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On Distinguishing Graphs by their Symmetric and Quasisymmetric functions

A Thesis

Submitted by

SAGAR SAWANT

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of

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Stay hungry. Stay foolish.

– Steve Jobs

To my family.

THESIS CERTIFICATE

This is to undertake that the Thesis titled **ON DISTINGUISHING GRAPHS BY THEIR SYMMETRIC AND QUASISYMMETRIC FUNCTIONS**, submitted by me to the Indian Institute of Technology Madras, for the award of **Doctor of Philosophy**, is a bona fide record of the research work done by me under the supervision of **Dr. Narayanan Narayanan**. The contents of this Thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

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LIST OF PUBLICATIONS

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II. Refereed journals (others)

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ABSTRACT

KEYWORDS chromatic symmetric function; U-polynomial; integer compositions; caterpillars; B-polynomial; caterpillars; Tutte polynomial; quasisymmetric functions

Stanley's Tree Isomorphism Conjecture posits that the chromatic symmetric function can distinguish non-isomorphic trees. This conjecture is already established for caterpillars and other subclasses of trees. We prove the conjecture's validity for a new class of trees that generalize proper caterpillars, thus confirming the conjecture for a broader class of trees.

On the digraph front, we focus on an analogue of the Stanley's Tree Isomorphism conjecture. The B-polynomial and quasisymmetric B-function, introduced by Awan and Bernardi, extends the widely studied Tutte polynomial and Tutte symmetric function to digraphs. We address one of the fundamental questions concerning these digraph invariants, which is, the determination of the classes of digraphs uniquely characterized by them. We solve an open question originally posed by Awan and Bernardi, regarding the identification of digraphs that result from replacing every edge of a graph with a pair of opposite arcs. Further, we address the more challenging problem of reconstructing digraphs using their quasisymmetric functions. In particular, we show that the quasisymmetric B-function reconstructs *partially symmetric* orientations of *proper* q-caterpillars. As a consequence, we establish that all orientations of paths and asymmetric proper q-caterpillars can be reconstructed from their quasisymmetric B-functions. These results enhance the pool of oriented trees distinguishable through quasisymmetric functions.

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NOTATION

(D, ω)	Weighted digraph
$[p]$	The set $\{1, 2, \ldots, p\}$
$\chi_G(x)$	Chromatic polynomial of graph G
$B_D(\mathbf{x}; y, z)$	quasisymmetric B-function of digraph D
$\mathbf{X}_G$	Chromatic symmetric function of graph G
$\Gamma^{>}(\mathbf{x})$	Strict order quasisymmetric function
$\Gamma^{\geq}(\mathbf{x})$	Weak order quasisymmetric function
$\kappa(G)$	Number of connected components in graph G
$\mathbf{X}^{>}_{\mathbf{D}}(\mathbf{x}; q)$	Chromatic quasisymmetric function of digraph D
$\mathbf{XB}_G(\mathbf{x}; y)$	Tutte symmetric function of graph G
$\mathrm{Comp}(C)$	Composition corresponding to q-caterpillar C
$\mathrm{diam}(G)$	Diameter of graph G
$\mathrm{QSym}_R(\mathbf{x})$	Algebra of quasisymmetric functions over ring R
$\mathrm{Sym}_R(\mathbf{x})$	Algebra of symmetric functions over ring R
$\mathrm{Mon}_d(\beta)$	$\{y^{asc(f)} z^{dsc(f)} \mid type(f) = \beta$ and $asc(f) + dsc(f) = d\}$
μ_{q+1}	Multiplicity of $q + 1$ in $\textsc{Twig}(T)$
$\mathbb{N}$	Set of positive integers including 0
$\vec{G}$	Digraph obtained by symmetrization of graph G
$\mathbb{P}$	Set of positive integers

p_λ	Power sum symmetric function with respect to partition λ
$\mathbb{Q}$	Set of rational numbers
$Surj(V,p)$	Set of subjective functions from V to $[p]$
$\textsc{Twig}(T)$	Multiset of twigs in tree T
T°	Trunk of the tree T
$\underline{D}$	Underlying graph of digraph D
$\widetilde{m}_\lambda$	Augmented monomial symmetric function with respect to partition λ
$\mathbb{Z}$	Set of integers
$B_D(x,y,z)$	B-polynomial of digraph D
$B_{(D,\omega)}(\mathbf{x};y,z)$	Vertex-weighted quasisymmetric B-function
$B_{p,p'}$	Bilateral set
$D(V,A)$	A digraph on vertex set V and with set of arcs A
$G(V,E)$	A graph on vertex set V and with set of edges E
$G[F]$	Spanning subgraph (V,F) of graph $G(V,E)$
M_δ	Monomial quasisymmetric function with respect to composition δ
m_λ	Monomial symmetric function with respect to partition λ
$P(v)$	Pendant(Path)-vector of spine vertex in oriented (q-)caterpillar
$T_G(x,y)$	Tutte polynomial of graph G
$U_G(\mathbf{x};y)$	U-polynomial of graph G

CHAPTER 1

INTRODUCTION

The study of graphs traces its origins to the mid-eighteenth century, initiated by L. Euler's investigation of the Königsberg Bridge problem. Subsequently, graph theory found applications in various fields, including the classification of surfaces, which marked the beginning of a new branch in mathematics known as topology. In recent years, graph theory has become pervasive across numerous disciplines, directly and indirectly impacting fields such as network analysis, molecular chemistry, communication networks, and more. With the rapid development of artificial intelligence, machine learning, and data science in various domains, the application of graph theory has emerged as a highly sought-after area of interest.

It is natural to understand which properties of graphs are sufficient to uniquely determine them. Equivalently, what data about the graphs distinguish one from another? A graph invariant is a property or object associated with graphs that remains the same for isomorphic graphs. For instance, the number of vertices, edges, connected components, and chromatic number are a few examples of such graph invariants. Thus, we are interested in identifying which graph invariants distinguish non-isomorphic graphs.

The study of chromatic invariants mainly revolves around the following questions.

- ✎ Which properties of graphs are determined by these chromatic invariants?
- ✎ Which classes of graphs are identifiable by these chromatic invariants?
- ✎ Do they distinguish non-isomorphic graphs?
- ✎ If non-isomorphic graphs can be distinguished by a chromatic invariant, can the graphs be reconstructed from it?

This thesis aims to address the above questions using the invariants chromatic symmetric function, B-polynomial and quasisymmetric B-function. These questions strongly relate to Stanley's tree isomorphism conjecture [41], which suggests that chromatic symmetric function distinguishes non-isomorphic trees. The conjecture has remained open for nearly 30 years and has been formulated in various versions for digraphs and posets. We study the chromatic symmetric function, B-polynomial, and its quasisymmetric extension with a focus on the tree isomorphism conjecture and its digraph analogues.

We begin with a brief history and motivation for the chromatic invariants and their development throughout the years.

1.1 BACKGROUND

1.1.1 Four coloring of maps

In 1852, Francis Guthrie attempted to color the map of England's counties with the condition that neighboring counties must be assigned different colors. One of his key observations was that four colors sufficed for coloring any map under the same conditions. He proposed this as a conjecture, which was later famously proven true and became known as the four-color map theorem.

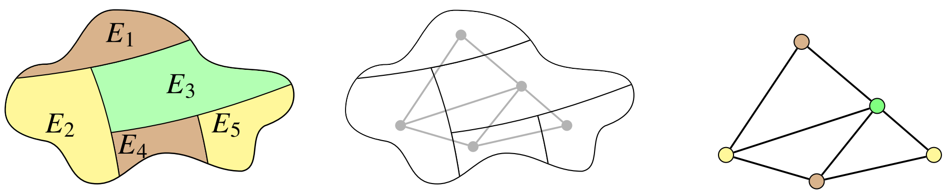


Figure 1.1: Map coloring and its corresponding graph coloring

Every map corresponds to a graph as follows: regions are represented by the vertices, and any two such vertices are connected by an edge if and only if the regions share a common boundary. The coloring of the map translates to the coloring of vertices such that adjacent vertices are assigned distinct colors (see Figure 1.1).

For a graph G on the vertex set V and edge set E, a proper k-coloring is a function from

V to $\{1, 2, \ldots, k\}$ such that adjacent vertices are assigned distinct colors. A graph is said to be planar if there exists a drawing of the graph without crossing of edges. Observing that the graph associated with maps does not admit any crossing of edges, the four-color theorem can be posed as follows.

Theorem 1.1 (Four-Color Theorem)**.** *Every planar graph admits a proper* 4*-coloring.*

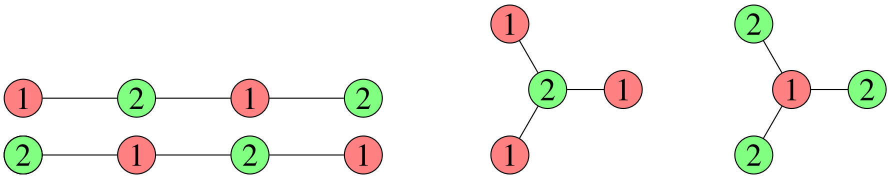
The first proof, presented by Kempe, relied on the notion of Kempe's chain [46]. Later, Tait proposed a proof using an edge-coloring formulation of the problem. However, both Kempe's and Tait's proofs were eventually shown to be false, by Heawood and Petersen, respectively [25, 20]. Nevertheless, the pursuit of the four-coloring problem significantly contributed to the development of graph theory. Nearly a century after the initial attempts, Appel and Haken produced a computer-aided proof, which built upon Kempe's chain concept and Heesch's ideas of unavoidability and reducibility [4, 5].

1.1.2 Chromatic polynomial

In pursuit of the four-color problem, George Birkhoff introduced a graph polynomial in 1912 [10], known as the chromatic polynomial, which studies the number of colorings of a map. For a graph G, the chromatic polynomial of the graph, denoted by $\chi(x)$, is a polynomial such that for any positive integer k, graph G admits $\chi(k)$ many proper k-colorings.

It has been shown that certain properties of graphs, such as the number of edges and connected components, can be recovered from their chromatic polynomial [39]. In [43], Stanley showed that evaluating the chromatic polynomial of a graph at negative integers yields the number of acyclic orientations satisfying specific properties. Particularly, the chromatic polynomial evaluated at -1 gives the number of acyclic orientations of the graph.

Furthermore, Greene and Zaslavsky provided a combinatorial interpretation of the derivatives of the chromatic polynomial in terms of orientations with special sources



(a) proper 2-colorings of a path

(b) proper 2-colorings of a star

Figure 1.2: Proper 2-colorings

and sinks [23]. These results highlight the diverse and extensive applications of the chromatic polynomial and the wealth of information it provides about the graph.

In light of the information provided by chromatic polynomials, it is interesting to know whether the graphs are uniquely determined by the chromatic polynomial. The answer to this is affirmative for trivial cases like edgeless graphs, complete graphs, and cycles. Since the chromatic polynomial of a graph determines the number of edges and connected components of the graph, it also indicates whether it is a tree or not. However, all the trees on n vertices share the same chromatic polynomial. In fact, a graph is a tree on n vertices if and only if the chromatic polynomial of the graph is $x(x-1)^{n-1}$. In other words, the chromatic polynomial does not distinguish between non-isomorphic trees.

Note that while the chromatic polynomial encodes quantitative information about colorings, it may lose crucial structural details about the underlying graph. In particular, even if the number of colorings of non-isomorphic trees is the same, the sizes of the corresponding color classes may differ.

For example, consider the following trees: a path on 4-vertices, and a star on 4-vertices.

(a) path graph on 4 vertices

(b) star graph on 4 vertices

Each of these graphs admits exactly two proper 2-colorings, as depicted in Figure 1.2. For a k-coloring f, we define *type* of f as the non-increasing tuple encoding the size of its color classes. In this context, the path graph in Figure 1.2 admits two colorings of type $(2,2)$, whereas the star graph has two colorings of type $(3,1)$. Thus, even though each graph admits two proper 2-colorings, the size of the color classes of their colorings are distinct. Thus, a polynomial that encodes the type of coloring would perhaps provide a better understanding of the structure of the underlying tree.

1.2 GENERALIZATIONS OF THE CHROMATIC POLYNOMIAL

1.2.1 Symmetric function generalization

In 1995, R. Stanley introduced a symmetric function generalization of the chromatic polynomial [41]. Let $\mathbf{x} = (x_1, x_2, \dots)$ be a list of indeterminates. Then, for a graph G, the chromatic symmetric function is a generating function over proper colorings, defined as:

$$\mathbf{X}_G := \sum_{\substack{f : V \to \mathbb{P} \\ f\, proper}} \left(\prod x_{f(v)} \right),$$

where $\mathbb{P}$ is the set of positive integers. The chromatic symmetric function determines the size of the color classes of proper colorings. Additionally, it encodes significant information about graphs, such as girth, the number of vertex partitions into independent sets, and the order of connected components in subgraphs [33, 41]. In particular, it has been proved that the degree sequence and path sequence of trees (see Section 2.1.1) can be recovered from the chromatic symmetric functions. This raises the question: does the chromatic symmetric function distinguish all non-isomorphic graphs? Unfortunately, the answer to this question is negative.

Stanley presented two non-isomorphic graphs with the same chromatic symmetric functions Figure 3.1. However, he observed that non-isomorphic trees with at most 4 vertices have distinct chromatic symmetric functions. He thus raised the question of whether chromatic symmetric functions distinguish all trees.

Development in this direction has led to the belief that the answer to this question is affirmative. This is commonly referred to as Stanley's Tree Isomorphism Conjecture. The progress on this conjecture is detailed in Section 3.1.

1.2.2 Tutte polynomial and its symmetric function generalization

R. M. Foster had observed that the chromatic polynomial satisfies the following deletion-contraction relation:

$$\mathcal{X}_G(x) = \mathcal{X}_{G\backslash e}(x) - \mathcal{X}_{G/e}(x).$$

W. Tutte's interest in deletion-contraction relations, particularly for counting perfect rectangles and spanning trees of graphs, led to the development of a bivariate polynomial known as the Tutte Polynomial [49]. This polynomial serves as a universal object for deletion-contraction polynomials, meaning that any graph polynomial that satisfies a deletion-contraction reduction is a specialization of the Tutte polynomial. As a consequence, the chromatic polynomial is a specialization of the Tutte polynomial.

The Tutte polynomial is defined recursively as follows:

Definition 1.2 (Tutte Polynomial)**.** For a graph G, its Tutte polynomial $T_G(x, y)$ is defined as

$$T_G(x,y) = \begin{cases} 1 & \text{if } G \text{ is edgeless,} \\ yT_{G\backslash e}(x,y) & \text{if } e \text{ is a loop,} \\ xT_{G/e}(x,y) & \text{if } e \text{ is a bridge,} \\ T_{G\backslash e}(x,y) + T_{G/e}(x,y) & \text{otherwise.} \end{cases}$$

The chromatic polynomial of a graph can be expressed as an evaluation of the Tutte polynomial as follows [16].

$$T_G(1-x, 0)x^{\kappa(G)}(-1)^{|V|-\kappa(G)} = \mathcal{X}_G(x).$$

The proof mainly follows from the inclusion-exclusion principle and the subset-sum expansion of the Tutte polynomial (see Definition 4.1).

In 1998, R. Stanley presented the following symmetric function generalization of the Tutte polynomial [44].

Definition 1.3 (Tutte symmetric function)**.** For a graph $G(V, E)$, the Tutte symmetric function of G is defined as

$$\mathbf{XB}_G(\mathbf{x}; y) = \sum_{f\colon V \to \mathbb{P}} \left(\prod_{v \in V} x_{f(v)} \right) (1 + y)^{|f^=|},$$

where $f^=$ is the set of edges with monochromatic vertices under f.

Analogous to the specialization of the chromatic polynomial from the Tutte polynomial, the Tutte symmetric function of a graph also determines its chromatic symmetric function. Formally, we have

$$\mathbf{XB}_G(\mathbf{x}; -1) = \mathbf{X}_G\,.$$

However, when restricted to trees, the Tutte symmetric function and chromatic symmetric function are equivalent graph invariants. That is, any two trees have the same Tutte symmetric function if and only if they have the same chromatic symmetric functions. Nevertheless, determining classes of graphs other than trees that can be distinguished by their Tutte symmetric function is still an active area to explore.

In 1999, Nobel and Welsh defined a weighted-graph polynomial, called the W-polynomial, which arises from chromatic invariants of knots [36]. This polynomial is defined recursively, similar to the Tutte-Grothendieck decomposition, but for weighted graphs. However, we focus on the unweighted graph variant of the polynomial. In the particular case wherein every graph can be considered as a weighted graph with all its vertices assigned weight 1, the W-polynomial is referred to as the U-polynomial.

Definition 1.4 (U-polynomial)**.** For a graph $G(V, E)$ and any edge subset $F \subseteq E$, let

$a_1, a_2, \ldots, a_k$ be the number of vertices in the connected components of $G(V, F)$. Then, the U-polynomial of G is defined as

$$U_G(\mathbf{x}; y) = \sum_{F \subseteq E} x_{a_1} x_{a_2} \ldots x_{a_k} (y-1)^{|F|+k-|V|}.$$

The U-polynomial of a graph G is equivalent to the Tutte symmetric function of the graph. As a consequence, the U-polynomial determines the chromatic symmetric function of graphs, and when restricted to trees, it is equivalent to the chromatic symmetric function.

1.3 CHROMATIC INVARIANTS OF DIGRAPH AND POSETS

Analogous to the chromatic polynomial of graphs, Stanley introduced weak and strict order polynomials for partially ordered sets that count the number of weak and strict order-preserving colorings of the poset, respectively [42]. These polynomials have been generalized to quasisymmetric functions as follows:

Definition 1.5 (Order quasisymmetric functions)**.** For a partially ordered set $(\mathcal{P}, \preceq)$, the weak and strict order quasisymmetric function is defined as

$$\Gamma^{\geqslant}(\mathbf{x}) = \sum_{\substack{f:\,\mathcal{P}\to\mathbb{P} \\ \text{weakly} \\ \text{order-preserving}}} \left(\prod_{v\in\mathcal{P}} x_{f(v)}\right)$$

and

$$\Gamma^{>}(\mathbf{x}) = \sum_{\substack{f:\,\mathcal{P}\to\mathbb{P} \\ \text{stricly} \\ \text{order-preserving}}} \left(\prod_{v\in\mathcal{P}} x_{f(v)}\right).$$

The weak and strict order quasisymmetric functions are equivalent invariants.

In [40], Shareshian and Wachs defined the quasisymmetric analogue of the chromatic symmetric function, known as the chromatic quasisymmetric function. Initially, this was defined for labeled graphs or, equivalently, acyclic digraphs. In [17], the chromatic quasisymmetric function was extended to digraphs, where the expansion of the function in various bases was studied.

Definition 1.6 (Chromatic quasisymmetric functions)**.** For a digraph $D(V, A)$, its chromatic quasisymmetric function is defined as

$$\mathbf{X}_D^{>}(\mathbf{x}; q) = \sum_{\substack{f\,:\,V \to \mathbb{P} \\ \text{proper coloring}}} \left(\prod x_{f(v)} \right) q^{asc(f)}$$

where $asc(f)$ is the number of arcs (u, v) in D satisfying $f(u) < f(v)$.

In [7], Awan and Bernardi defined a digraph generalization of the Tutte polynomial, called as B-polynomial. Furthermore, the B-polynomial of (acyclic) digraphs also determines the order polynomials of the induced posets.

Definition 1.7 (B-polynomial)**.** For a digraph $D(V, A)$, the B-polynomial $B_D(x, y, z)$ is a unique trivariate polynomial, such that for every positive integer k,

$$B_D(k, y, z) = \sum_{f:V \to [k]} y^{asc(f)} z^{dsc(f)},$$

where $[k] \coloneqq \{1, 2, \ldots, k\}$ and $asc(f)$ (resp. $dsc(f)$) denotes the number of arcs (u, v) in A such that $f(u) < f(v)$ (resp. $f(u) > f(v)$).

Combinatorial interpretations of evaluations of B-polynomials, generating function formulations in terms of order polynomials and subset-sum expansion in terms of activities of edges are explored in [7]. Further, they introduced the following quasisymmetric generalization of the B-polynomial that extends the Tutte symmetric function to digraphs.

