term $X$ on the right-hand side of Equation (4.3.1), or is a phylogenetic tree with at least two leaves, in which case we can separate the root and the rest of the tree and get a set of at least two subtrees each of which is again a phylogenetic tree, which, as illustrated in Figure 4.6, is an $\mathcal{E}_{\geq 2} \circ \mathcal{S}$-structure. $\square$

![Figure 4.6](image)

**Figure 4.6.** A phylogenetic tree with at least two leaves is a set of at least two subtrees each of which is a phylogenetic tree.
Equation (4.3.1) enables us to compute the first several terms of the associated series of $\mathcal{S}$ using Maple:

$$\mathcal{S}(x) = x + \frac{x^2}{2!} + 4 \frac{x^3}{3!} + 26 \frac{x^4}{4!} + 236 \frac{x^5}{5!} + 2752 \frac{x^6}{6!} + 39208 \frac{x^7}{7!} + 660032 \frac{x^8}{8!} + \cdots,$$

$$\hat{\mathcal{S}}(x) = x + x^2 + 2x^3 + 5x^4 + 12x^5 + 33x^6 + 90x^7 + 261x^8 + 766x^9 + \cdots,$$

$$Z_{\mathcal{S}} = p_1 + \left( \frac{1}{2} p_1^2 + \frac{1}{2} p_2 \right) + \left( \frac{2}{3} p_1^3 + p_1 p_2 + \frac{1}{3} p_3 \right)$$

$$+ \left( \frac{13}{12} p_1^4 + p_1^2 p_2 + \frac{2}{3} p_1 p_3 + \frac{3}{4} p_2^2 + \frac{1}{2} p_4 \right)$$

$$+ \left( \frac{59}{30} p_1^5 + \frac{4}{3} p_1^2 p_3 + 2 + \frac{5}{2} p_1 p_2^2 + \frac{13}{3} p_1^3 p_2 + p_1 p_4 + \frac{2}{3} p_2 p_3 + \frac{1}{5} p_5 \right)$$

$$+ \left( \frac{172}{45} p_1^6 + \frac{2}{5} p_1 p_5 + \frac{59}{6} p_1^4 p_2 + \frac{26}{9} p_1^3 p_3 + \frac{15}{2} p_1^2 p_2^2 + 2 p_1^2 p_4 + \frac{8}{3} p_1 p_2 p_3 \right.$$  

$$\left. + \frac{3}{2} p_2 p_4 + \frac{1}{2} p_6 \right) + \cdots.$$

Figure 4.7 shows the unlabeled phylogenetic trees with no more than 5 vertices.

![Figure 4.7](image-url)
Therefore, the molecular decomposition of $\mathcal{S}$ is

\[
\mathcal{S} = X + \mathcal{E}_2 + \left( X\mathcal{E}_2 + \mathcal{E}_3 \right) + \left( X^2\mathcal{E}_2 + \mathcal{E}_2 \circ \mathcal{E}_2 + \mathcal{E}_2^2 + X\mathcal{E}_3 + \mathcal{E}_4 \right) \\
+ \left( X^3\mathcal{E}_2 + X^2\mathcal{E}_3 + 3X\mathcal{E}_2^2 + 2X\mathcal{E}_2 \circ \mathcal{E}_2 + X\mathcal{E}_4 + 3\mathcal{E}_2\mathcal{E}_3 + \mathcal{E}_5 \right) + \cdots
\]

It is of interest to observe that different trees might have the same species expression. For example, the three unlabeled phylogenetic trees with 5 vertices listed in Figure 4.8 correspond to the same species $X\mathcal{E}_2^2$.

Figure 4.8. Unlabeled phylogenetic trees corresponding to the species $X\mathcal{E}_2^2$.

**Definition 4.3.5.** We define an *alternating phylogenetic tree* to be either a single vertex, or a phylogenetic tree with more than one labeled vertex whose internal vertices are colored black or white, where no two adjacent vertices are colored the same way.

We denote by $\mathcal{S}^*$ the species of alternating phylogenetic trees. The structure of alternating phylogenetic trees $\mathcal{S}^*$ was studied by Stanley [27, p. 89], MacMahon [16, 17], and Riordan and Shannon [24] under other names such as yoke-chains and series-parallel networks.

Note that any phylogenetic tree with more than one labeled vertex gives rise to two alternating phylogenetic trees, since the coloring of the internal vertices is uniquely
Figure 4.9. An alternating phylogenetic tree labeled on the set \([9]\), where the root is colored black.

determined by the coloring of the root, which has two choices. Therefore,

\[ J^* = 2J - X. \]

**Proof of Theorem 4.3.3.** In this proof, we will show how to transform an arbitrary graph into a bi-point-determining graphs. This transformation, with all information preserved using the structure of alternating phylogenetic trees, is reversible, and hence gives a bijection from the set of graphs with vertex set \(U\) to the set of triples of the form \((\pi, \varphi, \gamma)\) where \(\pi\) is a partition of \(U\), \(\varphi\) is a bi-point-determining on the blocks of \(\pi\), and \(\gamma\) is a set of alternating phylogenetic trees each of which is labeled on a block of \(\pi\). Such a bijection leads to the functional equation

\[ G = R \circ J^*. \]

Let \((g, h)\) be an ordered pair that satisfies the following conditions

**C1** \(g\) is a graph with vertex set \(u = \{u_1, u_2, \ldots\}\), where each \(u_i\) is a set, and the \(u_i\) are disjoint;

**C2** \(h\) is a set \(h = \{t_1, t_2, \ldots\}\), where each \(t_i\) is an alternating phylogenetic tree labeled on the vertex set \(u_i\). Such pairs \((g, h)\) are illustrated in Figures 4.10 and 4.11.
Next, we define two operations $O_Q$ and $O_P$ on pairs $(g, h)$ such that each operation sends $(g, h)$ to a new ordered pair $(g', h')$.

First, the operation $O_Q$ sends $(g, h)$ to a new pair $(g', h')$, where $g'$ is a graph and $h'$ is a set of alternating phylogenetic trees. More precisely, we start by defining an equivalence relation on the vertex set of $g$ such that two vertices are equivalent if they have the same augmented neighborhoods. We denote by

$$E = \{e_1, e_2, \ldots, e_m\}$$

the set of equivalence classes of $V(g)$, where each $e_i$ is a set of vertices of $g$, i.e.,

$$e_i = \{u_{i,1}, u_{i,2}, \ldots\}.$$

We let $w_1, w_2, \ldots$ be such that

$$w_i = u_{i,1} \cup u_{i,12} \cup \cdots.$$

We now let the $w_i$ be the vertices of $g'$, and two vertices $w_i$ and $w_j$ are adjacent in $g'$ if a vertex in the equivalence class $e_i$ is adjacent to a vertex in the equivalence class $e_j$.
$e_j$ in the graph $g$. Note that

$$w_1 \cup w_2 \cup \cdots = u_1 \cup u_2 \cup \cdots.$$  

We construct a set

$$h' = \{t'_1, t'_2, \ldots\}$$

by letting $t'_i$ be the alternating phylogenetic tree whose root is colored white and whose children are the trees $t_{i,1}, t_{i,2}, \ldots \in h$ labeled by the sets $u_{i,1}, u_{i,2}, \ldots \in V(g)$. Note that $t'_i$ could fail to be an alternating phylogenetic tree, because some of the alternating phylogenetic trees corresponding to the vertices $u_{i,1}, u_{i,2}, \ldots$ of $g$ have white roots. In this case, in order to make $t'_i$ have alternating colors on the internal vertices, we need to modify our construction of $t'_i$ by taking each white-rooted alternating phylogenetic tree, $t_{i,k}$, and attaching the children of the root of $t_{i,k}$ directly to the root of $t'_i$. We get a new pair $(g', h')$, where $g'$ is a graph on two vertices $w_1$ and $w_2$ with

$$w_1 = u_1, \quad w_2 = u_2 \cup u_3 \cup u_4,$$

and $h'$ is a set of two alternating phylogenetic trees, one on the set $w_1$, the other on the set $w_2$. Note that the alternating phylogenetic tree on $u_2$ has a white root, so we attach the children of this tree to the white root in the alternating phylogenetic tree on $w_2$.

Second, the operation $O_{\not\simeq}$ sends the ordered pair $(g, h)$ to a new ordered pair $(g', h')$ in a way similar to the operation $O_{\simeq}$, except that now the equivalence classes on the vertices of $g$ are taken over vertices with the same neighborhoods in $g$, and that the new root we attach to a set of alternating phylogenetic trees is colored black instead of white. Again, we modify our construction as in $O_{\not\simeq}$ to ensure that we get new alternating phylogenetic trees without violating the rule of alternating colors.
Figure 4.11.  a) An $O_{\varphi}$ application.  b) An $O_{\varphi}$ application.

Figure 4.12 illustrates the operation $O_{\varphi}$ on a pair $(g, h)$ in Figure 4.10, where

$$V(g) = \{u_1, u_2, u_3, u_4\},$$

$h$ is a set of alternating phylogenetic trees labeled on the set $u_i$ for $i = 1, 2, 3, 4$.

$g'$ with $V(g') = \{w_1, w_2\}$

$\quad \quad$ $\quad \quad$

$g'$ with $V(g') = \{w_1, w_2\}$

$h' = \{t'_1, t'_2\}$

Figure 4.12.  The operation $O_{\varphi}$ applied to a pair $(g, h)$ in Figure 4.10 requires a modification on the construction of alternating phylogenetic tree $t'_2$.  

103
It is straightforward to check that the new pair \((g', h')\) we get under either the application of \(O_Q\) or \(O_P\) satisfies conditions \(\text{C1}\) and \(\text{C2}\), and that the union of the vertices of \(g\) is equal to the union of the vertices of \(g'\). We further observe that the operation \(O_Q\) sends a graph \(g\) to a co-point-determining graph \(g'\), since in \(g'\), no two vertices have the same augmented neighborhoods. Similarly, the operation \(O_P\) sends a graph \(g\) to a point-determining graph \(g'\). That is why \(O_P\) and \(O_Q\) should be applied alternatingly, since \(O_P\) has no effect on a point-determining graph, and \(O_Q\) has no effect on a co-point-determining graph.

Now let \(G\) be a graph with vertex set

\[ U = \{v_1, v_2, \ldots\}. \]

We relabel \(G\) with the set

\[ U' = \{U_1, U_2, \ldots\}, \]

where each \(U_i = \{v_i\}\) is a singleton set, viewed as the label of a vertex of \(G\). We assign to \(G\) a set

\[ H = \{T_1, T_2, \ldots\}, \]

where each \(T_i\) is a single vertex \(v_i\). Then \((G, H)\) is an ordered pair satisfying conditions \(\text{C1}\) and \(\text{C2}\).

We keep applying the operations \(O_Q\) and \(O_P\) alternatingly on the pair \((G, H)\), until neither operation has any effect, that is, when we reach an ordered pair \((G_k, H_k)\) in which \(G_k\) is a bi-point-determining graph. Illustrated in Figure 4.13 is a sequence of alternating operations \(O_Q\) and \(O_P\), starting with \(O_P\), sending a pair \((G, H)\) to a pair \((G_k, H_k)\), where \(G_k\) is a bi-point-determining graph on a single vertex, and \(H_k\) is a set consists of a single alternating phylogenetic tree whose vertex set is the vertex of \(G_k\).
Figure 4.13. Alternating applications of $O_{\mathcal{D}}$ and $O_{\mathcal{D}}$ send a pair $(G, H)$ to a pair $(G_k, H_k)$.