Definition 1.8 (Quasisymmetric B-function)**.** For a digraph $D(V, A)$, the quasisymmetric B-function is defined as

$$B_D(\mathbf{x}; y, z) = \sum_{f\,:\,V \to \mathbb{P}} \left(\prod x_{f(v)} \right) y^{asc(f)} z^{dsc(f)}. \tag{1.1}$$

It is noteworthy that all the aforementioned graph polynomials and functions can be determined from the B-polynomial and quasisymmetric B-functions, respectively. In Figure 1.3, we illustrate the relations between the graph and digraph invariants described

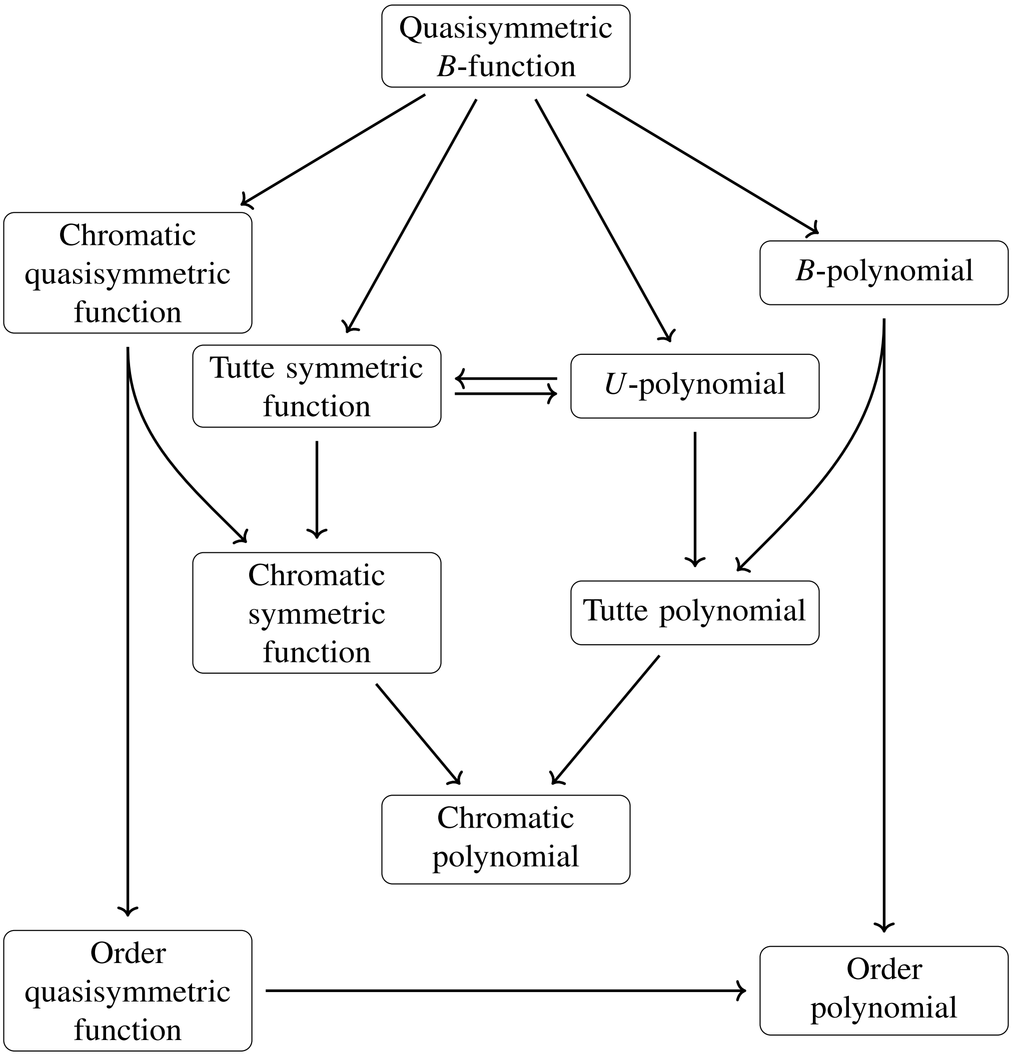


Figure 1.3: Relations among graph and digraph invariants: the invariant at the tail of an arrow determines the invariant at its head.

in Section 1.2 and Section 1.3.

1.4 CONTENT AND OUTLINE OF THE THESIS

We present a brief overview of the content and structure of the thesis.

In this thesis, we aim to address the problem of distinguishing (and reconstructing) trees and their orientations from the chromatic symmetric function and quasisymmetric B-functions, respectively.

In Chapter 2, we set up the necessary notations and preliminaries.

Chapter 3 aims to prove the validity of Stanley's tree isomorphism conjecture for a class of trees that extend proper caterpillars. We begin with a brief description of chromatic symmetric functions of graphs and their expansion in various bases, with a view towards Stanley's Tree Isomorphism Conjecture in Section 3.1. Furthermore, we introduce a generalization of caterpillars called *proper q-caterpillars* (see Definition 3.7) in Section 3.2. We show that whether a tree is a proper q-caterpillar or not can be recognized from its chromatic symmetric function (see Proposition 3.9). In Section 3.3, we recall the monoid of integer compositions introduced in [9, 3]. This monoid plays a key role in proving the validity of Stanley's trees isomorphism conjecture for proper q-caterpillars in Section 3.4

In the further chapters, we focus on distinguishing and reconstructing digraphs from their B-polynomial and quasisymmetric B-functions.

In Chapter 4, we solve an open question raised in [7] (see Question 4.5). We briefly recall the B-polynomial and its expansion in the binomial basis in Section 4.1. In Section 4.2, we exhibit a subset-sum expansion of the B-polynomial instrumental in the proof of Theorem 4.6. We conclude the chapter with some open questions.

In Chapter 5, we delve into a digraph analogue of Stanley's tree isomorphism conjecture concerning the quasisymmetric B-function. We commence with the expansion of the quasisymmetric B-function in a monomial quasisymmetric basis in Section 5.1. Following this, we provide a concise review of the literature pertaining to distinguishing digraphs by their various quasisymmetric functions in Section 5.2. In Section 5.3, we demonstrate that *partially symmetric* orientations of proper caterpillars can be reconstructed based on their quasisymmetric B-functions. The methods are further extended in Section 5.4 to prove that quasisymmetric B-functions distinguish certain orientations of proper q-caterpillars.

Consequently, we establish that all orientations of paths can be reconstructed from their quasisymmetric B-functions. These results offer a partial solution to the problem presented in [7, Question 10.7(ii)] and also encourage further exploration of [6, Conjectures 1.2 and 1.3].

We present non-isomorphic digraphs with equal quasisymmetric B-functions in Chapter 6. We achieve this by defining a vertex-weighted quasisymmetric B-function and show that this function satisfies a deletion-contraction relation with respect to symmetric arcs.

CHAPTER 2

PRELIMINARIES

2.1 GRAPHS AND DIRECTED GRAPHS

2.1.1 Graphs

A *graph* G is an ordered pair $((V(G), E(G))$, alternatively written as $G(V, E)$ consisting of a finite set V of *vertices*, and set E of 2-element subsets of V called the *edges*. Any two vertices u and v in a graph $G(V, E)$ are said to be *adjacent* to v if there exists an edge $\{u, v\}$ in G. For the sake of brevity, we denote the edge $\{u, v\}$ by uv. For a vertex u, its *neighborhood* $N(u)$ is the set of vertices in G adjacent to u, and its cardinality is called the *degree* of the vertex, denoted by $d(v)$. For a graph $G(V, E)$, we call $\{d(v)\}_{v \in V}$ as the degree sequence of the graphs.

A *subgraph* $H(W, F)$ of a graph $G(V, E)$ is a graph satisfying $W \subseteq V$ and $F \subseteq E$. For a graph $G(V, E)$, an *induced subgraph* on a vertex subset $W \subseteq V$ is a graph on vertex set W with the set of edges $\{uv \in E \mid u, v \in W\}$.

In a graph $G(V, E)$, a vertex u is said to be *connected* to a vertex v if there exists a path in G starting at u and ending at v. Observe that connectedness in a graph is an equivalence relation and, therefore, partitions the graph into equivalence classes called the *connected components* of the graphs. A graph is said to be *connected* if it has exactly one connected component, or equivalently, every pair of distinct vertices is connected. For a graph G, let $\kappa(G)$ denote its number of connected components.

The *length* of a path is the number of edges in the path. The length of the longest path in graph G is called the *diameter* of the graph G. Let π_i be the number of paths in graph G of length i. The tuple $(\pi_1, \pi_2, \ldots, \pi_n)$ is called the *path sequence* of the graph G.

A *tree* is a connected acyclic graph. Equivalently, any connected graph with n vertices and $n-1$ edges is a tree. An acyclic graph is called as *forest*. A graph G is a forest on n vertices if and only if it has $n-\kappa(G)$ edges.

We now recall the deletion and contraction operation on graphs. For a graph $G(V,E)$ and an edge $e \in E$, let $G \setminus e$ denote the graph on vertex set V and edge set $E \setminus \{e\}$. On the other hand, let G/uv denote by the graph obtained by identifying the vertices u and v to a new vertex w in the graph $G \setminus uv$. The graphs $G \setminus uv$ and G/uv are graphs obtained by *deletion* and *contraction* of the edge uv, respectively.

An edge in a graph is said to be a *bridge* if the number of connected components of $G \setminus e$ is more than the number of connected components of G. Observe that a graph G is a forest if and only if every edge of the graph is a bridge.

2.1.2 Digraphs

A *digraph* D is an ordered pair $(V(D), A(D))$, where $V(D)$ represents the finite set of vertices and $A(D)$ represents the multiset of *arcs in* D. An arc $(u,v) \in A(D)$ is said to be *outgoing from* u and *incoming to* v. It is important to note that adjacency in a graph is a symmetric relation, but this symmetry need not hold in a digraph. The cardinality of the multiset of arcs incoming to v and outgoing from v is referred to as the *in-degree* and *out-degree of vertex* v, respectively. The in-degree and out-degree of a vertex v is denoted by $d_i(v)$ and $d_o(v)$, respectively. The sequence $\{(d_i(v), d_o(v)\}_{v\in V}$ is called as the *in-out degree sequence* of the digraph D.

The *underlying graph of* D, denoted as $\underline{D}$, is the graph obtained by replacing every arc (u,v) in D with the edge $\{u,v\}$. Henceforth, whenever we refer to an edge in a digraph, we mean the corresponding edge in the underlying graph. A digraph D is said to be an orientation of a graph G if $\underline{D} = G$. A digraph is said to be *acyclic* if it does not contain a directed cycle.

2.2 INTEGER COMPOSITIONS AND PARTITIONS

The symmetric and quasisymmetric functions that we study in the subsequent chapters are parameterized by the integer partitions and compositions, respectively. Our aim in this section is to provide with a brief introduction of the partitions and compositions.

2.2.1 Integer Compositions

An integer composition α of n, denoted by $\alpha \vDash n \in \mathbb{P}$, is an ordered sequence of positive integers $(\alpha_1, \alpha_2, \ldots, \alpha_r)$ whose sum is n. The integer α_i is called the i^{th} component of α, and the length of the integer compositions α, denoted by $\ell(\alpha)$, is r. Let $\mathscr{C}_n$ denote the set of integer compositions of n, and $\mathscr{C} = \bigcup_{n \in \mathbb{P}} \mathscr{C}_n$.

For any $n \in \mathbb{P}$, there is a one-to-one correspondence between the integer compositions of n and subsets of the set $[n-1]$ given by

$$(\alpha_1, \alpha_2, \ldots, \alpha_r) \longmapsto \{\alpha_1, \alpha_1 + \alpha_2, \ldots, \sum_{k=1}^{r-1} \alpha_k\}, \text{ and}$$

$$\{s_1, s_2, \ldots, s_r\} \longmapsto (s_1, s_2 - s_1, s_3 - s_2, \ldots, s_r - s_{r-1}, n - s_r)$$

with $s_1 < s_2 < \cdots < s_r$. For an integer composition $\alpha \vDash n$, let $set(\alpha)$ denote the corresponding subset of $[n-1]$.

Let α and β be two integer compositions of n. Then β is said to be a *coarsening* of α if α is obtained by adding some (or no) consecutive parts of α, and is denoted by $\alpha \preceq \beta$. For example, $(2,3,2) \preceq (2,5)$. Let $(\mathscr{C}_n, \preceq)$ be the poset defined by the coarsening order. Observe that for any integer compositions α and β of n, we have

$$\alpha \preceq \beta \iff set(\alpha) \supseteq set(\beta).$$

As a consequence, $(\mathscr{C}_n, \preceq)$ is isomorphic to the boolean lattice $(2^{[n]}, \supseteq)$.

2.2.2 Integer Partitions

For a positive integer n, its *integer partition* is a finite sequence of non-increasing positive integers $\lambda = \lambda_1 \;\; \lambda_2 \;\; \cdots \;\; \lambda_t$ satisfying $\sum_{i=1}^{t} \lambda_i = n$. For $n \in \mathbb{P}$, let $\mathscr{P}_n$ denote the set of all partitions of n, and $\mathscr{P}$ be the set of all partitions.

The integers λ_i are called the *parts* of λ. The *length* of the partitions, denoted by $\ell(\lambda)$, is the number of parts in the partition, and the sum of the parts is denoted by $|\lambda|$.

Alternatively, an integer partition can be denoted by

$$\lambda = (1^{r_1}2^{r_2}\cdots)$$

where r_i is the multiplicity of the part i in λ. Let $r(\lambda) := r_1!r_2!\ldots$ for the integer partition $\lambda = (1^{r_1}2^{r_2}\cdots)$.

For a detailed exposition to integer partition and compositions, we refer the reader to [45].

2.3 ALGEBRA OF SYMMETRIC FUNCTIONS

Let $\mathbb{P}, \mathbb{Z}$ and $\mathbb{Q}$ denote the set of positive integers, integers, and rational numbers, respectively. Let $\mathbf{x}$ denote the list of indeterminates $x_1, x_2, \ldots$ indexed by $\mathbb{P}$.

Symmetric function occurs in diverse areas of mathematics, including representation theory, algebraic geometry, invariant theory, and more. The modern presentation of the symmetric function is accredited to M. Hirsch [21].

Let $\mathbb{Q}[\![\mathbf{x}]\!]$ be the $\mathbb{Q}$-algebra of formal power series. The *degree* of the monomial $x_{i_1}^{\alpha_1}x_{i_2}^{\alpha_2}\cdots x_{i_k}^{\alpha_k}$ is given by $\sum_{i=1}^{k}\alpha_i$. Further, formal power series has *finite degree* if there exists a positive integer m such that the degree of each monomial is bounded by m. A formal power series is said to be *homogenous* of degree m if each its monomial is of degree m. For a monomial $x_{i_1}^{\alpha_1}x_{i_2}^{\alpha_2}\cdots x_{i_k}^{\alpha_k}$ and $f \in \mathbb{Q}[\![\mathbf{x}]\!]$, let $[x_{i_1}^{\alpha_1}x_{i_2}^{\alpha_2}\cdots x_{i_k}^{\alpha_k}]f$ denote the coefficient of $x_{i_1}^{\alpha_1}x_{i_2}^{\alpha_2}\cdots x_{i_k}^{\alpha_k}$ in f.

Definition 2.1. A formal power series $f \in \mathbb{Q}[\![\mathbf{x}]\!]$ is a *symmetric function* if

1. f has finite degree,

2. for every composition $(\alpha_1, \alpha_2, \ldots, \alpha_k)$, the coefficients of $x_{i_1}^{\alpha_1} x_{i_2}^{\alpha_2} \cdots x_{i_k}^{\alpha_k}$ in f are equal for all distinct integers $i_1, i_2, \ldots, i_k$.

Note that the set of symmetric functions forms a subalgebra of $\mathbb{Q}[\![\mathbf{x}]\!]$, we denote this $\mathbb{Q}$-subalgebra by $\mathrm{Sym}_{\mathbb{Q}}(\mathbf{x})$. Equivalently, symmetric functions are finite degree formal power series that are invariant under the action of permutation of indeterminates.

2.3.1 Bases for the algebra of symmetric functions

In this section, we define various bases of the algebra of symmetric functions.

Monomial symmetric functions

For a partition $\lambda = \lambda_1 \quad \lambda_2 \quad \cdots \quad \lambda_k \vdash n$, consider the $\mathbb{P}$-tuple $(\lambda_1, \lambda_2, \ldots, \lambda_k, 0, 0, \ldots)$ obtained by padding 0's to the partition λ. Let $\mathrm{Perm}(\lambda)$ be the set of $\mathbb{P}$-tuples obtained by permutation of components of $(\lambda_1, \lambda_2, \ldots, \lambda_k, 0, 0, \ldots)$.

Definition 2.2. The *monomial symmetric function* for an integer partition λ is defined as

$$m_\lambda := \sum_{\alpha \in \mathrm{Perm}(\lambda)} x_1^{\alpha_1} x_2^{\alpha_2} \cdots . \tag{2.1}$$

It is straightforward to see that m_λ is a symmetric function for all $\lambda \vdash n$. Further, $\{m_\lambda\}_{\lambda \vdash n}$ forms a $\mathbb{Q}$-basis for the symmetric functions homogenous of degree n.

We further define the augmented monomial symmetric functions, which are scalar multiples of (2.1).

Definition 2.3. For an integer partition $\lambda = \lambda_1 \quad \lambda_2 \quad \ldots \quad \lambda_k = (1^{r_1} 2^{r_2} \cdots)$ of n, the *augmented monomial symmetric function* is defined as

$$\widetilde{m}_\lambda = m_\lambda (r_1! r_2! \ldots) = \sum_{\substack{i_1, i_2, \ldots, i_k \\ \text{distinct}}} x_{i_1}^{\lambda_1} x_{i_2}^{\lambda_2} \cdots x_{i_k}^{\lambda_k}. \tag{2.2}$$

Power sum symmetric functions

Definition 2.4. The power sum symmetric function is defined as follows:

1. for $k \in \mathbb{P}$, let $p_k := x_1^k + x_2^k + \cdots$.

2. for $\lambda = \lambda_1\ \lambda_2\ \cdots\ \lambda_r$, let $p_\lambda := p_{\lambda_1} p_{\lambda_2} \cdots p_{\lambda_r}$.

The symmetric functions $\{p_\lambda\}_{\lambda \vdash n}$ forms a $\mathbb{Q}$-basis for the symmetric function homogeneous of degree n. Furthermore, the $\mathbb{Q}$-algebra generated $\{p_i\}_{i \in \mathbb{P}}$ is equal to the algebra of symmetric functions over $\mathbb{Q}$.

Other important and well-studied bases of symmetric functions include elementary symmetric basis, complete homogeneous basis, Schur symmetric functions, and more. A detail exposition on these symmetric functions can be found in [32, 45].

2.4 ALGEBRA OF QUASISYMMETRIC FUNCTIONS

The algebra of quasisymmetric function was first introduced by Gessel [22] while studying the P-partitions. We recall the description of the algebra of quasisymmetric function over $\mathbb{Q}$, which is a subalgebra of the formal power series.

Definition 2.5. A formal power series $f \in \mathbb{Q}[\![\mathbf{x}]\!]$ is said to be *quasisymmetric function* if

1. f has finite degree,

2. for every composition $(\alpha_1, \alpha_2, \ldots, \alpha_k)$, the coefficients of $x_{i_1}^{\alpha_1} x_{i_2}^{\alpha_2} \cdots x_{i_k}^{\alpha_k}$ in f are equal for all strictly increasing k-tuples $i_1 < i_2 < \cdots < i_k$.

We denote the algebra of quasisymmetric function over $\mathbb{Q}$ by $\mathrm{QSym}_{\mathbb{Q}}(\mathbf{x})$. Let $\mathrm{QSym}_R^n(\mathbf{x})$ denote the collection of quasisymmetric functions homogeneous of degree n.

2.4.1 Bases for the algebra of quasisymmetric functions

We recall certain $\mathbb{Q}$-bases for the algebra of quasisymmetric functions.