The above discussion shows that we get from any graph $G$, we get a pair $(G_k, H_k)$ satisfies conditions $C_1$ and $C_2$. To be more precise, writing

$$V(G_k) = \{V_1, V_2, \ldots\}, \quad H_k = \{T_1, T_2, \ldots\},$$

we get a triple of the form $(\pi, \varphi, \gamma)$, where

i) $\pi = \{V_1, V_2, \ldots\}$ is a partition of $U$;

ii) $\varphi = G_k$ is a bi-point-determining graph with vertex set $\pi$.

iii) $\gamma = \{T_1, T_2, \ldots\}$, where for each $i$, $T_i$ is an alternating phylogenetic tree with vertex set $V_i$.

On the other hand, since all information is preserved using the alternating phylogenetic trees, the above procedure is reversible. Roughly speaking, on each step, the adjacency outside the equivalence classes are always preserved, while the adjacency between vertices with the same augmented neighborhoods are transformed into them.
located in the same alternating phylogenetic tree with a white common ancestor, where the common ancestor of two vertices \(a\) and \(b\) in a phylogenetic tree is defined to be such that if we take the unique shortest path from \(a\) to \(b\), say, \(w_0w_1 \cdots w_l\), with \(w_0 = a\) and \(w_l = b\), then the common ancestor of \(a\) and \(b\) is the unique \(w_i\) for which both \(w_{i-1}\) and \(w_{i+1}\) are children of \(w_i\).

More precisely, suppose we are given a triple \((\pi, \varphi, \gamma)\), where \(\pi = \{V_1, V_2, \ldots\}\) is a partition of \(U\), i.e., \(\bigcup_i V_i = U\), \(\varphi\) is a bi-point-determining graph on the blocks of \(\pi\), and \(\gamma\) is a set \(\{S_1, S_2, \ldots\}\) in which each \(S_i\) is an alternating phylogenetic tree labeled on the set \(V_i\). Then there is a unique graph \(G\) with vertex set \(U\) constructed in the way such that for any \(v_1, v_2 \in V(G)\), \(\{v_1, v_2\}\) is an edge of \(G\) if and only if exactly one of the following two conditions is satisfied:

- \(v_1, v_2 \in V_i\) for some \(i\), hence \(v_1\) and \(v_2\) are labels of vertices of \(S_i\). Then we require the common ancestor of those vertices labeled \(v_1\) and \(v_2\) in \(S_i\) to be colored white. The common ancestor of two vertices \(a\) and \(b\) in a phylogenetic tree is defined to be such that if we take the unique shortest path from \(a\) to \(b\), say, \(w_0w_1 \cdots w_l\), with \(w_0 = a\) and \(w_l = b\), then the common ancestor of \(a\) and \(b\) is the unique \(w_i\) for which both \(w_{i-1}\) and \(w_{i+1}\) are children of \(w_i\).

- \(v_1 \in V_i, v_2 \in V_j\) and \(i \neq j\). Then we require \(V_i\) and \(V_j\) to be adjacent to each other in the graph \(\varphi\).

The above can be concluded with a species equivalence

\[
G = \mathcal{R} \circ \mathcal{I}^*,
\]

which gives

\[
\mathcal{I} = \mathcal{R} \circ (2\mathcal{I} - X).
\]
Figure 4.14. Construct a graph $G$ from a given triple $(\pi, \varphi, \gamma)$.

We get from Theorem 4.3.3 a functional equation expressing the species $R$ in terms of the species $G$.

**Corollary 4.3.6.** Let $G$, $R$ be the species of graphs and the species of bi-point-determining graphs. Let $\Gamma$ be the virtual species as defined in Section 2.4. Then we have

$$R = G(2\Gamma - X).$$

**Proof.** First, we observe that since $S_0 = 0$ and $S_1 = X$, the same is true for $S^*$: $S^*_0 = 0$ and $S^*_1 = X$. Proposition 19 of [2, p. 130] says that there exists a unique virtual species $S^*(-1)$ such that

$$S^* \circ S^*(-1) = S^*(-1) \circ S^* = X.$$

Since Theorem 4.3.3 gives that

$$R = G(S^*(-1)),$$
it suffices to show that the compositional inverse of $S^*$ is $2\Gamma - X$.

But $2S - S^* = X$ implies that

$$S = \frac{X + S^*}{2}.$$ 

On the other hand, Equation (4.3.1) implies $2S - X = \mathcal{E}(S) - 1$. So

$$S^* = \mathcal{E}(S) - 1,$$

and

$$S^* + 1 = \mathcal{E}(S) = \mathcal{E}\left(\frac{X + S^*}{2}\right).$$

But from

$$\mathcal{E} \circ \Gamma(X) = X + 1,$$

we get

$$\mathcal{E} \circ \Gamma \circ S^* = X \circ S^* + 1,$$

so

$$\mathcal{E}(\Gamma(S^*)) = S^* + 1 = \mathcal{E}\left(\frac{X + S^*}{2}\right)$$

by Equation (4.3.3). So

$$\Gamma(S^*) = \frac{X + S^*}{2},$$

which gives that

$$X = 2\Gamma(S^*) - S^* = (2\Gamma - X) \circ S^*.$$ 

□
Equation (4.3.2) gives rise to several identities for computing the associated series of $R$:

\[
\mathcal{R}(x) = G(2 \log(1 + x) - x),
\]

\[
\tilde{\mathcal{R}}(x) = Z_{\mathcal{G}}(x - 2x^2, x^2 - 2x^4, \ldots),
\]

\[
Z_{\mathcal{R}} = Z_{\mathcal{G}}\left(2 \sum_{k \geq 1} \frac{\mu_k}{k} \log(1 + p_k) - p_1, 2 \sum_{k \geq 1} \frac{\mu_k}{k} \log(1 + p_{2k}) - p_2, \ldots\right).
\]

Using Maple, we get the following:

\[
\mathcal{R}(x) = \frac{x}{1!} + 12 \frac{x^4}{4!} + 312 \frac{x^5}{5!} + 13824 \frac{x^6}{6!} + 1147488 \frac{x^7}{7!} + 178672128 \frac{x^8}{8!} + \cdots,
\]

(4.3.4)

\[
\tilde{\mathcal{R}}(x) = x + x^4 + 6x^5 + 36x^6 + 324x^7 + 5280x^8 + 156088x^9 + 8415760x^{10} + \cdots,
\]

\[
Z_{\mathcal{R}} = p_1 + \left(\frac{1}{2} p_1^4 + \frac{1}{2} p_2^2\right) + \left(\frac{13}{3} p_1^5 + 3p_1 p_2^2 + \frac{2}{5} p_3\right) + \left(\frac{96}{5} p_1^6 + 11p_1^2 p_2^2 + \frac{4}{5} p_1 p_5 + \frac{11}{3} p_2^3 + p_3^2 + \frac{1}{3} p_6\right) + \cdots.
\]

It is interesting to observe from Equation (4.3.4) that there is no bi-point-determining graphs on 2 or 3 vertices. The unlabeled bi-point-determining graphs on 4 or 5 vertices are shown in Figure 4.15.

**Figure 4.15.** Unlabeled bi-point-determining graphs on $n$ vertices, $n = 4, 5$. 109
Therefore, we get the molecular decomposition of $R$:

$$R = X + \mathcal{E}_2 \circ X^2 + [5X(\mathcal{E}_2 \circ X^2) + \mathcal{D}_5] + \cdots,$$

where $\mathcal{D}_5 = X^5/D_5$ is the molecular species of regular pentagons with cycle index

$$Z_{\mathcal{D}_5} = Z(D_5) = \frac{1}{10}(p_1^5 + 5p_1p_2^2 + 4p_5).$$

Listed in Table 3 are numbers of labeled and unlabeled bi-point-determining graphs, denoted by $r_n^l$ and $r_n^u$.

**Table 3.** Numbers of labeled and unlabeled bi-point-determining graphs with no more than 15 vertices.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$r_n^l$</th>
<th>$r_n^u$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>12</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>312</td>
<td>6</td>
</tr>
<tr>
<td>6</td>
<td>13824</td>
<td>36</td>
</tr>
<tr>
<td>7</td>
<td>1147488</td>
<td>324</td>
</tr>
<tr>
<td>8</td>
<td>178672128</td>
<td>5280</td>
</tr>
<tr>
<td>9</td>
<td>52666091712</td>
<td>156088</td>
</tr>
<tr>
<td>10</td>
<td>29715982846848</td>
<td>8415760</td>
</tr>
<tr>
<td>11</td>
<td>32452221242518272</td>
<td>820793600</td>
</tr>
<tr>
<td>12</td>
<td>69259424722321036032</td>
<td>145063881480</td>
</tr>
<tr>
<td>13</td>
<td>291060255757818125657088</td>
<td>46793310149168</td>
</tr>
<tr>
<td>14</td>
<td>2421848956937579216663491584</td>
<td>27790808726803840</td>
</tr>
<tr>
<td>15</td>
<td>40050322614433939228627991906304</td>
<td>30630967638347575456</td>
</tr>
</tbody>
</table>

We denote by $R^c$ the species of connected bi-point-determining graphs.

**Theorem 4.3.7.** For species $R$, $R^c$, and $\mathcal{E}_+$, we have

$$R = X + (1 + X) \mathcal{E}_+(R^c - X).$$
**Proof.** Since a graph with a singleton vertex is an \( R^c \)-structure, we denote by \( R^c - X \) the species of connected bi-point-determining graphs with more than one vertex.

Let \( R \) be a bi-point-determining graph. Then \( R \) is both point-determining and co-point-determining. In particular, the decomposition of \( R \) into a set of its connected components is similar with that of a point-determining graph in that there is at most one connected component consisting of a singleton vertex. Hence such a decomposition can result in one of the following three situations:

i) \( R \) is a singleton vertex, in which case we get an \( X \)-structure.

ii) \( R \) has more than one vertex, and none of its connected components is a singleton vertex, in which case we get an \( E_+ (R^c - X) \).

iii) \( R \) has more than one vertex, and one of its connected components is a singleton vertex, in which case we get an \( X \cdot E_+ (R^c - X) \) species.

Therefore, we get the desired result. \( \square \)

We can compute the beginning terms of the associated series of \( R^c \) using Maple:

\[
R^c(x) = \frac{x}{1!} + 12 \frac{x^4}{4!} + 252 \frac{x^5}{5!} + 12312 \frac{x^6}{6!} + 1061304 \frac{x^7}{7!} + 170176656 \frac{x^8}{8!} + \cdots
\]

\[
\widetilde{R}^c(x) = x + x^4 + 5x^5 + 31x^6 + 293x^7 + 4986x^8 + \cdots,
\]

\[
Z_{\tilde{R}^c} = p_1 + \left( \frac{1}{2} p_1^4 + \frac{1}{2} p_2^2 \right) + \left( \frac{21}{10} p_1^5 + \frac{5}{2} p_1 p_2^2 + \frac{2}{5} p_5 \right) + \left( \frac{17}{10} p_1^6 + \frac{17}{2} p_1^2 p_2^2 + \frac{2}{5} p_1 p_5 + \frac{11}{3} p_2^3 + \frac{1}{3} p_3 \right) + \cdots.
\]

The calculation agrees with the observation from Figure 4.15 that the only unlabeled bi-point-determining graph on four vertices is connected, and among the six
unlabeled bi-point-determining graph on five vertices there is only one of them that is not connected.

4.4. 2-Colored Graphs and Connected 2-colored Graphs

**Definition 4.4.1.** A proper coloring of a graph is an assignment of colors to the vertices of the graph where no two adjacent vertices are assigned the same color. A 2-colored graph, also called a bi-colored graph by Harary [11, p. 93] and Hanlon [9], is a graph in which all vertices are properly 2-colored.

For simplicity, we call the two colors in a 2-colored graph white and black. We denote by $G(X, Y)$ the 2-sort species defined such that for a two-set $U = (V, W)$, $G[U]$ is a 2-colored graph in which the vertices colored white are elements of $V$ and the vertices colored black are elements of $W$.