Monomial quasisymmetric functions

Definition 2.6. For an integer composition $\delta = (\delta_1, \ldots, \delta_k) \vDash n$, the *monomial quasisymmetric function* M_δ is defined as

$$M_\delta := \sum_{i_1 < i_2 < \cdots < i_k} x_{i_1}^{\delta_1} x_{i_2}^{\delta_2} \cdots x_{i_k}^{\delta_k},$$

where the sum is over all increasing k-tuples of positive integers.

The collection $\{M_\delta\}_{\delta \vDash n}$ forms an $\mathbb{Q}$-basis of $\mathrm{QSym}^n_{\mathbb{Q}}(\mathbf{x})$ (see [45]). For a quasisymmetric function f, let $[M_\delta]f$ denote the coefficient of M_δ obtained by expressing f in the monomial quasisymmetric basis over $\mathbb{Q}$.

Fundamental quasisymmetric function

The fundamental quasisymmetric function was primarily studied for the P-partitions of posets and their linear extensions.

Definition 2.7. For an integer composition $\alpha \vDash n$, the *fundamental quasisymmetric function* is defined as

$$F_\alpha := \sum_{\beta \preceq \alpha} M_\beta \tag{2.3}$$

where $\preceq$ is the coarsening order defined in Section 2.2.1.

For example, $F_{(2,2)} = M_{(1,1,2)} + M_{(2,1,1)} + M_{(1,1,1,1)} + M_{(2,2)}$.

In terms of the indeterminates, the fundamental quasisymmetric function for an integer composition $\alpha \vDash n$ is defined as

$$F_\alpha = \sum_{(i_1, i_2, \ldots, i_k)} x_{i_1} x_{i_2} \cdots x_{i_k}, \tag{2.4}$$

where the sum is taken over all non-decreasing k-tuples $(i_1, i_2, \ldots, i_k)$ satisfying $i_j < i_{j+1}$ for $j \in set(\alpha)$.

Other bases of quasisymmetric functions include quasisymmetric Schur functions,

$\Phi-$power sum quasisymmetric functions, Ψ-power sum quasisymmetric functions, etc.

For further details, we refer the reader to [31, 8].

CHAPTER 3

CHROMATIC SYMMETRIC FUNCTION

In this chapter, we study the chromatic symmetric function of graphs and Stanley's Tree Isomorphism Conjecture, which posits that non-isomorphic trees are distinguished by their chromatic symmetric function. We define a generalization of caterpillars that we call *proper q-caterpillars*, and show that Stanley's Tree Isomorphism Conjecture holds for proper q-caterpillars, for all $q \geq 2$.

3.1 STANLEY'S TREE ISOMORPHISM CONJECTURE

We begin with the definition of the chromatic symmetric function, introduced by R. Stanley [41], that generalizes the chromatic polynomial of a graph to a symmetric function.

Definition 3.1 ([41])**.** The *chromatic symmetric function* of a graph $G = (V, E)$ is defined as

$$\mathbf{X}_G := \sum_{\substack{f:V\to\mathbb{P} \\ proper}} \mathbf{x}^{c(f)}. \tag{3.1}$$

where $c(f) = (|f^{-1}(1)|, |f^{-1}(2)|, \ldots)$.

Recall that the chromatic polynomial of a graph G, denoted as χ_G, evaluated at k yields the number of proper colorings of the graph G using k colors. In this context, the chromatic symmetric function generalizes the chromatic polynomial as follows:

Proposition 3.2 ([41, Proposition 2.2])**.** *For $k \in \mathbb{P}$, we have*

$$\mathbf{X}_G(\underbrace{1, 1, \ldots, 1}_{k}, 0, 0, \ldots) = \chi_G(k).$$

Note that the chromatic symmetric function is indeed symmetric in $\mathbf{x}$ since any permutation of the colors does not affect the properness of colorings. Moreover, the chromatic symmetric function $\mathbf{X}_G$ homogeneous in $\mathbf{x}$ with degree $|V|$. It is straightforward to see that for any two isomorphic graphs G and H with $\psi : G \xrightarrow{\simeq} H$ as a graph isomorphism, we have

$$X_G = \sum_{\substack{f:V(G)\to\mathbb{P} \\ proper}} \mathbf{x}^{c(f)} = \sum_{\substack{f\circ\psi^{-1}:V(H)\to\mathbb{P} \\ proper}} \mathbf{x}^{c(f)} = \sum_{\substack{g:V(H)\to\mathbb{P} \\ proper}} \mathbf{x}^{c(g)} = X_H.$$

Therefore, isomorphic graphs share the same chromatic symmetric functions, or equivalently, the chromatic symmetric function is a graph invariant. This raises the question of whether the chromatic symmetric function encodes sufficient information to distinguish non-isomorphic graphs. Unfortunately, the answer is negative. R. Stanley presented two non-isomorphic graphs, both containing cycles, that share the same chromatic symmetric function (see Figure 3.1).

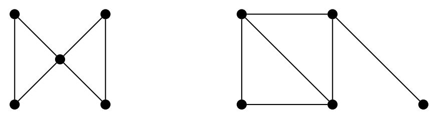


Figure 3.1: Non-isomorphic graphs with the same chromatic symmetric function

In fact, there exist infinitely many pairs of (unicyclic) non-isomorphic graphs with the same chromatic symmetric function [15, 37]. However, the question remains open for trees and is conjectured to be true, commonly known as Stanley's Tree Isomorphism Conjecture.

Conjecture 3.3. *The chromatic symmetric function distinguishes trees.*

The conjecture has been open for nearly three decades and is believed to be true. Substantial progress has been made in confirming the conjecture for various subclasses of trees. Martin et. al proved the conjecture for specific classes of caterpillars, spiders, and certain unicyclic graphs by establishing the connection between the chromatic symmetric function and the subtree polynomial [33, 12]. Additionally, Aliste-Prieto and Zamora [3] showed that the conjecture holds for proper caterpillars, while Loebl and Sereni [30] extended this result to all caterpillars. Tsujie proved that the trivially perfect graphs can be distinguished by their chromatic symmetric functions [48], while in [2], it was proven for certain trees with a diameter of at most 5. To explore additional examples of graphs that can be distinguished based on their chromatic symmetric function, refer to [13, 18, 27, 50]. The conjecture has been verified for all vertices up to 29 using computer-based computations [26].

3.1.1 Bases expansion of Chromatic Symmetric Function

We begin with expanding the chromatic symmetric function in certain bases of symmetric function, wherein the coefficients determine various statistics of the graphs.

Figure 3.2: Stable set partitions of the 4-cycle.

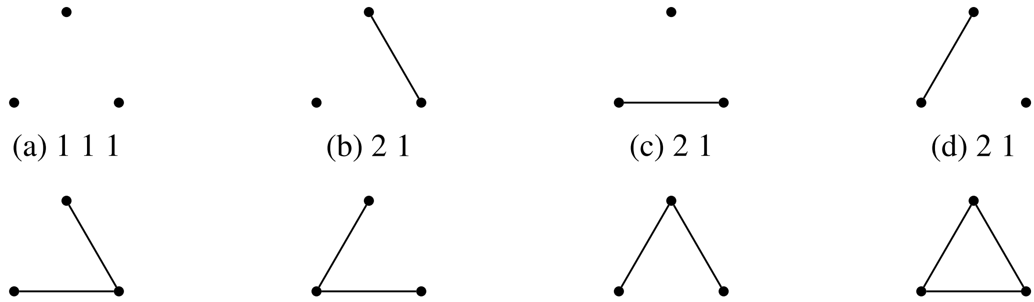
For a graph $G = (V, E)$, a set partition of V into non-empty sets is said to be *stable* if every block of the set partition is an independent set in G. The *type* of the set partition is the integer partition defined by the sizes of its blocks. The following proposition exhibits that the chromatic symmetric function expanded in augmented monomial symmetric function basis determines the number of stable set partitions of G having type λ. For example, Figure 3.2 exhibits all stable partitions of the 4-cycle.

Proposition 3.4 ([41, Proposition 2.3])**.** *For a graph $G = (V, E)$, let* Stab_λ *denote the collection of stable set partitions of G of type λ. Then, we have*

$$\mathbf{X}_G = \sum_{\lambda \vdash |V|} |\operatorname{Stab}_\lambda| \widetilde{m}_\lambda.$$

where $\{\widetilde{m}_\lambda\}_{\lambda \vdash |V|}$ is the set of augmented monomial symmetric functions.

For example, the expansion of the chromatic symmetric function of a 4-cycle in augmented



(a) 1 1 1 (b) 2 1 (c) 2 1 (d) 2 1

(e) 3 (f) 3 (g) 3 (h) 3

Figure 3.3: Spanning subgraphs of K_3 along with the partitions determined by the orders of their connected components.

monomial symmetric function basis is $\widetilde{m}_{22} + 2\widetilde{m}_{211} + \widetilde{m}_{1111}$.

Given a graph $G = (V, E)$ and a subset $F \subseteq E$, let $G[F]$ denote the spanning subgraph (V, F) of G. Let $\lambda[F]$ be the partition of $|V|$ formed by the orders of the connected components of the spanning subgraph $G[F]$.

Theorem 3.5 ([41, Theorem 2.5])**.** *For a graph G, the expansion of the chromatic symmetric function in the power sum symmetric function basis is*

$$\mathbf{X}_G = \sum_{F\subseteq E} (-1)^{|F|} p_{\lambda[F]}(\mathbf{x}). \tag{3.2}$$

where $\{p_\lambda\}_{\lambda\vdash|V|}$ *is the set of power sum symmetric functions.*

For example, we infer from Figure 3.3 that

$$\mathbf{X}_{K_3} = p_{111} - 3p_{21} + 3p_3 - p_3 = p_{111} - 3p_{21} + 2p_3.$$

Observe that the coefficient of $-p_{211\cdots1}$ in the chromatic symmetric function is the number of edges of the graph. Similarly, other properties like girth, number of connected components, diameter (of trees), etc. can be recovered from the chromatic symmetric function [35].

3.1.2 U-polynomial

We now recall the U-polynomial defined by Noble and Welsh [36], which establishes a strong connection with the chromatic symmetric function due to the expansion (3.2). For a partition $\lambda = \lambda_1 \lambda_2 \cdots \lambda_k \vdash n$, let $\mathbf{x}_\lambda$ denote the monomial $x_{\lambda_1} x_{\lambda_2} \cdots x_{\lambda_k}$,

Definition 3.6 ([36]). Given a graph $G = (V, E)$, the U-polynomial of the graph is defined as

$$U_G(\mathbf{x}; y) = \sum_{F \subseteq E} \mathbf{x}_{\lambda[F]} (y-1)^{|F|-|V|+\kappa(F)},$$

where $\kappa(F)$ is the number of connected components in the spanning subgraph $G[F]$, or equivalently the length of partition $\lambda[F]$.

For example, the U-polynomial of a 4-cycle is $x_1^3 + 3x_2x_1 + 3x_3 + x_3(y-1)$.

A subtle but key observation is that information about certain spanning subgraphs may be lost in the chromatic symmetric function due to the alternating sum. However, the U-polynomial encodes monomials with respect to each spanning subgraph, along with its cyclomatic number $(|F| - |V| + \kappa(F))$ (see [11] for an exposition on the cyclomatic number).

We now show that, when restricted to trees, both the chromatic symmetric function and the U-polynomial are equivalent graph invariants. Note that any spanning subgraph $T[F]$ of a tree $T = (V, E)$ must have $|V| - |F|$ connected components. This implies that $|F| - |V| + \kappa(F) = 0$ for all $F \subseteq E$. Therefore, for any tree T, we have

$$\begin{aligned} (-1)^{|V|} U_T(-p_1(\mathbf{x}), -p_2(\mathbf{x}), -p_3(\mathbf{x}), \dots; y) &= (-1)^{|V|} \left(\sum_{F \subseteq E} (-1)^{\kappa(F)} p_{\lambda[F]}(\mathbf{x}) (y-1)^0 \right) \\ &= \sum_{F \subseteq E} (-1)^{|V|-\kappa(F)} p_{\lambda[F]}(\mathbf{x}) \\ &= \sum_{F \subseteq E} (-1)^{|F|} p_{\lambda[F]}(\mathbf{x}) \\ &= \mathbf{X}_T \end{aligned} \quad (3.3)$$

This implies that any two trees have the same chromatic symmetric function if and only if they share the same U-polynomial. Therefore, Stanley's Tree Isomorphism Conjecture is equivalent to distinguishing trees by their U-polynomials. As the variable y is redundant for the U-polynomial of trees, we omit it for the remainder of this chapter.

3.2 PROPER *Q*-CATERPILLARS

A tree is said to be a caterpillar if deleting all its pendant vertices results in a path. Such a caterpillar is said to be *proper* if every non-pendant vertex is adjacent to at least one leaf. We consider the following generalization of proper caterpillars.

Definition 3.7 (proper q-caterpillars)**.** Let $q \geq 1$ be fixed. A proper q-caterpillar T is constructed as follows: We begin with a path $S = \langle v_1, \ldots, v_\ell \rangle$ (with endpoints v_1 and v_ℓ) called the spine, with $\ell > 0$. For every $1 \leq i \leq \ell$, we glue (endpoint of the path identified with a vertex on the spine) p_i additional paths of length exactly q to the vertices v_i, respectively, where $p_i \in \mathbb{P}$. (For example, see Figure 3.4.)

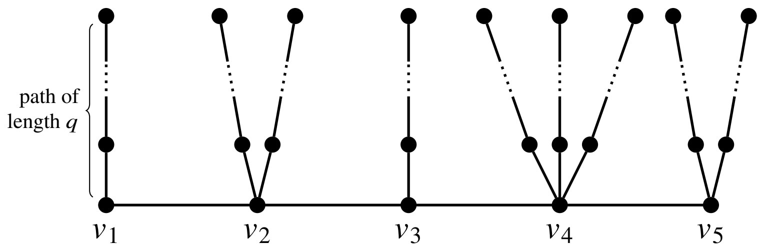


Figure 3.4: Example of a proper q-caterpillar with spine $\langle v_1, v_2, \ldots, v_5 \rangle$ with associated integer composition $(q + 1, 2q + 1, q + 1, 3q + 1, 2q + 1)$.

In this context, proper 1-caterpillars have been distinguished by their chromatic symmetric functions up to isomorphism [3]. For $q \geq 1$, we show that the chromatic symmetric function recognizes whether a tree is a proper q-caterpillar or not. Furthermore, we prove that for $q \geq 2$, proper q-caterpillars are distinguished by their chromatic symmetric functions.

The proof is based on ideas involved in [3], that is, associating proper q-caterpillars with integer compositions, and the interrelations of the chromatic symmetric function, U-polynomial and $\mathcal{L}$-polynomial. Note that for $q \geq 2$, every integer composition $(p_1, p_2, \ldots, p_\ell)$ with each component being positive corresponds to a unique proper q-caterpillar (up to isomorphism) with p_i many paths of length q incident on the vertex v_i of the spine $\langle v_1, v_2, \ldots, v_\ell \rangle$. Therefore, for each such integer composition lexicographically smaller than its reverse, there are infinitely many trees (one for each $q \geq 2$) that can be distinguished by chromatic symmetric function, thereby attaining a significant improvement in the pool of trees that are known to satisfy Stanley's Tree Isomorphism Conjecture.

We begin by characterizing proper q-caterpillars in terms of the statistics that can be retrieved from the chromatic symmetric function. This allows us to differentiate proper q-caterpillars from other types of trees.

Given a tree $T = (V, E)$, the *trunk* T° of T is the smallest subtree containing all vertices of degree at least three. For each pendant vertex u of T, there exists a unique path starting at u and ending at some vertex in the trunk such that all internal vertices of the path have degree two. Each such path is called a *twig*, and let $\textsc{Twig}(T)$ be the multiset representing the lengths of twigs in T. Evidently, every tree containing a vertex of degree at least three can be decomposed into the trunk T° and some twigs. L. Crew proved that the order of T°, and the multiset $\textsc{Twig}(T)$ can be determined by the chromatic symmetric function [13].

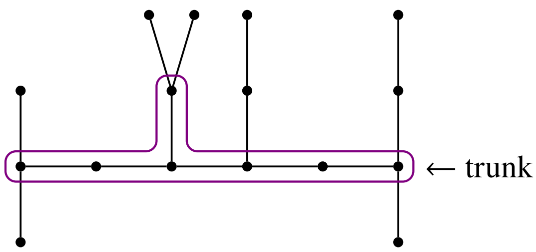


Figure 3.5: Decomposition of a tree T into trunk and twigs, with $|T^\circ| = 7$ and $\textsc{Twig}(T) = \{1, 1, 1, 1, 1, 2, 2\}$.

It is clear that a path T is a proper q-caterpillar if and only if its order is either $q+1, 2q+1$ or $2q+2$. For proper q-caterpillars that are not paths, we characterize the proper q-caterpillars using tree-invariants determined by the chromatic symmetric functions.

Theorem 3.8 ([12, 13, 33]). *For a tree $T(V, E)$, its order, degree sequence, diameter, order of the trunk T°, and the multiset* Twig(T) *can be recovered from its chromatic symmetric function.*

Proposition 3.9. *Let $q \geq 1$ be fixed and $T = (V, E)$ be a tree that is not a path. Then T is a proper q-caterpillar if and only if it satisfies the following:*

(i) $|T^\circ| = |V| - \delta_1 - \delta_2$ *where δ_i is the number of vertices of degree i in T.*

(ii) Twig(T) *only contains integers q and q+1, with $\mu_{q+1} \leq 2$ where μ_{q+1} is the multiplicity of q+1 in* Twig(T).

(iii) $\operatorname{diam}(T) = (|T^\circ| - 1) + 2q + \mu_{q+1}$.

Proof. ($\Rightarrow$) It is clear that every proper q-caterpillar that is not a path satisfies the above three conditions.

($\Leftarrow$) A tree satisfying $|T^\circ| = 1$ and (ii) is indeed a proper q-caterpillar. Thus we may assume that $|T^\circ| \geq 2$. Note that $\operatorname{diam}(T) \leq 2q + \operatorname{diam}(T^\circ) + \mu_{q+1}$ along with (iii) implies that $(|T^\circ| - 1) \leq \operatorname{diam}(T^\circ)$, and hence T° is a path, say $\langle w_1, w_2, \ldots, w_k \rangle$ (with endpoints w_1 and w_k). From (i), it follows that T° consists only of vertices of degree at least 3, owing to which every vertex of the trunk must be incident to at least one twig. To prove that T is a proper q-caterpillar, it suffices to prove that twigs of length $q+1$ (if they exist) are incident to the distinct endpoints of the trunk. For $1 \leq i \leq k$, let w_i be incident to n_i many twigs P_i^t $(1 \leq t \leq n_i)$. Let u_i^t be the pendant vertex of the twig $P_i^t (1 \leq t \leq n_i)$. In the resulting tree T, the distance between the vertices u_i^t and u_j^s is given by

$$d(u_i^t, u_j^s) = \ell(P_i^t) + |i - j| + \ell(P_j^s)$$

where $\ell(P_i^t)$ is the length of the twig with endpoint u_i^t. From the above computation, the endpoints of the path in T of length $\operatorname{diam}(T)$ must be w_1^t and w_k^s for some $1 \leq t \leq n_1$

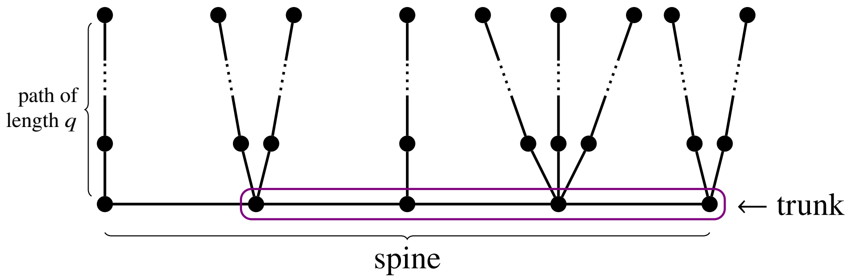


Figure 3.6: Example of a proper q-caterpillar with spine of order 5, trunk of order 4 and the multiset of twigs is $\{\underbrace{q, q, \ldots, q}_{8 \text{ times}}, q{+}1\}$.

and $1 \le s \le n_k$. This together with (ii) and (iii) dictates the position of q+1-twigs as follows:

$$\mu_{q+1} = \begin{cases} 0 & \text{if neither } w_1 \text{ nor } w_k \text{ is incident to a } q+1\text{-length twig,} \\ 1 & \text{if exactly one of } w_1 \text{ or } w_k \text{ is incident to } q+1\text{-length twig,} \\ 2 & \text{if both } w_1 \text{ and } w_k \text{ are incident to } q+1\text{-length twig.} \end{cases}$$

Therefore, the tree T is a proper q-caterpillar, and this completes the proof. ■

Note. The trunk of the proper q-caterpillar may not coincide with the spine (see Figure 3.6). However, it is always a subpath of the spine.