![Figure 4.16. The 2-sort species of 2-colored graphs $G(X, Y)$.](image)

**Proposition 4.4.2.** Let $G(X, Y)$ be the 2-sort species of 2-colored graphs. Then the exponential generating series of $G(X, Y)$ is given by

$$G(x, y) = \sum_{m,n=0}^{\infty} \frac{2^m x^m y^n}{m! n!}.$$
CHAPTER 4. POINT-DETERMINING GRAPHS

Proof. In a 2-colored graph, each edge must connect one vertex of sort $X$ and one vertex of sort $Y$. Hence there are $2^{mn}$ labeled 2-colored graphs with $m$ white vertices and $n$ black vertices. □

Theorem 4.4.3. Let $\mathcal{G}(X, Y)$ be the 2-sort species of 2-colored graphs. Then the cycle index of $\mathcal{G}(X, Y)$ is given by

$$Z_{\mathcal{G}(X,Y)} = \sum_{m,n \geq 0} \left( \sum_{\lambda \vdash m, \mu \vdash n} 2^{\sum_{i,j} \gcd(\lambda_i, \mu_j)} \frac{p_{\lambda}[x]}{z_{\lambda}} \frac{p_{\mu}[y]}{z_{\mu}} \right).$$

Proof. Let $(\lambda, \mu)$ be an ordered pair of partitions, and let $(\sigma, \pi)$ be an ordered pair of permutations with $\sigma$ having cycle type $\lambda$ and $\pi$ having cycle type $\mu$. Let $\text{fix}(\sigma, \pi) = \text{fix} \mathcal{G}[\lambda, \mu]$ be the number of 2-colored graphs fixed by $(\sigma, \pi)$.

To start with, we consider the simpler case when $\sigma$ is a $k$-cycle and $\pi$ is an $l$-cycle. Let $K_{k,l}$ denote the complete bipartite graph on $[k, l]$, and let $E(K_{k,l})$ be its edge set. Then $|E(K_{k,l})| = kl$. Without loss of generality, we let the labeling of left-hand side vertices of $K_{k,l}$ be $\{1, 2, \ldots, k\}$, and the labeling of right-hand side vertices of $K_{k,l}$ be $\{1', 2', \ldots, l'\}$. Then each edge of $K_{k,l}$ is represented by an ordered pair $(i, j')$, for some $i \in [k]$ and $j \in [l]$. The pair of permutations $(\sigma, \pi)$ acts on the set $E(K_{k,l})$ by letting $\sigma$ act on the set $\{1, 2, \ldots, k\}$ and $\pi$ act on the set $\{1', 2', \ldots, l'\}$. This action partitions the $kl$ edges of $K_{k,l}$ into orbits $\{A_1, A_2, \ldots\}$. We observe that there are $\text{lcm}(k, l)$ edges in each of the orbits, since all edges of the form $(i_r, j'_r)$, where $i_r = \sigma^r(i)$ and $j_r = \pi^r(j)$ for some $r = 1, 2, \ldots, \text{lcm}(k, l) - 1$, are in the same orbit as the edge $(i, j')$, and hence this action of $(\sigma, \pi)$ on the set $E(K_{k,l})$ results in $(kl)/\text{lcm}(k, l) = \gcd(k, l)$ orbits. Note that each 2-colored graph with vertex set $[k, l]$ can be identified with a subset of $E(K_{k,l})$. If a subset $S$ of $E(K_{k,l})$ is fixed by the pair of permutations $(\sigma, \pi)$, then whenever an edge $(i, j')$ is in $S$, all edges in the same orbit as $(i, j')$ under the action of $(\sigma, \pi)$ on $E(K_{k,l})$ is in $S$ as well. This means that the number of 2-colored
graphs fixed by the pair of permutations \((\sigma, \pi)\) is the same as the number of subsets of \(\{A_1, A_2, \ldots, A_{\gcd(k,l)}\}\). Therefore,
\[
\text{fix}(\sigma, \pi) = 2^{\gcd(k,l)}.
\]

For the general case, we write \(\lambda = (\lambda_1, \lambda_2, \ldots)\) and \(\mu = (\mu_1, \mu_2, \ldots)\). It is straightforward to see that each ordered pair \((\lambda_i, \mu_j)\), for some integers \(i\) and \(j\), gives rise to a factor \(2^{\gcd(\lambda_i, \mu_j)}\) in the number \(\text{fix}(\sigma, \pi)\), and hence
\[
\text{fix} \mathcal{G}[\lambda, \mu] = \prod_{i,j} 2^{\gcd(\lambda_i, \mu_j)} = 2^{\sum_{i,j} \gcd(\lambda_i, \mu_j)}.
\]

\[\square\]

**Remark 4.4.4.** The above argument also gives a way to count 2-colored graphs by the number of edges. Let \(b_{m,n}(x)\) be the ordinary generating function for 2-colored graphs, in which \(m\) vertices are colored white and \(n\) vertices colored black, by the number number of edges. We get the following expression for \(b_{m,n}(x)\), which agrees with the result of Harary and Palmer [11, p. 95]:
\[
b_{m,n}(x) = \sum_{\lambda \vdash m, \mu \vdash n} \frac{1}{z^{\lambda}z^{\mu}} \prod_{k,l=1}^{m,n} \left(1 + x^{\lcm(k,l)}\right)^{c_k(\lambda)c_l(\mu)\gcd(k,l)},
\]
where \(c_i(\lambda)\) denotes the number of parts in \(\lambda\) with length \(i\). For example, the coefficient of \(x^4\) in \(b_{2,3}(x)\) is 3, as shown in Figure 4.17.

![Figure 4.17](image)
CHAPTER 4. POINT-DETERMINING GRAPHS

Theorem 4.4.3 enables us to calculate the associated series of \( \mathcal{G}[X,Y] \):

\[
\mathcal{G}(x, y) = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{y}{1!} + \frac{y^2}{2!} + \frac{y^3}{3!} + 2 \frac{x}{1!} \frac{y}{1!} + 4 \frac{x^2}{2!} \frac{y}{1!} + 4 \frac{x}{1!} \frac{y^2}{2!} + \cdots ,
\]

\[
\widetilde{\mathcal{G}}(x, y) = 1 + x + y + 2xy + x^2 + y^2 + 3x^2y + 3xy^2 + x^3 + y^3 + \cdots ,
\]

\[
Z_{\mathcal{G}(X,Y)} = 1 + (p_1[x] + p_1[y]) + \left( \frac{1}{2} p_1^2[x] + \frac{1}{2} p_2[x] + 2 p_1[x] p_1[y] + \frac{1}{2} p_2[y] + \frac{1}{2} p_1^2[y] \right)
\]

\[
+ \left( \frac{1}{6} p_1^3[x] + \frac{1}{2} p_1[x] p_2[x] + \frac{1}{3} p_3[x] + p_2[x] p_1[y] + 2 p_1^2[x] p_1[y] + 2 p_1[x] p_1^2[y] \right)
\]

\[
+ 2 p_1[x] p_1^2[y] + p_1[x] p_2[y] + \frac{1}{3} p_3[y] + \frac{1}{2} p_1[y] p_2[y] + \frac{1}{6} p_1^3[y] \right) + \cdots .
\]

Figure 4.18 shows the unlabeled 2-colored graphs on at most 4 vertices, where each vertex is either a white vertex, a black vertex, or a vertex that can be colored in both colors. For example, there are two unlabeled 2-colored graph on one vertex, one color black the other colored white.

![Unlabeled 2-colored graphs](image)

**FIGURE 4.18.** Unlabeled 2-colored graphs with no more than 4 vertices.

A 2-colored graph is called *connected* if the underlying graph is connected.
Theorem 4.4.5. Let $\mathcal{G}^c(X,Y)$ be the species of connected 2-colored graphs. Then

$$\mathcal{G}(X,Y) = \mathcal{E}(\mathcal{G}^c(X,Y)).$$

Proof. The canonical decomposition of a graph into connected components applies to 2-colored graphs.

Equation (4.4.1) is equivalent to

$$\mathcal{G}^c(X,Y) = \Gamma(\mathcal{G}(X,Y)),$$

which enables us to compute the associated series of $\mathcal{G}^c[X,Y]$ using Maple:

$$\mathcal{G}^c(x,y) = \frac{x}{1!} + \frac{y}{1!} + \frac{xy}{2!} + \frac{x^2y + xy^2}{3!} + \frac{x^3y + 5x^2y^2 + xy^3}{4!} + \cdots,$$

$$\tilde{\mathcal{G}}^c(x,y) = x + y + xy + xy^2 + x^2y + x^3y + xy^3 + 2x^2y^2 + x^4y + 4x^3y^2 + 4x^2y^3 + \cdots,$$

$$Z_{\mathcal{G}^c(X,Y)} = (p_1[x] + p_1[y]) + p_1[x]p_1[y] + \left(\frac{1}{2} p_1^2[x]p_1[y] + \frac{1}{2} p_1[x]p_1^2[y] + \frac{1}{2} p_2[x]p_1[y] + \frac{1}{2} p_1[x]p_2[y]\right) + \cdots.$$

Figure 4.19. Unlabeled connected 2-colored graphs with no more than 4 vertices.
4.5. Point-Determining 2-Colored Graphs

**Definition 4.5.1.** A 2-colored graph is called *point-determining* if the underlying graph is point-determining. A 2-colored graph is called *semi-point-determining* if all vertices of the same color have distinct neighborhoods.

Note that the notion of co-point-determining 2-colored graphs is not interesting, since any two adjacent vertices in a 2-colored graph are colored differently, so that there is no vertex that could be adjacent to both of them.

We denote by $\mathcal{P}(X, Y)$ the species of point-determining 2-colored graphs, by $\mathcal{P}^s(X, Y)$ the species of semi-point-determining 2-colored graphs, and by $\mathcal{P}^c(X, Y)$ the species of connected point-determining 2-colored graphs.

**Theorem 4.5.2.** For species $\mathcal{P}(X, Y)$, $\mathcal{P}^s(X, Y)$ and $\mathcal{P}^c(X, Y)$, we have

\begin{align}
\mathcal{P}^s(X, Y) &= (1 + X)(1 + Y) \cdot \mathcal{E}(\mathcal{P}^c_{\geq 2}(X, Y)), \\
\mathcal{P}(X, Y) &= (1 + X + Y) \cdot \mathcal{E}(\mathcal{P}^c_{\geq 2}(X, Y)).
\end{align}

**Proof.** Let $G_1$ be a semi-point-determining 2-colored graph. We observe that a connected component of $G_1$ could be either a single vertex colored white, a single vertex colored black, or a connected point-determining 2-colored graph with at least two vertices. At the same time, $G_1$ can have at most one isolated vertex colored with each color, due to the fact that all vertices in $G_1$ of the same color must have distinct neighborhoods. Equation (4.5.1) follows by translating the above into species equivalence.

Let $G_2$ be a point-determining 2-colored graph. As in the above discussion we see that a connected component of $G_2$ could be either a single vertex colored white, a single vertex colored black, or a connected point-determining 2-colored graph with at
least two vertices. But this time, since the underlying graph of $G_2$ is point-determining graph, $G_2$ can have at most one isolated vertex in all. Hence the term $(1+X)(1+Y)$ in (4.5.1) is replaced with the term $1+X+Y$ in (4.5.2).

\[ P^s(X, Y) = (1+X)(1+Y) \mathcal{E}(P^c_{\geq 2}(X, Y)). \]

\[ P(X, Y) = (1+X+Y) \mathcal{E}(P^c_{\geq 2}(X, Y)). \]

**Theorem 4.5.3.** For the species $\mathcal{G}(X, Y)$ and $\mathcal{P}^s(X, Y)$, we have

\[ \mathcal{G}(X, Y) = \mathcal{P}^s(\mathcal{E}_+(X), \mathcal{E}_+(Y)). \]

**Proof.** The proof use the same idea as the proof of Theorem 4.1.3. To be more precise, given any 2-colored graph, we define equivalence relations on the vertex set by setting two same-colored vertices to be equivalent if they have the same neighborhoods, and get a new 2-colored graph whose vertex set is the set of equivalence
classes and the adjacency in the original graph is accordingly preserved. We observe that the resulting new graph is a semi-point-determining 2-colored graph, and the rest is straightforward.