3.3 MONOID OF INTEGER COMPOSITIONS

Before proceeding to the main theorem of this chapter, we revisit the factorization of integer compositions introduced in [9]. This factorization is instrumental for determining the isomorphism classes of proper q-caterpillars.

3.3.1 $\mathcal{L}$-polynomial

Let $\mathscr{C}$ denote the set of all integer compositions. Recall that an integer composition β is said to be a *coarsening* of an integer composition α if β is obtained by adding some (or no) consecutive parts of α, denoted by $\alpha \preceq \beta$. For example, $(5, 5, 3, 5) \preceq (10, 8)$. Let $(\mathscr{C}, \preceq)$ be the poset with the coarsening order. Note that for a fixed integer n, the poset of integer compositions of n under the coarsening order form a complete boolean lattice of order n. In [9], Billera, Thomas and Willigenburg defined an equivalence relation on $\mathscr{C}$ based on the equality of the multiset

$$\mathcal{M}(\alpha) := \{\lambda(\beta) \in \mathscr{C} \mid \alpha \leq \beta\},$$

where $\lambda(\beta)$ is the partition obtained by arranging the components of β in non-increasing order. We consider the polynomial interpretation of this equivalence relation called the $\mathcal{L}$-polynomial (or the composition-lattice polynomial) introduced in [3].

The $\mathcal{L}$-polynomial of an integer composition α is defined as

$$\mathcal{L}(\mathbf{x};\alpha) = \sum_{\beta \succeq \alpha} x_{\beta_1} x_{\beta_2} \ldots x_{\beta_r}.$$

For instance, the $\mathcal{L}$-polynomial of the composition $(5,5,3,5)$ is $x_3x_5^3 + x_3x_5x_{10} + 2x_5^2x_8 + 2x_5x_{13} + x_8x_{10} + x_{18}$.

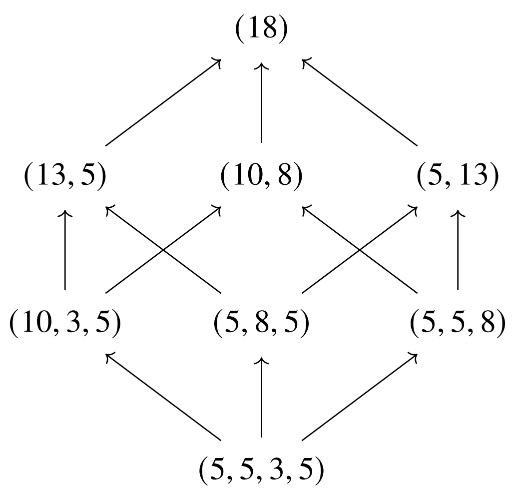


Figure 3.7: Coarsening of $(5,5,3,5)$.

3.3.2 Factorization of integer compositions

Note that the equality of the $\mathcal{L}$-polynomial induces an equivalence relation on the integer compositions. Let $[\alpha]_{\mathcal{L}}$ denote the equivalence class of α under this equivalence relation.

We recall its description using the "unique" factorization defined on the set of integer compositions.

Definition 3.10. For any two compositions $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_r)$ and $\beta = (\beta_1, \beta_2, \ldots, \beta_s)$, their *concatenation* is given by

$$\alpha \cdot \beta := (\alpha_1, \alpha_2, \ldots, \alpha_r, \beta_1, \beta_2, \ldots, \beta_s),$$

whereas the *near-concatenation* operation is defined as

$$\alpha \odot \beta := (\alpha_1, \alpha_2, \ldots, \alpha_{r-1}, (\alpha_r + \beta_1), \beta_2, \ldots, \beta_s).$$

Let $\alpha^{\odot q}$ denote the q-fold near-concatenation $\underbrace{\alpha \odot \alpha \odot \cdots \odot \alpha}_{q \text{ times}}$, for any positive integer q.

The *composition* of two integer compositions is given by

$$\alpha \circ \beta := \beta^{\odot \alpha_1} \cdot \beta^{\odot \alpha_2} \cdot \cdots \cdot \beta^{\odot \alpha_r}.$$

For example, $(2, 1) \circ (2, 3) = ((2, 3) \odot (2, 3)) \cdot (2, 3) = (2, 5, 3) \cdot (2, 3) = (2, 5, 3, 2, 3)$.

Proposition 3.11 ([9, Proposition 3.3])**.** *$(\mathscr{C}, \circ)$ is a non-commutative associative monoid with the integer composition 1 as the identity element.*

A factorization $\alpha = \varepsilon \circ \eta$ is said to be *trivial* if one of the following is satisfied:

a) either ε or η is the identity composition 1,

b) both ε and η are of length 1,

c) both ε and η have all parts equal to 1.

An integer composition is said to be *irreducible* if it admits only trivial factorizations. A factorization $\alpha = \eta_1 \circ \eta_2 \circ \cdots \circ \eta_k$ is said to be an *irreducible factorization* if each integer composition η_i is irreducible and no $\eta_i \circ \eta_{i+1}$ is a trivial factorization.

Theorem 3.12 ([9, Theorem 3.6])**.** *Every integer composition admits a unique irreducible factorization.*

This factorization can be compared to the prime factorization within a unique factorization domain. In this analogy, compositions of length 1 with all parts equal to 1 in $\mathscr{C}$ can be seen as analogous to units in the UFD.

We now revisit the characterization of integer compositions that share the same $\mathcal{L}$-polynomial as the integer compositions α, based on the irreducible factorization of α. Let α^* be the integer composition obtained by reversing α, that is, the i^{th} component of α^* is $\alpha_{\ell(\alpha)-i+1}$ for $1 \leq i \leq \ell(\alpha)$.

Theorem 3.13 ([9, Theorem 4.1]). *Let $\alpha = \eta_1 \circ \eta_2 \circ \cdots \circ \eta_k$ be the irreducible factorization of α. Then*

$$[\alpha]_{\mathcal{L}} = \{\varepsilon_1 \circ \varepsilon_2 \circ \cdots \circ \varepsilon_k \mid \varepsilon_i = \eta_i \text{ or } \varepsilon_i = {\eta_i}^*, \text{ for all } i = 1, 2, \ldots k\},$$

Example 3.14. Consider the integer composition $(4, 10, 4, 10)$ with its irreducible factorization given by $(1, 1) \circ (2, 5) \circ (2)$. Then the equivalence class

$$[(4, 10, 4, 10)]_{\mathcal{L}} = \{(1, 1)\circ(2, 5)\circ(2), (1, 1)\circ(5, 2)\circ(2)\} = \{(4, 10, 4, 10), (10, 4, 10, 4)\}.$$

3.4 DISTINGUISHING PROPER q-CATERPILLARS

We showed in Proposition 3.9 whether a tree is a proper q-caterpillars or not can be determined by the statistics recoverable by its chromatic symmetric function. We now proceed to show that the chromatic symmetric function distinguishes non-isomorphic proper q-caterpillars. We accomplish this by associating each proper q-caterpillar with a unique integer composition. In Lemma 3.16, we relate the U-polynomial of proper q-caterpillars with the $\mathcal{L}$-polynomial of corresponding integer composition. Further, we show that any two proper q-caterpillars are isomorphic if and only if their corresponding compositions are either the same or reverses of one another. Finally, we combine these ideas to prove that the chromatic symmetric function distinguishes proper q-caterpillars.

Let $q \geq 2$, and T be a proper q-caterpillar. Let $\langle v_1, v_2, \ldots v_\ell \rangle$ denote the spine of T. Let

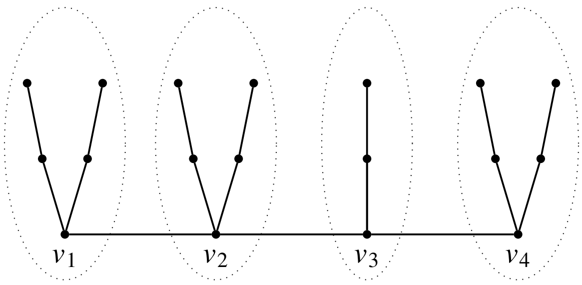


Figure 3.8: Proper 2-caterpillar T with $\varphi(T) = (5, 5, 3, 5)$.

p_i represent the number of paths in T of length q, starting from a leaf and ending at v_i. We define a composition $\varphi(T)$ of length ℓ whose i^{th} component is $q{\cdot}p_i + 1$. Conversely, for any integer composition α with all components greater than one and congruent to 1 modulo q, we construct a proper q-caterpillar $\tau(\alpha)$ as follows: consider a path with $\ell(\alpha)$ vertices, which serves as the spine, and glue $\frac{\alpha_i - 1}{q}$ new paths of length q to the i^{th} vertex of the spine. The mapping φ and τ are inverses of each other. For instance, see Figure 3.8.

Proposition 3.15. *Any two proper q-caterpillars S and T are isomorphic if and only if $\varphi(S) = \varphi(T)$ or $\varphi(S) = \varphi(T)^*$.*

Proof. ($\Leftarrow$) It is straightforward to see that $\varphi(S) = \varphi(T)$ or $\varphi(S) = \varphi(T)^*$ implies that S and T are isomorphic.

($\Rightarrow$) Let $\Psi\colon S \to T$ be an isomorphism. Then, when restricted to the spine $\langle v_1, v_2, \dots, v_\ell\rangle$, the isomorphism Ψ either maps $v_i \mapsto v_i$ for all $i = 1, 2, \dots, \ell$, or $v_i \mapsto v_{\ell-i+1}$ for all $i = 1, 2, \dots, \ell$. Consequently, $\varphi(S) = \varphi(T)$ in the former case, whereas $\varphi(S) = \varphi(T)^*$ in the latter case. ■

The following lemma is a generalization of [3, Proposition 2.5], that obtains $\mathcal{L}(\varphi(T); \mathbf{x})$ as an evaluation of the U-polynomial $U_T(\mathbf{x})$, for a proper q-caterpillar T.

Lemma 3.16. *Let $q \geq 1$. For any proper q-caterpillar $T = (V, E)$ and the composition $\varphi(T)$ associated to T, we have*

$$U_T(\underbrace{0, 0, \dots, 0}_{q\ \textit{times}}, x_{q+1}, x_{q+2}, \dots) = \mathcal{L}(\varphi(T); \mathbf{x}).$$

Proof. The U-polynomial with $x_1 = x_2 = \cdots = x_q = 0$ can be interpreted as the subset-sum over $F \subseteq E$ such that each connected component of the induced subgraph $T[F]$ has order at least $q + 1$. This implies that such an F must contain all non-spine edges (otherwise, the induced subgraph $T[F]$ would contain a connected component of order at most q). Thus every monomial $\mathbf{x}_{\lambda[F]}$ in $U_T(0, 0, \ldots, 0, x_{q+1}, x_{q+2}, \ldots)$ corresponds to the subset $F' := F \cap S$, where S is the set of spine edges. Any such subset F' of spine-edges determines a unique coarsening $\varphi(T)^{F'}$ of the composition $\varphi(T)$ in the poset $(\mathscr{C}, \preceq)$ obtained as follows: for maximal paths $\langle v_1, \ldots, v_{i_1}\rangle, \langle v_{i_1+1}, \ldots, v_{i_2}\rangle, \ldots, \langle v_{i_k+1}, \ldots, v_\ell\rangle$ in $T[F']$ with $1 \le i_1 < i_2 < \cdots < i_k \le \ell$, define

$$\varphi(T)^{F'} := \left(\sum_{j=1}^{i_1} \varphi(T)_j, \sum_{j=i_1+1}^{i_2} \varphi(T)_j, \ldots, \sum_{j=i_k+1}^{\ell} \varphi(T)_j\right).$$

Observe that the monomial contributed by the subset F in $U_T(0, 0, \ldots, 0, x_{q+1}, x_{q+2}, \ldots)$ is same as the monomial contributed by the coarsening $\varphi(T)^{F'}$ in $\mathcal{L}(\varphi(T); \mathbf{x})$. (See Figure 3.9 for an example.) Therefore we have

$$U_T(0, 0, \ldots, 0, x_{q+1}, x_{q+2}, \ldots) = \sum_{\substack{F \subseteq E \\ F \text{ contains all} \\ \text{non-spine edges}}} \mathbf{x}_{\lambda[F]} = \mathcal{L}(\varphi(T); \mathbf{x}).$$

■

Lemma 3.16 along with the equivalence of chromatic symmetric function and U-polynomial implies that the chromatic symmetric function determines the $\mathcal{L}$-polynomial. The following lemma plays a vital role in the irreducible factorization of the integer compositions associated with the proper q-caterpillars.

Lemma 3.17. *Let $q \ge 2$ and h be positive integers such that q does not divide h. Let γ be an integer composition in which each component is congruent to h modulo q and the greatest common divisor (gcd) of all components is* 1*. Then either γ is irreducible or its irreducible factorization is $\gamma = (1^m) \circ \omega$ where ω is an integer composition and (1^m) denotes the integer composition $\underbrace{(1, 1, \ldots, 1)}_{m}$, for some $m \ge 1$.*

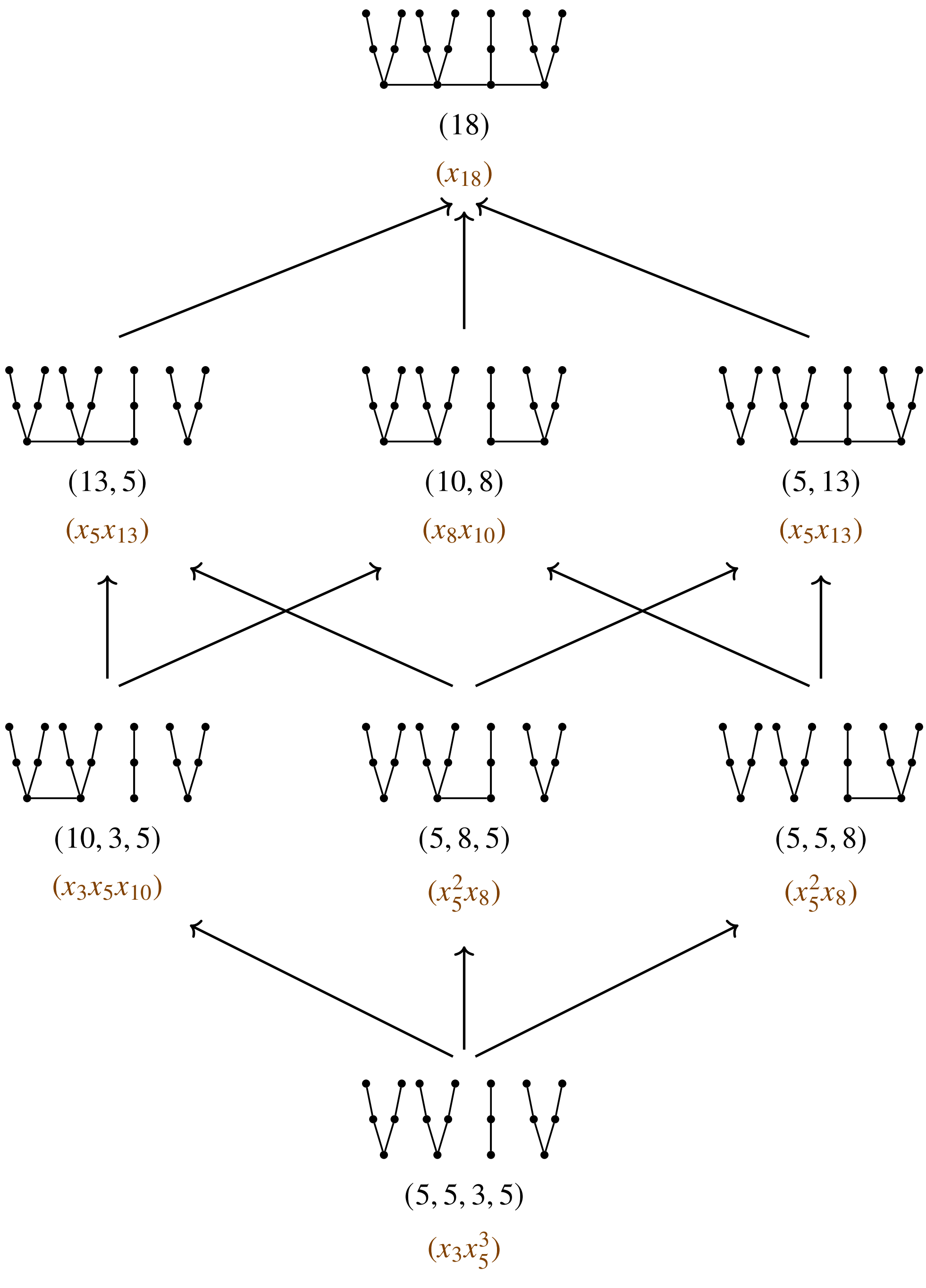


Figure 3.9: Bijection between coarsenings of integer composition and subgraphs of proper 2-caterpillar corresponding to $(5, 5, 3, 5)$ containing all non-spine edges.

Proof. We may assume that γ is not irreducible. We prove using induction on length of γ. Let $\gamma = \zeta \circ \eta$ be a non-trivial factorization of γ. We claim that each component of ζ must be equal to 1. Assume to the contrary that ζ contains at least one component greater than 1, and let i be the smallest index with the i^{th} component $\zeta_i > 1$. The gcd of all components of γ being 1 implies that the length of η must be at least 2. Since $\gamma_1 = \eta_1$ and $\gamma_{\ell(\gamma)} = \eta_{\ell(\eta)}$, both η_1 and $\eta_{\ell(\eta)}$ are congruent to h modulo q. For $k = \ell(\eta) \cdot i$, consider the k^{th} component of $\gamma = \zeta \circ \eta$. By the given hypothesis, we get γ_k to be congruent to h modulo q, but the factorization implies

$$\varepsilon_k = (\zeta \circ \eta)_k = \eta_1 + \eta_{\ell(\eta)} \equiv 2h \pmod{q}.$$

This is not possible because h is non-zero modulo q. Therefore ζ must have all the components equal to 1, that is, $\gamma = (1^r) \circ \eta$ for some $r \geq 2$. Note that η satisfies the given hypothesis and its length $\ell(\eta) < \ell(\gamma)$. Using induction, either η is irreducible or its irreducible factorization is $(1^s) \circ \omega$, and consequently, the irreducible factorization of γ is $(1^r) \circ \eta$ or $(1^{rs}) \circ \omega$, respectively. Thus γ admits the required irreducible factorization. ∎

Using Lemma 3.17, we can conclude that the proper q-caterpillars are distinguished by the chromatic symmetric functions up to isomorphism.