We make use of the virtual species $\Gamma$ defined in Section 2.4 again, and get from Theorem 4.5.3 that

$$P^s(X, Y) = \mathcal{G}(\Gamma(X), \Gamma(Y)),$$

which, together with Equations 4.5.1 and 4.5.2, allows us to compute the associated series of the species of semi-point-determining 2-colored graphs, the species of point-determining 2-colored graphs, and the species of connected point-determining 2-colored graphs as follows:

$$P^s(x, y) = 1 + \frac{x}{1!} + \frac{y}{1!} + 2 \frac{x}{1!} \frac{y}{1!} + 2 \frac{x}{1!} \frac{y^2}{2!} + 2 \frac{x^2}{2!} \frac{y}{1!} + 10 \frac{x^2}{2!} \frac{y^2}{2!} + 24 \frac{x^2}{2!} \frac{y^3}{3!}$$

$$+ 24 \frac{x^3}{3!} \frac{y^2}{2!} + \cdots,$$

$$\tilde{P}^s(x, y) = 1 + x + y + 2xy + x^2y + xy^2 + 3x^2y^2 + 3x^3y^2 + 3x^2y^3 + \cdots,$$

$$Z_{P^s(X, Y)} = 1 + \left( p_1[x] + p_1[y] \right) + \left( 2p_1[x]p_1[y] \right) + \left( p_2[x]p_1[y] + p_1[x]p_2[y] \right)$$

$$+ \left( \frac{1}{2} p_2[x]p_2[y] + \frac{5}{2} p_1^2[x]p_1^2[y] \right)$$

$$+ \left( p_1p_2[x]p_2[y] + p_2[x]p_1p_2[y] + 2p_2[x]p_2[y] + 2p_2^2[x]p_2^2[y] + 2p_1^2[x]p_2^2[y] \right) + \cdots.$$

$$P(x, y) = 1 + \frac{x}{1!} + \frac{y}{1!} + \frac{x}{1!} \frac{y}{1!} + 2 \frac{x}{1!} \frac{y^2}{2!} + 2 \frac{x^2}{2!} \frac{y}{1!} + 6 \frac{x^2}{2!} \frac{y^2}{2!} + 24 \frac{x^2}{2!} \frac{y^3}{3!}$$

$$+ 24 \frac{x^3}{3!} \frac{y^2}{2!} + \cdots,$$

$$\tilde{P}(x, y) = 1 + x + y + xy + x^2y + xy^2 + 2x^2y^2 + 3x^3y^2 + 3x^2y^3 + \cdots,$$

$$Z_{\mathcal{P}(X, Y)} = 1 + \left( p_1[x] + p_1[y] \right) + \left( p_1[x]p_1[y] \right) + \left( p_2[x]p_1[y] + p_1[x]p_2[y] \right)$$

$$+ \left( \frac{1}{2} p_2[x]p_2[y] + \frac{3}{2} p_1^2[x]p_1^2[y] \right)$$
CHAPTER 4. POINT-DETERMINING GRAPHS

\[
+ (p_1 p_2[x] p_2[y] + p_2[x] p_1 p_2[y] + 2 p_1^2[x] p_2^2[y] + 2 p_2^2[x] p_1^3[y]) + \cdots .
\]

\[
\mathcal{P}(x, y) = \frac{x}{1!} + \frac{y}{1!} + \frac{x y}{1! 1!} + \frac{4 x^2 y^2}{2! 2!} + \frac{6 x^2 y^3}{2! 3!} + \frac{6 x^3 y^2}{3! 2!} + \cdots ,
\]

\[
\widetilde{\mathcal{P}}(x, y) = x + y + x y + x^2 y^2 + x^3 y^2 + x^2 y^3 + \cdots ,
\]

\[
Z_{\mathcal{P}(X, Y)} = (p_1[x] + p_1[y]) + (p_1[x] p_1[y]) + (p_2[x] p_1^2[y])
\]

\[
+ \left( \frac{1}{2} p_1 p_2[x] p_2[y] + \frac{1}{2} p_2[x] p_1 p_2[y] + \frac{1}{2} p_1^3[x] p_1^2[y] + \frac{1}{2} p_2^2[x] p_1^3[y] \right) + \cdots .
\]

**Figure 4.22.** Unlabeled point-determining 2-colored graphs with no more than 5 vertices.

We can write down the molecular decomposition of a 2-sort species. For example, Figure 4.22 gives the first terms of the molecular decomposition of \(\mathcal{P}(X, Y)\).

\[
\mathcal{P}(X, Y) = 1 + (X + Y) + X Y + (X + Y)(X Y) + (\mathcal{E}_2(X) \mathcal{E}_2(Y) + X^2 Y^2)
\]

\[
+ [2(X + Y) \mathcal{E}_2(X Y) + X^3 Y^2 + X^2 Y^3] + \cdots ,
\]

where the terms \(2(X + Y) \mathcal{E}_2(X Y) + X^3 Y^2 + X^2 Y^3\) correspond to the unlabeled point-determining 2-colored graphs with 5 vertices as shown in Figure 4.23.
Figure 4.23. Unlabeled point-determining 2-colored graphs with 5 vertices.
APPENDIX A

Index of Species

0  empty species.
1  singleton set species.
\(X\)  species of singletons.
\(X^n\)  species of linear orders of order \(n\).
\(X^n/A\)  molecular species of (left) cosets of \(A\) in \(S_n\).
\(\mathcal{A}(X, Y)\)  2-sort species of rooted trees.
\(\mathcal{C}(X)\)  species of oriented cycles.
\(\mathcal{D}_n(X)\)  molecular species \(X^n/D_n\).
\(\mathcal{E}(X)\)  species of sets.
\(\mathcal{E}_k(X)\)  species of \(k\)-element sets.
\(\mathcal{E}_k\langle F \rangle\)  exponential composition of species \(F\) of order \(k\), for \(k \geq 1\).
\(\mathcal{E}\langle F \rangle\)  exponential composition of species \(F\).
\(\mathcal{K}(X)\)  species of complete graphs.
\(\mathcal{G}(X)\)  species of (simple) graphs.
\(\mathcal{G}^c(X)\)  species of connected graphs.
\(\mathcal{G}(X, Y)\)  2-sort species of 2-colored graphs, or bi-colored graphs.
\(\mathcal{G}^c(X, Y)\)  2-sort species of connected 2-colored graphs.
Γ(\(X\)) virtual species of “connected (1 + X)-structures”, or 
compositional inverse of \(e_+\).

\(L(\(X\))\) species of linear orders.

\(N(\(X\))\) species of (2-)rectangles.

\(N^{(k)}(\(X\))\) species of \(k\)-rectangles.

\(N_N\) species of \(k\)-dimensional cubes on \([N]\), or \(e_n^{\geq k}[N]\), where \(N = n^k\).

\(O_G(\(X\))\) species associated to a graph \(G\).

\(P(\(X\))\) a) species of point-determining graphs (in chapter 4);

b) species of prime graphs.

\(P^c(\(X\))\) species of connected point-determining graphs.

\(P(\(X, Y\))\) 2-sort species of point-determining 2-colored graphs.

\(P^s(\(X, Y\))\) 2-sort species of semi-point-determining 2-colored graphs.

\(P^c(\(X, Y\))\) 2-sort species of connected point-determining 2-colored graphs.

\(\Phi(\(X\))\) species of permutations.

\(\Psi^{(k)}(\(X\))\) species of partitions into \(k\) blocks.

\(Q(\(X\))\) species of co-point-determining graphs.

\(Q^c(\(X\))\) species of connected co-point-determining graphs.

\(R(\(X\))\) species of bi-point-determining graphs.

\(R^c(\(X\))\) species of connected bi-point-determining graphs.

\(S(\(X\))\) species of phylogenetic trees.

\(S^*(\(X\))\) species of alternating phylogenetic trees, or yoke-chains, or 
series-parallel networks.
APPENDIX B

General Notations

$A \star B$  product of groups $A$ and $B$ acting on the set $[m+n]$.  
$A \times B$  product of groups $A$ and $B$ acting on the set $[mn]$.  
$B \wr A$  wreath product of groups $A$ and $B$.  
$B^A$  exponentiation group of $A$ and $B$.  
$\text{aut}(G)$  automorphism group of a graph $G$.  
$\mathbb{B}$  category of finite sets with bijections.  
$\mathbb{B}^k$  category of $k$-sets with bijective multifunctions.  
$b_n$  number of unlabeled prime graphs of order $n$.  
$\mathcal{C}$  set of unlabeled connected graphs.  
$\mathcal{CM}$  monoid algebra associated with a free commutative monoid $M$.  
$c_k(\lambda)$  number of parts of length $k$ in a partition $\lambda$.  
$c_n$  number of labeled connected graphs of order $n$.  
$\tilde{c}_n$  number of unlabeled connected graphs of order $n$.  
$c.t.(\sigma)$  cycle type of a permutation $\sigma$.  
$d_\lambda$  number of permutations with cycle type $\lambda$.  
$D_n$  dihedral group of order $n$.  
$\mathcal{D}(F)$  Dirichlet exponential generating function of a species $F$.  
$\mathcal{D}(G)$  Dirichlet exponential generating function of a graph $G$.  

124
$E(G)$  edge set of a graph $G$.

gcd$(k, l)$ greatest common divisor of integers $k$ and $l$.

$f_1 * f_2$ image of $f_2$ under the operator obtained by substituting the
operator $I_r$ for the variables $p_r$ in $f_1$.

$F(x)$ exponential generating series of a species $F$.

$\tilde{F}(x)$ type generating series of a species $F$.

$F_1 + F_2$ sum of species $F_1$ and $F_2$.

$F_1 \cdot F_2$ product of species $F_1$ and $F_2$.

$F_1 \circ F_2$ composition of species $F_1$ and $F_2$.

$F_1 \boxtimes F_2$ arithmetic product of species $F_1$ and $F_2$.

$G_1 \odot G_2$ Cartesian product of graphs $G_1$ and $G_2$.

$\lambda_i$ $i$th part of the partition $\lambda = (\lambda_1, \lambda_2, \ldots)$, arranged in
weakly decreasing order.

$K_{k,l}$ complete bipartite graph on the set $[k,l]$.

$l(G)$ number of vertices in a graph $G$.

$L(G)$ number of graphs isomorphic to $G$ with vertex set $V(G)$.

$lcm(k, l)$ least common multiple of integers $k$ and $l$.

$\mathbb{N}$ set of natural numbers.

$\Omega$ $\mathbb{Q}$-algebra generated by the operators $\{I_k\}$.

$\mathbb{P}$ set of prime numbers.

$\mathbb{P}$ set of unlabeled prime graphs with respect to the Cartesian
multiplication.
$p_n$ power sum symmetric function of order $n$.

$p_\lambda$ power sum symmetric function indexed by the partition $\lambda$.

$p_\lambda \boxtimes p_\mu$ an operation defined by Definition 1.2.3.

$\text{Par}_n$ set of partitions of $n$.

$\text{Par}^k_n$ set of sequences of $k$ partitions of $n$.

$\mathbb{Q}$ set of rational numbers.

$\mathfrak{R}$ ring of polynomials in the variables $p_1, p_2, \ldots$ with the operation $\boxtimes$.

$\mathfrak{S}_n$ symmetric group of order $n$.

$V(G)$ vertex set of a graph $G$.

$z_\lambda$ number of permutations commute with a permutation of cycle type $\lambda$.

$Z(A)$ Pólya’s cycle index polynomial of a permutation group $A$.

$Z_F$ cycle index of $F$.

$Z(G) = Z_{\tilde{\mathfrak{S}}}$ cycle index of the species associated to the graph $G$.  

126
Bibliography