Theorem 3.18. *For $q \geq 2$, the chromatic symmetric function distinguishes isomorphism classes of proper q-caterpillars.*

Proof. Let $q \geq 2$. Let S and T be two proper q-caterpillars with the same chromatic symmetric function. Lemma 3.16 implies that the $\mathcal{L}$-polynomial of $\varphi(S)$ and $\varphi(T)$ are equal as well. Note that it suffices to prove the equivalence class $[\varphi(T)]_{\mathcal{L}} = \{\varphi(T), \varphi(T)^*\}$, as it would imply $\varphi(S) = \varphi(T)$ or $\varphi(S) = \varphi(T)^*$. This, along with Proposition 3.15 would imply that S is isomorphic to T. If the gcd of all components of $\varphi(T)$ is 1, then by Lemma 3.17 either $\varphi(T)$ is irreducible or its irreducible factorization is $(1^r) \circ \omega$ for some integer composition ω. On the other hand, if the gcd of all components is d which is greater than 1, then factorize $\varphi(T) = \varepsilon \circ d$. Note that the gcd of all components of ε is 1, and each component is congruent to h modulo q, where h is the least positive integer satisfying $d \cdot h \equiv 1 \pmod{q}$. By Lemma 3.17, either ε is irreducible or its irreducible factorization must be $(1^r) \circ \omega$ for some $r \geq 2$. This implies that the irreducible factorization of $\varphi(T)$ is $\varepsilon \circ d$ or $(1^r) \circ \omega \circ d$. In either case, the irreducible factorization of $\varphi(T)$ contains at most one non-palindrome composition. This, along with Theorem 3.13 implies that $[\varphi(T)]_{\mathcal{L}} = \{\varphi(T), \varphi(T)^*\}$. This completes the proof. ■

We believe that further generalizations of Lemma 3.16 might hold for other classes of trees. The future prospects in this direction are discussed in Chapter 7

CHAPTER 4

TUTTE POLYNOMIAL OF DIRECTED GRAPHS

In this chapter, we study the B-polynomial introduced by Awan and Bernardi, which is a digraph analogue of the Tutte Polynomial. We provide an affirmative answer to the question raised by Awan and Bernardi in [7]; does the B-polynomial of a digraph determine whether the digraph is a symmetrization of some graph or not?

4.1 B-POLYNOMIAL

We begin by recalling the Tutte polynomial and the Potts polynomial with respect to graphs. The Tutte polynomial of graphs, originally defined by W. Tutte is a universal object for the polynomials that satisfy deletion-contraction relation. Formally, all graph polynomials that are multiplicative with respect to disjoint union and admit a deletion-contraction reduction, can be expressed as a certain evaluation of the Tutte polynomial. The Tutte polynomial coincides with the rank generating function of Whitney, introduced in [51] and therefore admits an edge subset-sum expansion.

Definition 4.1 (Tutte Polynomial)**.** For a graph $G(V, E)$, the Tutte polynomial of G is defined as

$$T_G(x, y) = \sum_{F\subseteq E} (x-1)^{\kappa(G[F])-\kappa(G)}(y-1)^{|S|-\kappa(G[F])+|V|},$$

where $\kappa(G[F])$ denotes the number of connected components in the spanning subgraph $G[F]$.

A detailed exposition of the Tutte polynomial can be found in [16, 28].

In [19], Fortuin and Kasteleyn showed that the following Potts model (or polynomial) [38] is an evaluation of the Tutte polynomial [49].

Definition 4.2 ([7])**.** For a graph $G(V, E)$, the Potts polynomial $P(x, t)$ is a bivariate

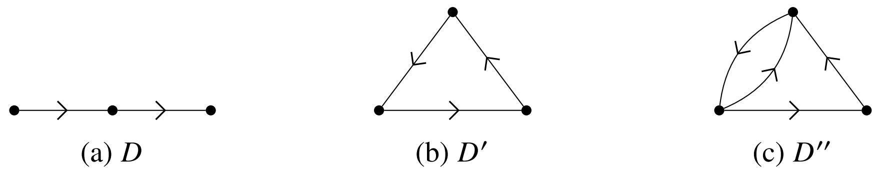


Figure 4.1: Digraphs

polynomial, such that for every positive integer k,

$$P(k,t) = \sum_{f:\, V\to[k]} t^{|f^{\neq}|}$$

where $f^{\neq}$ is the collection of edges whose endpoints are monochromatic under f.

The generalization of the Tutte polynomial to digraph uses above Potts's polynomial as an intermediary.

Definition 4.3 ([7, Theorem 3.1])**.** For a digraph $D(V,A)$, the B-polynomial $B_D(x,y,z)$ is the unique trivariate polynomial, such that for every positive integer k,

$$B_D(k,y,z) = \sum_{f:V\to[k]} y^{asc(f)} z^{dsc(f)},$$

where $[k] := \{1,2,\dots,k\}$ and $asc(f)$ (resp. $dsc(f)$) denotes the number of arcs uv in A such that $f(u) < f(v)$ (resp. $f(u) > f(v)$).

The B-polynomial admits the following expansion in the binomial basis,

$$B_D(x,y,z) = \sum_{p=1}^{|V|} \binom{x}{p} \left(\sum_{g\in Surj(V,p)} y^{asc(g)} z^{dsc(g)} \right), \tag{4.1}$$

where $Surj(V,p)$ is the collection of surjective colorings from V to $[p]$.

Example 4.4. The B-polynomials of the digraphs in Figure 4.1 are

$$B_D(x,y,z) = \binom{q}{1} + \binom{q}{2}(2y+2yz+2z) + \binom{q}{3}(y^2+4yz+z^2),$$
$$B_{D'}(x,y,z) = \binom{q}{1} + \binom{q}{2}(6yz) + \binom{q}{3}(3yz^2+3y^2z),$$
$$B_{D''}(x,y,z) = \binom{q}{1} + \binom{q}{2}(2yz+2y^2z+2yz^2) + \binom{q}{3}(y^3z+4y^2z^2+yz^3).$$

Let $\overleftrightarrow{G}$ be the graph obtained by replacing every edge in G with a pair of opposite arcs. The digraph $\overleftrightarrow{G}$ is called as *symmetrization* of the graph G. It is straightforward to see that

$$P_G(x, yz) = B_{\overleftrightarrow{G}}(x, y, z). \tag{4.2}$$

Further, the Tutte polynomial and Potts polynomial satisfy the following [16, Theorem 9.6.6]:

$$T_G(x, y) = \frac{y^{|E|}}{(y-1)^{|V|}(x-1)^{\kappa(G)}} P_G((x-1)(y-1), \frac{1}{y}). \tag{4.3}$$

Combining (4.2) and (4.3), we obtain an equivalence between the Tutte polynomial of a graph G and the B-polynomial of the digraph $\overleftrightarrow{G}$.

In what follows, we denote the arc (u, v) by uv for the simplicity of writing.

4.2 B-POLYNOMIAL AND SYMMETRIC DIGRAPHS

In this section, we address an open question posed in [7] regarding the identification of digraphs obtained by symmetrization. For any graph G, it follows from (4.2) that the B-polynomial of a digraph $\overleftrightarrow{G}$ can be expressed in terms of variables x and yz. Awan and Bernardi raised the question of whether the converse holds true.

Question 4.5 ([7, Question 10.3])**.** *Is it true that $B_D(x, y, z)$ is a function of x and yz if and only if D is a symmetrization of some graph G?*

In Theorem 4.6, we prove that the answer to the above question is in the affirmative. In other words, we establish that the B-polynomial differentiates the classes of digraphs obtained through symmetrization, from all other digraphs.

Theorem 4.6. *A digraph D is a symmetrization of some undirected graph G if and only if its B-polynomial is a function of x and yz.*

Prior to the proof of aforementioned theorem, we present a subset-sum expansion for $B_D(x, y, z)$. This expansion is derived through the repeated application of following

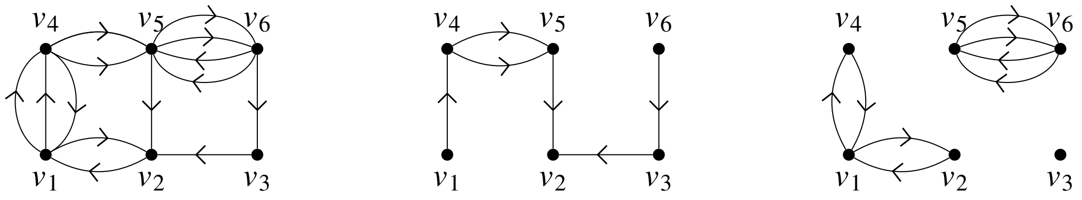


Figure 4.2: Partition of the arc set A into arc sets $A' = \{v_1v_4, v_3v_2, 2 \cdot v_4v_5, v_5v_2, v_6v_2\}$ and $A'' = \big\{\{v_1v_2, v_2v_1\}, \{v_1v_4, v_4v_1\}, 2 \cdot \{v_5v_6, v_6v_5\}\big\}$.

recurrence relation concerning opposite arcs proved in [7, Lemma 4.1]. For a digraph $D(V, A)$, and pair of opposite arcs $e = \{uv, vu\}$ in A,

$$B_D(x, y, z) = (yz)B_{D\backslash e}(x, y, z) + (1 - yz)B_{D/e}(x, y, z). \tag{4.4}$$

Let $A = A' \sqcup A''$ be a partition of the arc set A such that A'' is expressible as a disjoint union of opposite arc pairs $\{uv, vu\}$, and A' consists of arcs uv such that the opposite arc vu does not belong to A' (see Figure 4.2). The following proposition presents a subset-sum expansion of B-polynomial with respect to the set A''.

Proposition 4.7. *For digraph $D(V, A)$, we have*

$$B_D(x, y, z) = \sum_{R \sqcup S = A''} (yz)^{|R|}(1 - yz)^{|S|} B_{D\backslash R/S}(x, y, z), \tag{4.5}$$

where A'' is the set of doubletons containing a pair of opposite arcs, and $D/S\backslash R$ is the digraph obtained by deleting and contracting the pair of opposite arcs in R and S, respectively.

Proof. The proof mainly follows from (4.4) and induction on $|A''|$. The base case $|A''| = 1$ follows from (4.4). Assume the result for all proper subsets of A''. For a pair of opposite arcs $e = \{uv, vu\} \in A''$, we have the following:

$$\begin{aligned} B_D(x, y, z) &= (yz)B_{D\backslash e}(x, y, z) + (1 - yz)B_{D/e}(x, y, z) \\ &= (yz) \sum_{R \sqcup S = A''\backslash e} (yz)^{|R|}(1 - yz)^{|S|} B_{D\backslash (R\cup e)/S}(x, y, z) \end{aligned}$$

$$
\begin{aligned}
&+ (1 - yz) \sum_{R \sqcup S = A'' \setminus e} (yz)^{|R|}(1 - yz)^{|S|} B_{D \setminus R/(S \cup e)}(x, y, z) \\
&= \sum_{R \sqcup S = A'' \setminus e} (yz)^{|R \cup e|}(1 - yz)^{|S|} B_{D \setminus (R \cup e)/S}(x, y, z) \\
&+ \sum_{R \sqcup S = A'' \setminus e} (yz)^{|R|}(1 - yz)^{|S \cup e|} B_{D \setminus R/(S \cup e)}(x, y, z) \\
&= \sum_{R \sqcup S = A''} (yz)^{|R|}(1 - yz)^{|S|} B_{D \setminus R/S}(x, y, z).
\end{aligned}
$$

The second line in the above equality follows from the induction hypothesis. In the third line, the two summations are over the subset-sum wherein the pair e is deleted in the former and contracted in the latter. This observation implies the last line of the equation, which completes the proof. ■

We now proceed to the proof of Theorem 4.6. The main idea of the proof involves eliminating pair of opposite arcs using the proposition mentioned above and extract the highest degree term of the B-polynomial.

Proof of Theorem 4.6. ($\Leftarrow$) We prove that if a digraph $D(V, A)$ is not a symmetrization of any undirected graph G, then its B-polynomial does not lie in $\mathbb{Q}[x, yz]$. We treat $B_D(x, y, z)$ as a polynomial over x with coefficients in ring $\mathbb{Q}[y, z]$. From (4.1), it follows that the largest exponent of x in $B_D(x, y, z)$ is equal to the number of vertices of D. Since contraction of arcs reduces the number of vertices, the largest exponent $x^{|V|}$ appears only in the summand where no pair of opposite arcs is contracted, that is, when $R = A''$ in (4.5). This leads to the following equality.

$$
\begin{aligned}
\left[\binom{x}{|V|}\right] B_D(x, y, z) &= \left[\binom{x}{|V|}\right] (yz)^{|A''|} B_{D \setminus A''}(x, y, z) \\
&= (yz)^{|A''|} \sum_{g \in Surj(V, |V|)} y^{asc_{A'}(g)} z^{dsc_{A'}(g)}.
\end{aligned}
\tag{4.6}
$$

This implies that the leading coefficient of the B-polynomial of D is $(yz)^{|A''|}$ times the leading coefficient of $D(V, A')$. Hence it suffices to prove the existence of a $|V|$-coloring of $D(V, A')$ with distinct number of ascents and descents. Since $D \neq \overleftrightarrow{G}$, the set of

(a) A 6-coloring f having exactly 3 ascents and 3 descents.

(b) A 6-coloring g obtained from f by reassigning colorings 5 and 6.

Figure 4.3: 6-colorings of digraph $D(V, A')$, with blue and red colored arcs depicting ascents and descents of the colorings.

non-symmetric arcs A' is non-empty. Let $uv \in A'$ and f be any surjective $|V|$-coloring such that $f(u) = |V| - 1$ and $f(v) = |V|$. If the number of ascents and descents of f are distinct, we are done. Suppose to the contrary that $asc(f) = dsc(f)$. We define the coloring g obtained by interchanging the colors of u and v under f as follows:

$$g(w) = \begin{cases} |V| & \text{if } w = u, \\ |V| - 1 & \text{if } w = v, \\ f(w) & \text{otherwise.} \end{cases}$$

Let $\mathrm{Asc}(f)$ and $\mathrm{Dsc}(f)$ respectively denote the multiset of arcs occurring as ascents and descents under f. Note that the set of ascents and descents of f and g restricted to $A' \setminus \{uv\}$ are the same, whereas $\{uv\} = \mathrm{Asc}(f) \setminus \mathrm{Asc}(g) = \mathrm{Dsc}(g) \setminus \mathrm{Dsc}(f)$. This implies that $asc(g) = asc(f) - 1$ and $dsc(g) = dsc(f) + 1$, and consequently $asc(g) \neq dsc(g)$ (see Figure 4.1). Thus $B_D(x, y, z) \notin \mathbb{Q}[x, yz]$. ∎

4.3 CONCLUDING REMARKS

After the identification of symmetric digraphs from the B-polynomial, a natural question would be to know whether the B-polynomial distinguishes non-isomorphic digraphs. However, this is not true. One way to obtain such pairs is by considering reverse digraphs. For a digraph $D(V, A)$, let $rev(D)$ denote the digraph obtained by reversing all the arcs of D. Then, we observe that the B-polynomials of the digraph D and $rev(D)$ are the same. For any positive integer k, the permutation $\sigma\colon [k] \to [k]$ mapping $i \mapsto k - i + 1$ acts as an involution on $Surj(V, k)$. Therefore for all $k \in \mathbb{P}$,

$$\begin{aligned} B_D(k, y, z) &= \sum_{f\colon V \to [k]} y^{asc(f)} z^{dsc(f)} \\ &= \sum_{\substack{\sigma\circ g\colon V \to [k] \\ \sigma\circ g = f}} y^{asc(f)} z^{dsc(f)} \\ &= \sum_{g\colon V \to [k]} y^{dsc(g)} z^{asc(g)} \\ &= B_{rev(D)}(k, y, z). \end{aligned} \tag{4.7}$$

The last equality follows from the observation that for any coloring $f\colon V \to [k]$, the multiset of ascents and descents satisfy $\mathrm{Asc}_D(f) = \mathrm{Dsc}_{rev(D)}(f)$ and $\mathrm{Dsc}_D(f) = \mathrm{Asc}_{rev(D)}(f)$.

However, the computations using `SageMath` affirm that for oriented trees up to order 8, the digraph and its reverse are the only pair of non-isomorphic digraph having the same B-polynomial. Therefore, investigating the uniqueness of B-polynomials of digraphs up to isomorphism and reversals is an interesting question worth exploring.

Question 4.8. *Does the B-polynomial distinguish acyclic digraphs up to isomorphism and reverses?*

CHAPTER 5

DISTINGUISHING AND RECONSTRUCTING DIRECTED GRAPHS

The digraph polynomials and functions arising through the colorings are invariants that encode various statistics associated with the digraphs. One of the most sought-after problems with respect to these digraph invariants is the following: can these invariants uniquely determine the digraphs? If not, which classes of digraphs are distinguishable by these invariants. These questions have been investigated for various invariants [34, 24, 52, 29, 6], and are to some extent digraph analogues of Stanley's tree isomorphism conjecture.

5.1 QUASISYMMETRIC B-FUNCTION

From (4.7), it follows that the B-polynomial is ineffective in distinguishing orientations of a fixed graph, as there are numerous pairs of non-isomorphic digraphs with the same B-polynomial (for example see Figure 5.1(a)). This is one of the motivations for introducing a quasisymmetric extension of the B-polynomial and investigation of the classes of digraphs that can be distinguished by the extension. One may view this phenomenon as an analogy to the fact that all trees of a fixed order have the same chromatic polynomial, but the chromatic symmetric function holds potential to distinguish all trees.

We begin with the definition of the quasisymmetric B-function introduced by Awan and Bernardi in [7].

Definition 5.1 (Section 8, [7]). Let $\mathbb{P}$ be the set of positive integers and $\mathbf{x} = (x_1, x_2, \dots)$ denote a list of commutative indeterminates. For a digraph $D(V, A)$, the quasisymmetric

B-function is defined as

$$B_D(\mathbf{x}; y, z) = \sum_{f : V \to \mathbb{P}} \left(x_1^{|f^{-1}(1)|} x_2^{|f^{-1}(2)|} x_3^{|f^{-1}(3)|} \cdots \right) y^{asc(f)} z^{dsc(f)}. \tag{5.1}$$

We now show that the above function is indeed quasisymmetric. For any fixed k-tuple $\delta = (\delta_1, \delta_2, \ldots, \delta_k) \in \mathbb{P}^k$ and $i_1 < i_2 < \cdots < i_k$, let $F^{\delta}_{i_1,\ldots,i_k}$ denote the set of $\mathbb{P}$-colorings corresponding to monomial $x_{i_1}^{\delta_1} x_{i_2}^{\delta_2} \cdots x_{i_k}^{\delta_k}$ to $B_D(\mathbf{x}; y, z)$. For any $i_1 < i_2 < \cdots < i_k$ and $j_1 < j_2 < \cdots < j_k$ we have the order-preserving bijections $\sigma : \{i_1, i_2, \ldots, i_k\} \to [k]$ and $\tau : \{j_1, j_2, \ldots, j_k\} \to [k]$. This maps induce a bijection from $F^{\delta}_{i_1,\ldots,i_k}$ to $F^{\delta}_{j_1,\ldots,j_k}$ wherein $f \mapsto \tau^{-1} \circ \sigma \circ f$. Furthermore, the bijection preserves the number of ascents and descents of the colorings. This implies that for any $i_1 < i_2 < \cdots < i_k$ and $j_1 < j_2 < \cdots < j_k$,

$$[x_{i_1}^{\delta_1} x_{i_2}^{\delta_2} \cdots x_{i_k}^{\delta_k}] B_D(\mathbf{x}; y, z) = [x_{j_1}^{\delta_1} x_{j_2}^{\delta_2} \cdots x_{j_k}^{\delta_k}] B_D(\mathbf{x}; y, z).$$

Recall that for $n \in \mathbb{P}$, the monomial quasisymmetric functions over all integer compositions of n (see Definition 2.6) form a $\mathbb{Q}[y, z]$-basis for $\mathrm{QSym}^n_{\mathbb{Q}[y,z]}(\mathbf{x})$. The following proposition expresses the quasisymmetric B-function in the monomial quasisymmetric basis .

Proposition 5.2 ([7]). *For any digraph $D(V, A)$, we have*

$$B_D(\mathbf{x}; y, z) = \sum_{p=1}^{|V|} \sum_{f \in Surj(V,p)} M_{type(f)} y^{asc(f)} z^{dsc(f)},$$

where $type(f)$ is the tuple $(|f^{-1}(1)|, |f^{-1}(2)|, \ldots, |f^{-1}(p)|)$ called the type of f.

We briefly recall that the in-out degree sequence of a digraph (see Section 2.1.2) can be recovered from its quasisymmetric B-function. Given a digraph $D(V, A)$ and $v \in V$, consider the coloring f_v that assigns color 1 to the vertex v and color 2 to the remaining vertices. Observe that every surjective coloring of type $(1, |V| - 1)$ uniquely corresponds to a coloring f_v for some $v \in V$, and satisfies $y^{asc(f_v)} z^{dsc(f_v)} = y^{outdegree\ of\ v} z^{indegree\ of\ v}$.

Therefore, we have

$$[M_{(1,|V|-1)}]B_D(\mathbf{x};y,z) = \sum_{v\in V} y^{asc(f_v)}z^{dsc(f_v)} = \sum_{v\in V} y^{outdegree\ of\ v}z^{indegree\ of\ v}. \tag{5.2}$$

For an integer composition β of n, we define the following multisets containing the monomials of fixed degree corresponding to the surjective colorings.

$$\mathrm{Mon}_d(\beta) := \{y^{asc(f)}z^{dsc(f)} \mid type(f) = \beta \text{ and } asc(f) + dsc(f) = d\},$$
$$\mathrm{Mon}(\beta) := \bigcup_{d\geq 0} \mathrm{Mon}_d(\beta).$$

The above digraph invariant is a quasisymmetric analogue of the following Tutte symmetric function introduced by Stanley in [44].

Definition 5.3. For a graph $G(V,E)$, the Tutte symmetric function is defined as

$$T_G(\mathbf{x};t) = \sum_{V\to\mathbb{P}} \left(x_1^{|f^{-1}(1)|}x_2^{|f^{-1}(2)|}x_3^{|f^{-1}(3)|}\cdots\right)(1+t)^{|f^{=}|},$$

where $f^{=}$ is the multiset of edges whose endpoints are monochromatic under f.

It is straightforward to see that for any graph $G(V,E)$,

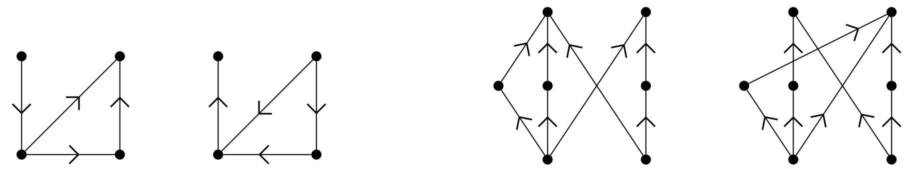
$$B_{\overleftrightarrow{G}}(\mathbf{x};y,z) = (yz)^{|E|}T_G\left(\mathbf{x};\frac{1}{yz}-1\right). \tag{5.3}$$

The quasisymmetric B-function determines other digraph and poset invariants such as order quasisymmetric function, P-partition enumerator of naturally labelled posets and chromatic quasisymmetric function [42, 40].

5.2 BACKGROUND ON CHROMATIC INVARIANTS OF DIGRAPHS

Note that using (5.3), every pair of non-isomorphic graphs with equal Tutte symmetric functions leads to non-isomorphic digraphs with the same quasisymmetric B-functions. Therefore, we are interested in the investigation of the following general question.

Question 5.1 (Question 10.7(i), [7])**.** *Does the quasisymmetric B-function distinguish*



(a) Non-isomorphic digraphs with the same chromatic quasisymmetric function.

(b) Digraphs whose corresponding poset have the same P-partition enumerator.

Figure 5.1: The pair of digraphs in (a) and (b) have distinct quasisymmetric B-functions.

acyclic digraphs?

Every acyclic digraph induces a partial order on its vertex-set defined by the reachability. A canonical way to obtain a poset from an acyclic digraph D is by defining a partial order $u \leq v$ iff there is a directed path from u to v in D. Under this correspondence, the study of distinguishing digraphs and posets by their quasisymmetric functions is closely related and actively investigated: In [24], it was proven that the order quasisymmetric function distinguishes rooted trees, which coincides with the class of $(\mathsf{N}, \bowtie)$-free naturally labeled posets. Furthermore, in [29], they demonstrated that all N-free naturally labeled posets can be distinguished by the P-partition enumerator. Additionally, in [6], labeled rooted trees, along with certain weak edges, are distinguished by their (P, ω)-partition enumerator.

A stronger and somewhat more challenging problem than distinguishing digraphs is their "reconstruction". The previously mentioned results focus on distinguishing non-isomorphic orientations but do not provide a mechanism for their reconstruction. However, J. Zhou has addressed the reconstruction of rooted trees based on their order quasisymmetric function in [52].

In this chapter, we primarily focus on the reconstruction of digraphs from their quasisymmetric B-functions. Certainly, the quasisymmetric B-function is a stronger invariant than the chromatic quasisymmetric function and P-partition enumerator (see Figure 5.1). This is because the quasisymmetric B-function determines certain

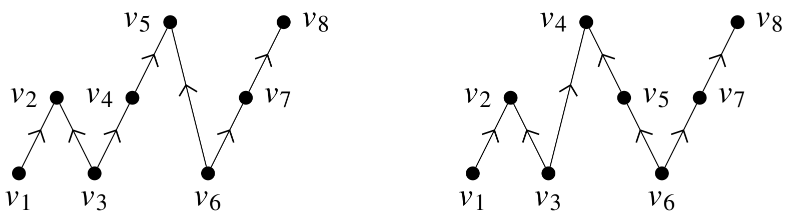


Figure 5.2: Two non-isomorphic oriented paths containing 'N', and having the same in-out degree sequence and height-profile $(3, 3, 2)$.

interesting statistics of a digraph.

A vertex V in an acyclic digraph D is said to be of *height* k if the length of the longest directed path ending at v is $k - 1$. The *height-profile* of an acyclic digraph D is a tuple $(h_0, h_1, \ldots, h_{r-1})$, where h_k is the number of vertices in D of height k. The quasisymmetric B-function encodes the in-out degree sequence and height-profile of acyclic digraphs. However, these quantities are not sufficient to distinguish the orientations of even simple graphs such as paths. For example, Figure 5.2 depicts non-isomorphic orientations of paths with the same in-out degree sequence and height-profile. Therefore the problem of distinguishing orientations of path by quasisymmetric functions is still open.

To the best of our knowledge, Corollary 5.2 along with Theorems 5.11 and 5.12 mark the first instance of reconstructing digraphs containing 'N' using a quasisymmetric function.

We adopt certain change in notations for brevity. For a graph $G(V, E)$, we denote an edge incident to vertices u and v by $\{u, v\}$. On the other hand, an arc in a digraph $D(V, A)$ that is *outgoing from* u and *incoming to* v is denoted by uv. The *underlying graph of* D, denoted as $\underline{D}$, is the graph obtained by replacing every arc uv in D with the edge $\{u, v\}$. Henceforth, whenever we refer to an edge in a digraph, we mean the corresponding edge in the underlying graph.

Recall that for a positive integer p and a graph $G(V, E)$ (or $D(V, A)$), a *p-coloring of* G

is a mapping that assigns a color from the set $[p]$ to each vertex in V. An edge (or arc) is said to be *non-monochromatic* under a coloring if its endpoints are assigned distinct colors.

5.3 DISTINGUISHING ORIENTATIONS OF CATERPILLARS

We show that *semi-symmetric* orientations (see Definition 5.10) of certain caterpillars can be reconstructed from their quasisymmetric B-functions. A tree is said to be a caterpillar if all the vertices of degree at least two induce a (unique) path, which we call as the *spine* of the caterpillar. We consider the following subclasses of caterpillars.

Definition 5.4. (a) A *proper caterpillar* is a caterpillar that has every vertex of the spine adjacent to at least one pendant vertex.

(b) A proper caterpillar is said to be an *asymmetric proper caterpillar* if the number of pendant vertices adjacent to each spine vertex is distinct.

(c) A proper caterpillar is said to be *palindromic* if the associated integer composition is a palindrome.

The class of caterpillars has been shown to be reconstructible from chromatic symmetric functions [3, 30, 33]. Since the chromatic symmetric function of the underlying digraph is determined by the quasisymmetric B-function, it is sufficient to focus on the reconstruction problem of the orientations while fixing the underlying caterpillar. For proper caterpillars, we establish in Theorem 5.11 that their *semi-symmetric* orientations are reconstructible. Implementing the methods involved in reconstruction of the spine, we are able to reconstruct all the orientations of paths up to isomorphism. Using this and the fact that in-out degree sequence is extractible from the quasisymmetric B-functions, we prove the reconstruction of all orientations of asymmetric proper caterpillars in Theorem 5.12.

For proper caterpillars, we establish in Theorem 5.11 that the semi-symmetric orientations of proper caterpillars are reconstructible. Implementing the methods involved in the reconstruction of the spine, we are able to reconstruct all the orientations of paths up to isomorphism. Using this and the fact that in-out degree sequence is extractible from the quasisymmetric B-functions, we prove the reconstruction of all orientations of asymmetric proper caterpillars in Theorem 5.12.

An equivalent characterization of a *caterpillar* is that it is a tree where the deletion of all its pendant vertices results in a path. This resultant path is in fact the *spine* of the caterpillar. For a caterpillar C, we denote its spine by $\langle v_1, v_2, \ldots, v_\ell \rangle$ that starts at v_1 and ends at v_ℓ. Let $u_{k1}, u_{k2}, \ldots$ denote the pendant vertices adjacent to v_k. Let $\text{Comp}(C)$ be the unique integer composition $(\alpha_1, \alpha_2, \ldots, \alpha_\ell)$ associated to C such that for $i = 1, 2, \ldots, \ell$, the spine vertex v_i has exactly $\alpha_i - 1$ many neighbors with degree 1. Note that the integer compositions associated with isomorphic caterpillars are either the same or reverses of each other.

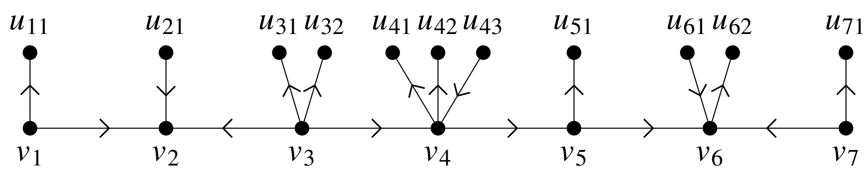


Figure 5.3: An oriented proper caterpillar with associated composition $(2, 2, 3, 4, 2, 3, 2)$.

For an oriented caterpillar $\overrightarrow{C}$ and its spine vertex v_k, let O_k and I_k denote the number of outgoing and incoming pendant arcs of v_k. The tuple $P(v_k) := (O_k, I_k)$ is called as the pendant vector of the spine vertex v_k. For instance, the pendant vector of the spine vertex v_4 in Figure 5.3 is $(2, 1)$. Note that any orientation of a fixed caterpillar C is uniquely determined by (a) the orientation of the spine $\langle v_1, v_2, \ldots, v_\ell \rangle$, and (b) the pendant vector $P(v_k)$ of each spine vertex v_k.

For an integer composition $\delta \vDash |V(T)|$, let $F_T(\delta)$ denote the set of surjective colorings of T having type δ with exactly $\ell(\delta) - 1$ many non-monochromatic edges. The following observations enable us to characterize the colorings of trees, their non-monochromatic arcs and the corresponding monomials.

Observation 5.5. Let $T(V,E)$ be a tree and $\beta = (\beta_1, \beta_2, \ldots, \beta_k)$ be an integer composition of $|V|$. Then

(a) A coloring f is in $F_T(\beta)$ if and only if the deletion of its non-monochromatic edges results in k many connected components of orders $\beta_1, \beta_2, \ldots, \beta_k$.

(b) If each component of β is greater than 1, then the endpoints of the non-monochromatic edges of colorings in $F_T(\beta)$ must have degree greater than 1 in T. Particularly for caterpillars, the non-monochromatic edges of such colorings must lie on the spine.

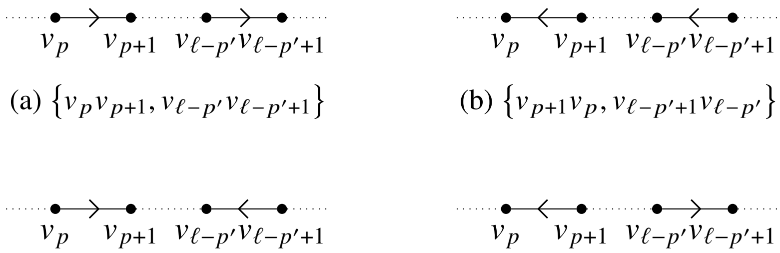
The above observations follow from the fact that every edge of a tree is a cut-edge. We begin with the classification of the spine edges of all caterpillars according to the partial sums of the corresponding integer compositions. Let $C(V,E)$ be a caterpillar with associated composition $\mathrm{Comp}(C) = (\alpha_1, \alpha_2, \ldots, \alpha_\ell)$. For $p = 1, 2, \ldots, \ell$, let $L_p := \sum_{i=1}^{p} \alpha_i$ and $R_p := \sum_{i=1}^{p} \alpha_{\ell-i+1}$ be the left and right justified partial sums of $\mathrm{Comp}(C)$, respectively. We now define the bilateral edges based on the equality of these partial sums. Let

$$\mathcal{B} = \left\{(p,p') \in [\ell] \times [\ell] \;\middle|\; L_p = R_{p'} \text{ and } L_p, R_{p'} \leq \lfloor |V|/2 \rfloor \right\}.$$

For $(p,p') \in \mathcal{B}$, let $B_{p,p'}$ denote the set of edges $\left\{\{v_p, v_{p+1}\}, \{v_{\ell-p'}, v_{\ell-p'+1}\}\right\}$. We call $B_{p,p'}$ as a *bilateral set*, and a spine edge is said to be *bilateral* if it belongs to $B_{p,p'}$ for some $1 \leq p, p' \leq \ell$. Note that $|B_{p,p'}|$ is either one or two, and the former scenario occurs if and only if $|V|$ is even and $L_p = R_{p'} = |V|/2$. For an oriented caterpillar, we denominate the orientation of the bilateral set $B_{p,p'}$ according to its bilateral edges as follows:

Definition 5.6. Let $\overrightarrow{C}(V,E)$ be an oriented caterpillar. For $2 \leq L_p = R_{p'} \leq \lfloor |V|/2 \rfloor$, the bilateral set $B_{p,p'}$ admitting the orientation

- $\left\{v_p v_{p+1}, v_{\ell-p'} v_{\ell-p'+1}\right\}$ are called *right directed* (Figure 5.4:(i)),



(a) $\{v_p v_{p+1}, v_{\ell-p'} v_{\ell-p'+1}\}$ (b) $\{v_{p+1} v_p, v_{\ell-p'+1} v_{\ell-p'}\}$

(c) $\{v_p v_{p+1}, v_{\ell-p'+1} v_{\ell-p'}\}$ (d) $\{v_{p+1} v_p, v_{\ell-p'} v_{\ell-p'+1}\}$

Figure 5.4: Orientations of the bilateral set $B_{p,p'}$.

- $\{v_{p+1} v_p, v_{\ell-p'+1} v_{\ell-p'}\}$ are called *left directed* (Figure 5.4:(ii)),
- $\{v_p v_{p+1}, v_{\ell-p'+1} v_{\ell-p'}\}$ is called *inward* directed (Figure 5.4:(iii)),
- $\{v_{p+1} v_p, v_{\ell-p'} v_{\ell-p'+1}\}$ is called *outward* directed (Figure 5.4:(iv)).

A bilateral set is called *uni-directed* if it is either left directed or right directed. For example, the bilateral sets $B_{1,1}$ and $B_{3,3}$ in Figure 5.3 are inward and right directed, respectively.

The following proposition asserts that the orientation of the spine arcs can be read from the multiset $\text{Mon}_1(s, |V| - s)$ up to uni-direction of bilateral sets.

Proposition 5.7. *Let $\vec{C}(V, E)$ be an oriented caterpillar with $\text{Comp}(C) = (\alpha_1, \alpha_2, \ldots, \alpha_\ell)$. For $L_p, R_{p'} \leq \lfloor |V|/2 \rfloor$ such that the arcs with endpoints $\{v_p, v_{p+1}\}$ and $\{v_{\ell-p'}, v_{\ell-p'+1}\}$ are not bilateral, the multiset*

$$\text{Mon}_1(L_p, |V| - L_p) = \begin{cases} \{y\} & \textit{iff } v_p v_{p+1} \in A, \\ \{z\} & \textit{iff } v_{p+1} v_p \in A. \end{cases} \tag{5.4}$$

and

$$\text{Mon}_1(R_{p'}, |V| - R_{p'}) = \begin{cases} \{y\} & \textit{iff } v_{\ell-p'+1} v_{\ell-p'} \in A, \\ \{z\} & \textit{iff } v_{\ell-p'} v_{\ell-p'+1} \in A. \end{cases} \tag{5.5}$$

For the bilateral set $B_{p,p'}$ with $s = L_p = R_{p'}$, we have

$$\mathrm{Mon}_1(s, |V| - s) = \begin{cases} \{y, z\} & \textit{iff } B_{p,p'} \textit{ is uni-directed,} \\ \{y, y\} & \textit{iff } B_{p,p'} \textit{ is inward directed,} \\ \{z, z\} & \textit{iff } B_{p,p'} \textit{ is outward directed.} \end{cases} \tag{5.6}$$

Proof. According to Observation 5.5(b), the non-monochromatic edges of the colorings from $F_C(L_p, |V| - L_p)$ and $F_C(R_{p'}, |V| - R_{p'})$ are $\{v_p, v_{p+1}\}$ and $\{v_{\ell-p'}, v_{\ell-p'+1}\}$, respectively. The coloring(s) in $F_C(L_p, |V| - L_p)$ (resp. $F_C(R_{p'}, |V| - R_{p'})$) assigns color 1 to the vertex v_p (resp. $v_{\ell-p'+1}$). Therefore, the orientations of the non-monochromatic edges correspond to the asserted multisets in (5.4), (5.5) and (5.6). ■

This leads us to the following corollary.

Corollary 5.8. *Let $\overrightarrow{C}(V, E)$ be an oriented caterpillar. If none of the bilateral sets $B_{p,p'}$ of $\overrightarrow{C}$ are uni-directed, then the orientation of the spine can be determined by the quasisymmetric B-function.*

It is worth noting that the information of the non-uni-directed bilateral sets, along with the already known digraph-statistics from the quasisymmetric B-function like in-out degree sequence and height-profile are insufficient to distinguish the orientation of the spine. In fact, there exist non-isomorphic orientations of paths that agree on the above quantities (see Figure 5.2). Therefore the determination of uni-directed bilateral sets is crucial and non-trivial. By imposing certain conditions on the underlying caterpillars, we show that the orientations of the spine including the uni-directed bilateral sets can be reconstructed from the quasisymmetric B-function.

5.3.1 Recovering orientation of the spine of proper caterpillars

Recall that a caterpillar is said to be *proper* if every vertex of the spine is adjacent to at least one pendant vertex. Equivalently, they are the caterpillars whose associated compositions have each component of size at least two. The advantage of studying the

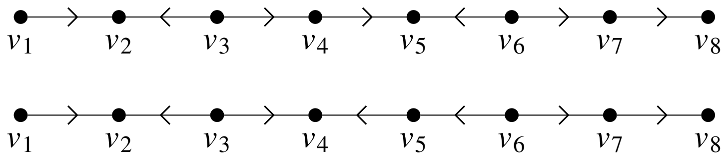


Figure 5.5: Two non-isomorphic oriented paths having the same non-oriented having the same in-out degree sequence and height-profile $(3, 3, 2)$.

proper caterpillars over non-proper caterpillars is that the composition corresponding to proper caterpillars have all parts greater than 1. Therefore the compositions obtained by adding some consecutive components must also have all parts greater than 1. From Observation 5.5(b), it follows that the non-monochromatic edges of the colorings of these type always lie on the spine. This avoids the conflict arising due to the involvement of the pendant vector while retrieving the spine. With this, we begin with reconstructing the spine of the proper caterpillars.

For the sake of brevity, we denote the multiset $\{a_{ij} \cdot y^i z^j \mid i, j \in \mathbb{N}\}$ where a_{ij} is the multiplicity of the monomial $y^i z^j$.

Proposition 5.9. *The orientation of the spine of oriented proper caterpillars can be reconstructed from their quasisymmetric B-functions.*

Proof. Let $\overrightarrow{C}$ be an orientation of a proper caterpillar C such that $\text{Comp}(C) = (\alpha_1, \alpha_2, \ldots, \alpha_\ell)$ is lexicographically smaller than its reverse. Let θ be the least positive integer (if exists) such that $B_{\theta,\theta'}$ is uni-directed. In the first step of the proof, we use $B_{\theta,\theta'}$ as our pivot to determine whether the other bilateral sets are oriented in the same direction as $B_{\theta,\theta'}$ or not. In the second step, we aim to determine the direction of this $B_{\theta,\theta}$, which will in turn discern the orientation of every other uni-directional bilateral set. Let π be the least positive integer (if exists) such that the edge $\{v_\pi, v_{\pi+1}\}$ is not a bilateral edge. The choice of $\text{Comp}(C)$ being lexicographically smaller than its reverse implies $L_\pi \leq \lfloor |V/2| \rfloor$. Since the orientation of the non-uni-directed bilateral sets is determined by quasisymmetric B-function (from

Proposition 5.7), the orientation of edge $\{v_\pi, v_{\pi+1}\}$ in $\overrightarrow{C}$ is known. This arc acts as our pivot in the second step to determine the orientation of the uni-directed bilateral set $B_{\theta,\theta'}$.

Any two uni-directed bilateral sets of $\overrightarrow{C}$ are said to be in *unison* if either both are left directed or both are right directed.

(Step I): We proceed by induction on $s \in \{L_p \mid B_{p,p'} \text{ is uni-directed}, p \geq \theta, p' \geq \theta'\}$. Suppose that for all $q < p$ and $q' < p'$, we know whether $B_{q,q'}$ is in unison with $B_{\theta,\theta'}$ are not. To determine the direction of $B_{p,p'}$, we consider the surjective 3-colorings whose non-monochromatic arcs belong to $B_{p,p'}$ or $B_{\theta,\theta'}$. In particular, to have

$$\big\{\{v_\theta, v_{\theta+1}\}, \{v_p, v_{p+1}\}\big\} \text{ or } \big\{\{v_{\ell-\theta'}, v_{\ell-\theta'+1}\}, \{v_{\ell-p'}, v_{\ell-p'+1}\}\big\}. \tag{5.7}$$

as non-monochromatic edges, the natural choice would be to consider the colorings such that removal of their non-monochromatic edges results in connected components of order $L_\theta, L_p - L_\theta$ and $|V| - L_p$. While doing so, we may encounter some other colorings in this set. However by induction hypothesis, the orientations of the non-monochromatic edges of these intermediary colorings are already known. The occurrence of the intermediary arcs is based on whether $L_p - L_\theta$ occurs as a partial sum of parts of $\mathrm{Comp}(C)$. The proof follows from the case-by-case analysis of the non-monochromatic arcs of these intermediary colorings. We accomplish this by considering set of colorings $F_C(L_\theta, L_p - L_\theta, |V| - L_p)$ or $F_C(L_\theta, |V| - L_p, L_p - L_\theta)$. We show that for each possible orientation of intermediary arcs, the multisets associated with the unison of $B_{p,p'}$ and $B_{\theta,\theta'}$ differs from the case when they are not in unison. If none of the partial sum of the parts equal $L_p - L_\theta$, then

$$\mathrm{Mon}_2(L_\theta, |V| - L_p, L_p - L_\theta) = \begin{cases} \{2yz\} & \text{if } B_{p,p'} \text{ and } B_{\theta,\theta'} \text{ are in unison,} \\ \{y^2, z^2\} & \text{otherwise.} \end{cases}$$

(Case 1): $L_p - L_\theta = L_q = R_{q'}$ for some $q \leq p$ and $q' \leq p'$.

The computation of monomials in $\mathrm{Mon}_2(L_\theta, L_p - L_\theta, |V| - L_p)$ and $\mathrm{Mon}_2(L_\theta, |V| -$

Colorings	Spine vertices corresponding to color classes		
	$v_1, \ldots, v_i$	$v_{i+1}, \ldots, v_j$	$v_{j+1}, \ldots, v_\ell$
g_1	1	2	3
f_1	1	3	2
	$v_1, \ldots, v_i$	$v_{i+1}, \ldots, v_{\ell-k'}$	$v_{\ell-k'+1}, \ldots, v_\ell$
g_2	1	3	2
f_2	1	2	3
	$v_1, \ldots, v_k$	$v_{k+1}, \ldots, v_j$	$v_{j+1}, \ldots, v_\ell$
g_3	2	1	3
f_3	3	1	2
	$v_1, \ldots, v_k$	$v_{k+1}, \ldots, v_{\ell-i'}$	$v_{\ell-i'+1}, \ldots, v_\ell$
g_4	2	3	1
f_4	3	2	1
	$v_1, \ldots, v_{\ell-j'}$	$v_{\ell-j'+1}, \ldots, v_{\ell-k'}$	$v_{\ell-k'+1}, \ldots, v_\ell$
g_5	3	1	2
f_5	2	1	3
	$v_1, \ldots, v_{\ell-j'}$	$v_{\ell-j'+1}, \ldots, v_{\ell-i'}$	$v_{\ell-i'+1}, \ldots, v_\ell$
g_6	3	2	1
f_6	2	3	1

Table 5.1: Set of colorings $F_C(L_i, L_j - L_i, |V| - L_j) = \{g_1, g_2, \ldots, g_6\}$ and $F_C(L_i, |V| - L_i, L_j - L_i) = \{f_1, f_2, \ldots, f_6\}$ where $L_i = R_{i'}$, $L_j = R_{j'}$ and $L_j - L_i = L_k = R_{k'}$.

$L_p, L_p - L_\theta)$ in accordance with Table 5.1 (where $i = \theta, j = p$ and $k = q$) lead to the following. In the first three rows of the following computation table, we calculate the multiset $\mathrm{Mon}_2(L_\theta, L_p - L_\theta, |V| - L_p)$, while the last row represents the multiset $\mathrm{Mon}_2(L_\theta, |V| - L_p, L_p - L_\theta)$.

Orientation of $B_{q,q'}$	$B_{p,p'}$ is in unison with $B_{\theta,\theta'}$	$B_{p,p'}$ is not in unison with $B_{\theta,\theta'}$
inward directed	$\{2y^2, 2yz, 2z^2\}$	$\{y^2, 4yz, z^2\}$
outward directed	$\{2y^2, 2yz, 2z^2\}$	$\{y^2, 4yz, z^2\}$
not in unison with $B_{\theta,\theta'}$	$\{3y^2, 3z^2\}$	$\{y^2, 4yz, z^2\}$
unison with $B_{\theta,\theta'}$	$\{y^2, 4yz, z^2\}$	$\{3y^2, 3z^2\}$

(Case 2): Either $L_p - L_\theta$ is equal to L_p for some $q \le p$, or $R_{q'}$ for some $q' \le p'$ (but not both).

Apart from (5.7), the other non-monochromatic edges of the colorings in $F_C(L_\theta, |V| - L_p, L_p - L_\theta)$ are

$$\begin{array}{ll} \big\{\{v_q, v_{q+1}\}, \{v_p, v_{p+1}\}\big\}, \big\{\{v_q, v_{q+1}\}, \{v_{\ell-\theta'}, v_{\ell-\theta'+1}\}\big\} & \text{if } L_p - L_\theta = L_q, \\ \big\{\{v_{\ell-q'}, v_{\ell-q'+1}\}, \{v_p, v_{p+1}\}\big\}, \big\{\{v_{\ell-q'}, v_{\ell-q'+1}\}, \{v_{\ell-\theta'}, v_{\ell-\theta'+1}\}\big\} & \text{if } L_p - L_\theta = R_{q'}. \end{array}$$

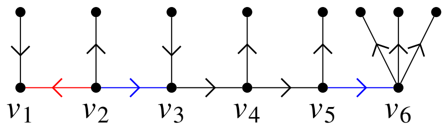
Therefore, when $v_q v_{q+1}$ or $v_{\ell-q'+1} v_{\ell-q'}$ occur in $\overrightarrow{C}$, we have

$$\mathrm{Mon}_2(L_\theta, |V| - L_p, L_p - L_\theta) = \begin{cases} \{3yz, z^2\} & \text{if } B_{p,p'} \text{ and } B_{\theta,\theta'} \text{ are in unison,} \\ \{y^2, yz, 2z^2\} & \text{if } B_{p,p'} \text{ and } B_{\theta,\theta'} \text{ are not in unison.} \end{cases}$$

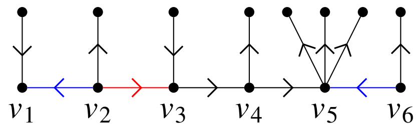
Otherwise if $v_{q+1} v_q$ or $v_{\ell-q'} v_{\ell-q'+1}$ occur in $\overrightarrow{C}$, we get

$$\mathrm{Mon}_2(L_\theta, |V| - L_p, L_p - L_\theta) = \begin{cases} \{y^2, 3yz\} & \text{if } B_{p,p'} \text{ and } B_{\theta,\theta'} \text{ are in unison,} \\ \{2y^2, yz, z^2\} & \text{if } B_{p,p'} \text{ and } B_{\theta,\theta'} \text{ are not in unison.} \end{cases}$$

Since the multiset associated with the unison of $B_{p,p'}$ and $B_{\theta,\theta'}$ are distinct from the case when they are not in unison,we conclude that the uni-directed bilateral arcs that are in



(a) A semi-symmetric orientation with pivot v_2v_1 and uni-directed bilateral sets $B_{2,1}$ and $B_{3,2}$.



(b) A semi-symmetric orientation with pivot v_2v_3 and uni-directed bilateral sets $B_{1,1}$ and $B_{3,2}$.

Figure 5.6: Proper caterpillars with associated compositions (a) (2,2,2,2,2,4) and (b) (2,2,2,2,4,2).

unison with $B_{\theta,\theta'}$ can be determined from the quasisymmetric B-function.

Note that if the underlying proper caterpillar C is palindromic, then every edge is a bilateral edge. Therefore, by assuming $B_{\theta,\theta'}$ being right directed, we are fixing an orientation from the isomorphism class of $\overrightarrow{C}$, and the direction of every other bilateral set in this orientation can be determined. Thus, if $\mathrm{Comp}(C)$ is a palindrome, then orientation of spine can be reconstructed from (Step I). We now proceed to determine the direction of $B_{\theta,\theta'}$ when the underlying composition is not a palindrome.

(Step II): The direction of $B_{\theta,\theta'}$ is discerned by comparing it with the orientation of the pivot non-bilateral edge $\{v_\pi, v_{\pi+1}\}$. Note that the edge $\{v_\pi, v_{\pi+1}\}$ may occur either before or after the bilateral edge $\{v_\theta, v_{\theta+1}\}$ on the spine (see Figure 5.6), that is, either $\pi < \theta$ (in the former scenario) or $\pi > \theta$ (in the latter scenario).

For $\pi < \theta$, the computations are based on the Table 5.1 with $i = \pi$, $j = \theta$ and $k = q$.

(Case 1.a): Suppose $\pi < \theta$, and $L_\theta - L_\pi$ is not a partial sum of components of $\mathrm{Comp}(C)$. The multiset $\mathrm{Mon}_2(L_\pi, |V| - L_\theta, L_\theta - L_\pi)$ contains a unique monomial contributed by the coloring with non-monochromatic edge set $\big\{\{v_\pi, v_{\pi+1}\}, \{v_\theta, v_{\theta+1}\}\big\}$. From Table 5.1, we conclude that

$$\mathrm{Mon}_2(L_\pi, |V| - L_\theta, L_\theta - L_\pi) = \begin{cases} \{y^2\} & \text{if } v_\pi v_{\pi+1} \in A \text{ and } B_{\theta,\theta'} \text{ is right directed,} \\ \{z^2\} & \text{if } v_{\pi+1} v_\pi \in A \text{ and } B_{\theta,\theta'} \text{ is left directed,} \\ \{yz\} & \text{otherwise.} \end{cases}$$

(Case 1.b): Let $L_\theta - L_\pi$ be either L_q or $R_{q'}$ (but not both) for some $1 \le q \le \theta$ and $1 \le q' \le \theta'$.

The distinctness of the multiset $\mathrm{Mon}_2(L_\pi, |V| - L_\theta, L_\theta - L_\pi)$ is exhibited in the respective scenarios by the following:

	$v_\pi v_{\pi+1}$		$v_{\pi+1} v_\pi$	
$B_{\theta,\theta'}$	right directed	left directed	right directed	left directed
$v_q v_{q+1}$	$\{2yz\}$	$\{2y^2\}$	$\{yz, z^2\}$	$\{y^2, yz\}$
$v_{q+1} v_q$	$\{yz, z^2\}$	$\{y^2, yz\}$	$\{2z^2\}$	$\{2yz\}$
$v_{\ell-q'} v_{\ell-q'+1}$	$\{y^2, 2yz\}$	$\{3y^2\}$	$\{2yz, z^2\}$	$\{y^2, 2yz\}$
$v_{\ell-q'+1} v_{\ell-q'}$	$\{2yz, z^2\}$	$\{y^2, 2yz\}$	$\{3z^2\}$	$\{2yz, z^2\}$

where the first two rows and the last two rows corresponds to $L_\theta - L_\pi$ being L_q or $R_{q'}$, respectively.

(Case 1.c): Let $L_\theta - L_\pi = L_q = R_{q'}$ for some $1 \le q \le \theta$ and $1 \le q' \le \theta'$.

By the choice of $B_{\theta,\theta'}$ (least uni-directed bilateral set), the bilateral sets $B_{q,q'}$ must be either inward directed or outward directed. The monomials computed using Table 5.1 gives the following:

	$v_\pi v_{\pi+1}$		$v_{\pi+1} v_\pi$	
$B_{q,q'}$ \ $B_{\theta,\theta'}$	right directed	left directed	right directed	left directed
inward directed	$\{3yz, z^2\}$	$\{y^2, 2yz, z^2\}$	$\{yz, 3z^2\}$	$\{2yz, 2z^2\}$
outward directed	$\{2y^2, 2yz\}$	$\{3y^2, yz\}$	$\{2yz, 2z^2\}$	$\{y^2, 3yz\}$

where the the multiset $\mathrm{Mon}_2(L_\theta, |V| - L_\pi, L_\pi - L_\theta)$ is computed corresponding to the orientation of $B_{q,q'}, B_{\theta,\theta'}$ and $\{v_\pi, v_{\pi+1}\}$. This concludes that the direction of $B_{\theta,\theta'}$ can be reconstructed when the pivot arc $\{v_\pi, v_{\pi+1}\}$ occurs before the bilateral set $B_{\theta,\theta'}$.

We now proceed with the final case, that is $\theta < \pi$. The monomials are computed using Table 5.1 with $i = \theta, j = \pi$ and $k = q$.

(Case 2.a): If $L_\pi - L_\theta$ is not equal any partial sum, then the multisets $\mathrm{Mon}_2(L_\theta, |V| - L_\pi, L_\pi - L_\theta)$ is the same as (Case 1.a) with the roles of θ and π interchanged.

(Case 2.b): Suppose $L_\pi - L_\theta = L_q = R_{q'}$ for some $1 \leq q \leq \pi$ and $1 \leq q' \leq \pi'$. We resolve this case pertaining to the orientation of the bilateral set $B_{q,q'}$. The colorings from the first four rows of Table 5.1 contribute the monomials occurring in the multisets.

	$v_\pi v_{\pi+1}$		$v_{\pi+1} v_\pi$	
$B_{q,q'}$ \ $B_{\theta,\theta'}$	right directed	left directed	right directed	left directed
inward directed	$\{3yz, z^2\}$	$\{2yz, 2z^2\}$	$\{y^2, yz, 2z^2\}$	$\{2yz, 2z^2\}$
outward directed	$\{2y^2, 2yz\}$	$\{2y^2, yz, z^2\}$	$\{2y^2, 2yz\}$	$\{y^2, 3yz\}$
unison with $B_{\theta,\theta'}$	$\{y^2, 2yz, z^2\}$	$\{2y^2, 2z^2\}$	$\{2y^2, yz, z^2\}$	$\{y^2, 2yz, z^2\}$
not in unison with $B_{\theta,\theta'}$	$\{3y^2, z^2\}$	$\{y^2, 2yz, z^2\}$	$\{y^2, 2yz, z^2\}$	$\{y^2, 3z^2\}$

where the multiset $\mathrm{Mon}_2(L_\theta, |V| - L_\pi, L_\pi - L_\theta)$ is computed for the first three rows, and the last row corresponds to the multiset $\mathrm{Mon}_2(L_\theta, L_\pi - L_\theta, |V| - L_\pi)$.

For fixed orientations of $\{v_\pi, v_{\pi+1}\}$ and $B_{q,q'}$, the multisets corresponding to $B_{\theta,\theta'}$ being right directed and left directed are distinct. Therefore the orientation of $B_{\theta,\theta'}$ can be reconstructed. This completes the proof. ■

The following corollary is an immediate consequence of the above proposition.

Corollary 5.2. *The orientations of paths can be reconstructed from their quasisymmetric*

B-function up to isomorphism.

Proof. We associate the integer composition $(1, 1, \ldots, 1)$ of length $|V|$ to the oriented path $\overrightarrow{P}(V, A)$. The orientations of the bilateral sets $B_{p,p}$ for $p = 1, 2, \ldots, \lfloor |V|/2 \rfloor$ can be obtained from (5.6) up to uni-direction. The method for determining the uni-directed bilateral sets is identical to the (Step I) in the proof of Theorem 5.11. ■

5.3.2 semi-symmetric orientations of proper caterpillars

Even though the non-uni-directed bilateral sets are straightforward to determine from the quasisymmetric B-function, they cause hindrance in recovering the pendant vectors (see Figure 5.8). This imposes the constraint of considering orientations of proper caterpillars in which certain pendant vectors corresponding to inward and outward directed bilateral sets exhibit symmetry.

Definition 5.10. Let C be a proper caterpillar. An orientation $\overrightarrow{C}$ is said to be *semi-symmetric* if for every inward and outward directed bilateral set $B_{p,p'}$, the pendant vectors $P(v_p)$ and $P(v_{\ell-p'+1})$ are equal. We denote the set of isomorphism classes of semi-symmetric orientation of C by $\bar{O}(C)$.

The oriented proper caterpillar in Figure 5.3 is a semi-symmetric orientation, whereas the oriented caterpillars in Figure 5.8 are not. We now prove that the pendant vectors in semi-symmetric orientations of proper caterpillars can be retrieved from the quasisymmetric B-function.

Theorem 5.11. *The semi-symmetric orientations of proper caterpillars can be distinguished by their quasisymmetric B-functions.*

Proof. We have already established the reconstruction of spine in Proposition 5.9. It suffices to prove that the pendant vectors in semi-symmetric orientations can be determined by their quasisymmetric B-function. Let $\overrightarrow{C}$ be a semi-symmetric orientation of a proper caterpillar C. The idea involves consideration of in-out degree sequence of the digraph, and surjective 3-colorings whose non-monochromatic edges comprise of one spine edge and one pendant edge. In particular, we are examining the multiset $\mathrm{Mon}(1, |V| - 1)$, and colorings in which the deletion of non-monochromatic edges leads to connected components of sizes either $1, L_p - 1$ and $|V| - L_p$, or $1, R_{p'} - 1$ and $|V| - R_{p'}$.

We prove by induction on $s \in \left\{L_p, R_{p'} \mid 2 \leq L_p, R_{p'} \leq \lfloor |V|/2 \rfloor \text{ and } p, p' \geq 1\right\}$ where the $\mathrm{Comp}(C)$ is lexicographically smaller than its reverse. We prove the base step by using the multiset $\mathrm{Mon}_2(1, |V| - 1)$ that encodes the in-out degree sequence of the vertices of degree 2 (see (5.2)). For the base step $s = 2$, we have either $s = L_1 \neq R_1$ or $s = L_1 = R_1$. In the former scenario, v_1 is the unique vertex of degree 2 in C, and therefore the multiset

$$\mathrm{Mon}_2(1, |V| - 1) = \begin{cases} \{y^2\} & \text{iff } v_1 v_2 \in A \text{ and } P(v_1) = (1, 0), \\ \{z^2\} & \text{iff } v_2 v_1 \in A \text{ and } P(v_1) = (0, 1), \\ \{yz\} & \text{otherwise.} \end{cases}$$

In the latter case, v_1 and v_ℓ are the only vertices of degree 2, and we have four possibilities for the orientation of $B_{1,1}$. The following computation table depicts that in all four cases, the multiset $\mathrm{Mon}_2(1, |V| - 1)$ containing the in-out degree sequence of v_1 and v_ℓ distinguishes the occurrences of the pendant vectors of $P(v_1)$ and $P(v_\ell)$ in semi-symmetric orientations.

Orientation of bilateral set $B_{1,1}$								
right directed		left directed		inward directed		outward directed		$\mathrm{Mon}_2(1, \lvert V\rvert - 1)$
$P(v_1)$	$P(v_\ell)$	$P(v_1)$	$P(v_\ell)$	$P(v_1)$	$P(v_\ell)$	$P(v_1)$	$P(v_\ell)$	
$(1,0)$	$(0,1)$	$(0,1)$	$(1,0)$					$\{y^2, z^2\}$
$(1,0)$	$(1,0)$	$(1,0)$	$(1,0)$					$\{y^2, yz\}$
$(0,1)$	$(0,1)$	$(0,1)$	$(0,1)$					$\{yz, z^2\}$
$(0,1)$	$(1,0)$	$(1,0)$	$(0,1)$	$(0,1)$	$(0,1)$	$(1,0)$	$(1,0)$	$\{2yz\}$
				$(1,0)$	$(1,0)$			$\{2y^2\}$
						$(0,1)$	$(0,1)$	$\{2z^2\}$

Assume by induction that we already have the knowledge of the pendant vectors $P(v_q)$ and $P(v_{\ell-q'+1})$ for $L_q, R_{q'} < s$. Now, consider the case where $s = L_p = R_{p'}$. According to Observation 5.5, we deduce that the set of non-monochromatic edges of the colorings in $F_C(s-1, |V|-s, 1)$ are $\big\{\{v_p, v_{p+1}\}, \{v_q, u_{qi}\}\big\}$ or $\big\{\{v_{\ell-p}, v_{\ell-p+1}\}, \{v_{\ell-q'+1}, u_{\ell-q'+1\,i}\}\big\}$ for $q = 1, 2, \ldots, p$ and $q' = 1, 2, \ldots, p'$. Let $[y^2]$, $[z^2]$ and $[yz]$ denote the multiplicity of y^2, z^2 and yz in $\mathrm{Mon}_2(s-1, |V|-s, 1)$ respectively. Then, the partial sums of pendant vectors are given by:

$$\sum_{k=1}^{p} P(v_k) = \begin{cases} ([y^2], s-p-[y^2]) & \text{if } B_{p,p'} \text{ is right directed,} \\ (s-p-[z^2], [z^2]) & \text{if } B_{p,p'} \text{ is left directed.} \end{cases} \tag{5.8}$$

$$\sum_{k=1}^{p'} P(v_{\ell-k+1}) = \begin{cases} (s-p'-[z^2], [z^2]) & \text{if } B_{p,p'} \text{ is right directed,} \\ ([y^2], s-p'-[y^2]) & \text{if } B_{p,p'} \text{ is left directed.} \end{cases} \tag{5.9}$$

$$\sum_{k=1}^{p} P(v_k) + \sum_{k=1}^{p'} P(v_{\ell-k+1}) = \begin{cases} ([y^2], [yz]) & \text{if } B_{p,p'} \text{ is inward directed,} \\ ([yz], [z^2]) & \text{if } B_{p,p'} \text{ is outward directed.} \end{cases} \tag{5.10}$$

This implies that we can determine both $P(v_p)$ and $P(v_{\ell-p'+1})$ when $B_{p,p'}$ is uni-directed. On the other hand, if $\{v_p, v_{p+1}\}$ and $\{v_{\ell-p'}, v_{\ell-p'+1}\}$ are not bilateral edges, then (5.8) and (5.9) can be used to derive the pendant vectors of $P(v_p)$ and $P(v_{\ell-p'+1})$ as well. However, when $B_{p,p'}$ is not uni-directed, we can extract $P(v_p)+P(v_{\ell-p'+1})$, and therefore compute the pendant vectors of both vertices v_p and $v_{\ell-p'+1}$ when $\overrightarrow{C}$ is a semi-symmetric orientation. Note that if $|V|/2 \notin \{L_p\}_{p=1}^{\ell}$, then there exist a unique spine vertex v_t such that $L_{t-1} \leq \lfloor |V|/2 \rfloor < L_t$ (For example, in Figure 5.3, the partial sum $L_3 \leq 8 < L_4$). The equations mentioned above cover the computation of all pendant vectors except for $P(v_t)$. Nonetheless, we can determine this pendant vector by subtracting $\sum_{k\in[\ell]\setminus\{t\}} I_k$ and $\sum_{k\in[\ell]\setminus\{t\}} O_k$ from the multiplicity of y and z in the degree multiset $\mathrm{Mon}(1, |V|-1)$, respectively. Thus, the orientation of $\overrightarrow{C}$ can be reconstructed from the quasisymmetric B-function up to isomorphism. ■

The above theorem and the result that caterpillars are reconstructible from their chromatic symmetric function, leads us to the following.

Corollary 5.3. *The semi-symmetric orientations of proper caterpillars can be reconstructed by their quasisymmetric B-functions.*

5.3.3 Asymmetric proper caterpillars.

Recall the Definition 5.4(b) of asymmetric proper caterpillars, which dictates that the components of their associated composition must be distinct. We show that all oriented asymmetric proper caterpillars can be reconstructed from their quasisymmetric B-functions. We use the fact that no more than two pairs of non-pendant vertices can have the same degree. Consequently, we can sequentially compute the pendant vectors by removing the terms contributed by the spine arcs connected to each spine vertex.

Theorem 5.12. *The quasisymmetric B-function distinguishes orientations of proper caterpillars up to isomorphism.*

Proof. Without loss of generality, we assume that $\mathrm{Comp}(C) = (\alpha_1, \alpha_2, \ldots, \alpha_\ell)$ is lexicographically smaller than its reverse. For $i = 1, 2, \ldots, \ell$, let h_i be the coloring in

$F_C(1, |V| - 1)$ that assigns the unique color 1 to the spine vertex v_i. Thus, we have

$$m_{h_i} := y^{asc(h_i)} z^{dsc(h_i)} = y^{\text{outdegree of } v_i} z^{\text{indegree of } v_i} \tag{5.11}$$

From Proposition 5.9, the orientation of spine of $\overrightarrow{C}$ is known. This implies that the above monomials can be computed from the pendant vector of the vertices. On the other hand, the internal vertices can be identified with their unique corresponding monomials due to the equality of degree, and the pendant vector of such vertices can be retrieved by the following:

$$P(v_i) = \begin{cases} \left(\deg_y \dfrac{m_{h_i}}{y^2}, \deg_z \dfrac{m_{h_i}}{y^2}\right) & \text{if } v_i v_{i-1},\ v_i v_{i+1} \in A, \\ \left(\deg_y \dfrac{m_{h_i}}{z^2}, \deg_z \dfrac{m_{h_i}}{z^2}\right) & \text{if } v_{i-1} v_i,\ v_{i+1} v_i \in A, \\ \left(\deg_y \dfrac{m_{h_i}}{yz}, \deg_z \dfrac{m_{h_i}}{yz}\right) & \text{otherwise.} \end{cases} \tag{5.12}$$

Due to asymmetry of the caterpillar, all the monomials in $\mathrm{Mon}(1, |V| - 1) \setminus \{m_{h_1}, m_{h_\ell}\}$ have distinct total degrees. Consequently, we can easily identify the corresponding internal vertices and compute their pendant vectors using (5.12). Therefore it suffices to compute the pendant vertices $P(v_1)$ and $P(v_\ell)$. Note that $\alpha_1 \neq \alpha_\ell$ implies that $\{v_1, v_2\}$ is not a bilateral edge, allowing us to compute $P(v_1)$ from Theorem 5.11. Furthermore, the pendant vector for $P(v_\ell)$ can be determined using Theorem 5.11, except when a non-uni-directed bilateral set $B_{k,1}$ exists. However, when there exists a non-uni-directed bilateral set $B_{k,1}$, we use (5.10) to determine the partial sum $P(v_\ell) + \sum_{i=1}^{k} P(v_i)$. Since the $P(v_1)$ is known, and the degree of the internal vertices $v_2, v_3, \ldots, v_k$ are less than $\deg(v_\ell)$, their corresponding monomials in $\mathrm{Mon}(1, |V| - 1) \setminus \{m_{h_1}\}$ can be identified. This enables us to compute the pendant vectors of the internal vertices $v_2, v_3, \ldots, v_k$, and as a result, the pendant vector $P(v_\ell)$ can be computed as well. This completes the proof. ∎

Particularly for the asymmetric proper caterpillars, we obtain the following.

Corollary 5.4. *Let $\overrightarrow{C}(V, A)$ be an oriented asymmetric proper caterpillar. Then $\overrightarrow{C}$ can be reconstructed from its quasisymmetric B-function up to isomorphism.*

5.4 DISTINGUISHING ORIENTATIONS OF PROPER Q-CATERPILLARS

We proved in Chapter 3 that the chromatic symmetric function distinguishes proper q-caterpillars, for $q \geq 2$. We now employ the methods from Section 5.3 to show that certain orientations of proper q-caterpillars can be distinguished by their quasisymmetric B-functions.

Recall that for $q \geq 2$, a q-caterpillar is a tree containing a path $S = \langle v_1, \dots, v_\ell \rangle$ (with endpoints v_1 and v_ℓ) called the spine, with $\ell > 0$ and paths of length exactly q glued to the spine vertices v_i. These q-length paths are called as the *branches* of the q-caterpillar. Further, a q-caterpillar is said to *proper* if every vertex of the spine is adjacent to at least one branch.

For a proper q-caterpillar C, with spine $\langle v_1, v_2, \dots, v_\ell \rangle$, let $p_1, p_2, \dots, p_\ell$ be the number of branches glued to the vertices $v_1, v_2, \dots, v_\ell$, respectively. Let $\mathrm{Comp}(C)$ be the integer composition $(qp_1 + 1, qp_2 + 1, \dots, qp_\ell + 1)$ associated to C for $i = 1, 2, \dots, \ell$. The notion of the partial sums and the bilateral sets defined associated with proper caterpillars in Section 5.3 extends canonically to the proper q-caterpillars.

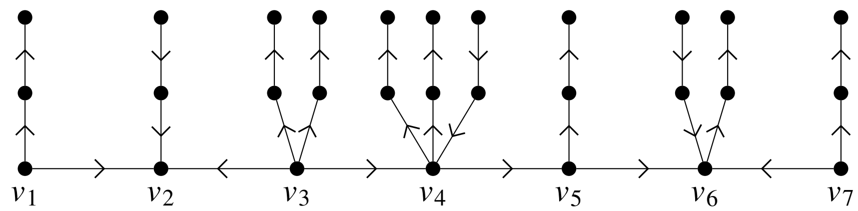


Figure 5.7: An admissible orientation of proper 2-caterpillar with associated composition $(3, 3, 5, 7, 3, 5, 3)$.

We restrict ourselves to orientations of proper q-caterpillars wherein the branches are directed paths.

Definition 5.13 (*Admissible orientation)***.** An orientation of a proper q-caterpillar is said to be *admissible* if each branch is either oriented towards the spine or away from the spine. That is, each branch is a directed path.

For example, Figure 5.7 is an admissible orientation of a proper 2-caterpillar. For an admissible orientation of proper q-caterpillar $\overrightarrow{C}$ and its spine vertex v_k, let O_k and I_k denote the number of outgoing and incoming directed branches incident on v_k. The *path vector* of the spine vertex v_k is the tuple $P(v_k) := (O_k, I_k)$. For instance, the path vector of the spine vertex v_6 in Figure 5.3 is $(1, 1)$. Similar to the proper caterpillars, any admissible orientation of a fixed q-caterpillar C is uniquely determined by (a) the orientation of the spine $\langle v_1, v_2, \ldots, v_\ell \rangle$, and (b) the path vector $P(v_k)$ of each spine vertex v_k.

Proposition 5.14. *Let $C(V, A)$ be an oriented proper q-caterpillar. Then the orientation of the spine can be determined by the quasisymmetric B-function.*

Proof. The proof is verbatim to the proof of Proposition 5.9. ∎

An admissible orientation of proper q-caterpillars is said to be *semi-symmetric* if for every inward or outward directed bilateral set $B_{p,p'}$, the path vectors (O_p, I_p) and $(O_{\ell-p'+1}, I_{\ell-p'+1})$ are equal, where ℓ is the length of the spine.

The methods involved in recovering the path vectors are almost similar to that of determining the pendant vectors of proper caterpillars. The key difference lies in determining the path vectors of the end vertices of the spine. Recall that we used the degree 2 monomials from the multiset of in-out degree of the vertices, which corresponded to the end vertices v_1 and v_ℓ. However, for $q \geq 2$, the proper q-caterpillars have more than two vertices of degree 2. We observe that in an admissible orientation of proper q-caterpillars, the non-spine vertices of degree 2 have exactly one in-degree and one out-degree. Thus, they contribute yz to the degree multiset $\mathrm{Mon}_2(1, |V| - 1)$. We

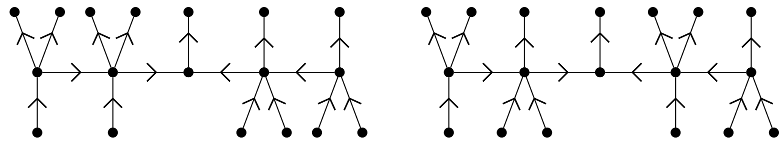


Figure 5.8: Two non-isomorphic graphs having same in-out degree sequence, height-profile and aforementioned statistics.

purge the contribution of the non-spine vertices of degree 2 as follows:

$$\widetilde{\mathrm{Mon}}_2(1, |V| - 1) := \mathrm{Mon}_2(1, |V| - 1) \setminus \left\{ (\sum_{i=1}^{\ell} (q-1) p_i) \cdot yz \right\}.$$

With this minor adjustment, the path vectors of semi-symmetric admissible orientations can be retrieved from the quasisymmetric function. Thus, we have the following.

Theorem 5.15. *The semi-symmetric admissible orientations of proper q-caterpillars can be distinguished by their quasisymmetric B-functions.*

Proof. The proof is the same as the proof of Theorem 5.11, wherein $\mathrm{Mon}_2(1, |V| - 1)$ is replaced by $\widetilde{\mathrm{Mon}}_2(1, |V| - 1)$. ■

5.5 CONCLUDING REMARKS

We showed that degree 2 monomials of certain subjective 3-colorings are sufficient for distinguishing semi-symmetric orientations of proper caterpillars. However, the statistics discussed in Section 5.3 are insufficient to distinguish non-semi-symmetric orientations. The Figure 5.8 exhibits two non-isomorphic oriented proper caterpillars for which the statistics discussed in the proofs of Theorem 5.11 are equal, but their corresponding quasisymmetric B-functions are distinct. Also, we do not know how to distinguish semi-symmetric orientations from the non-semi-symmetric orientations. Nevertheless, we believe that the method to distinguish these two types of orientations will shed light on reconstruction of the non-semi-symmetric orientations. We would like to highlight that the proof was based on examining monomials of degree at most 2 of surjective 3 colorings and the degree multiset. Moreover, the methods used in Proposition 5.9 and Theorem 5.11 can be applied to determine the semi-symmetric orientation of trees in which vertices with a degree of at least 3 induce a path. Computational evidence suggests that the higher degree terms can distinguish the non-semi-symmetric orientations, but providing their combinatorial interpretation with respect to the caterpillar is a tedious task. As mentioned earlier, the challenge in studying non-proper caterpillars lies in dealing with the presence of pendant arcs while investigating the orientation of the spine. However, we hope that one may overcome this obstacle by considering the examination of various coefficients together.

CHAPTER 6

DIGRAPHS WITH EQUAL QUASISYMMETRIC B-FUNCTIONS

Similar to the Tutte polynomial, the B-polynomial satisfies a deletion-contraction relation with respect to a symmetric edge $\{uv, vu\}$. However, this property does not hold for the quasisymmetric B-function, primarily because of its homogeneity in degree $|V|$.

In [14], L. Crew and S. Spirkl introduced the vertex-weighted chromatic symmetric function that satisfies the deletion-contraction property. Additionally, the vertex-weighted Tutte symmetric function was defined, along with exhibiting non-isomorphic graphs with the same Tutte symmetric functions [1].

Applying similar methods, we introduce the vertex-weighted quasisymmetric B-function and showcase certain pairs of digraphs that share the same quasisymmetric B-functions.

6.1 VERTEX-WEIGHTED QUASISYMMETRIC B-FUNCTIONS

Let $D(V, A)$ be a digraph. Let $\omega : V \to \mathbb{P}$ be a map that assigns each vertex of D a positive weight. We call the pair (D, ω) a weighted digraph. We define the quasisymmetric B-function of a weighted digraph as follows:

Definition 6.1. Let (D, ω) be a weighted digraph. The vertex-weighted quasisymmetric B-function is defined as:

$$B_{(D,\omega)}(\mathbf{x}; y, z) := \sum_{f:V\to\mathbb{P}} \left(\prod_{v\in V} x_{f(v)}^{\omega(v)} \right) y^{asc(f)} z^{dsc(f)} \tag{6.1}$$

For $A \subseteq V$, let $|A|_\omega$ denote the sum of weights of the vertices in A. We now present the expansion of the weighted quasisymmetric B-function in the monomial quasisymmetric basis.

Proposition 6.1. *For any weighted digraphs (D,ω),*

$$B_{(D,\omega)}(\mathbf{x};y,z) = \sum_{p=1}^{|V|} \sum_{g\in Surj(V,p)} M_{(|g^{-1}(1)|_\omega,|g^{-1}(2)|_\omega,\dots,|g^{-1}(p)|_\omega)} y^{asc(g)} z^{dsc(g)} \tag{6.2}$$

Proof. Let f be a $\mathbb{P}$-coloring of (D,ω). Let $\tilde{f} := \sigma \circ f$ where $\sigma : f(V) \to [f(V)]$ is an order preserving bijection. Note that $\tilde{f}$ is a surjective $[f(V)]$-coloring, and the ascent and descent sets of $\tilde{f}$ coincide respectively with the ascent and descents of f. ■

Let $e = \{u_1u_2, u_2u_1\}$ be a symmetric arc in a weighted digraph (D,ω). We define the weight $\omega_{\backslash e} := \omega$, and

$$\omega_{/e}(v) := \begin{cases} \omega(v) & \textit{if } v \in V \setminus \{u_1,u_2\} \\ \omega(u_1)+\omega(u_2) & \textit{if } v \textit{ is the vertex obtained by identifying } u_1 \textit{ and } u_2 \end{cases}$$

Proposition 6.2. *Let $D(V,A,\omega)$ be a weighted graph and $e = \{uv, vu\}$ be a pair of opposite arcs. Then*

$$B_{(D,\omega)}(\mathbf{x};y,z) = (yz)B_{(D_{\backslash e},\omega_{\backslash e})}(\mathbf{x};y,z) + (1-yz)B_{(D_{/e},\omega_{/e})}(\mathbf{x};y,z) \tag{6.3}$$

Proof. Consider the vertex-weighted quasisymmetric B-function of (D,ω),

$$\begin{aligned} B_{(D,\omega)}(\mathbf{x};y,z) &= \sum_{f:V\to\mathbb{P}} \left(\prod_{v\in V} x_{f(v)}^{\omega(v)}\right) y^{asc_A(f)} z^{dsc_A(f)} \\ &= \sum_{\substack{f:V\to\mathbb{P} \\ f(u)\neq f(v)}} \left(\prod_{v\in V} x_{f(v)}^{\omega(v)}\right) y^{asc_A(f)} z^{dsc_A(f)} + \sum_{\substack{f:V\to\mathbb{P} \\ f(u)= f(v)}} \left(\prod_{v\in V} x_{f(v)}^{\omega(v)}\right) y^{asc_A(f)} z^{dsc_A(f)} \\ &=(yz) \sum_{\substack{f:V\to\mathbb{P} \\ f(u)\neq f(v)}} \left(\prod_{v\in V} x_{f(v)}^{\omega(v)}\right) y^{asc_{A\backslash e}(f)} z^{dsc_{A\backslash e}(f)} \\ &\quad + \sum_{\substack{f:V\to\mathbb{P} \\ f(u)= f(v)}} \left(\prod_{v\in V} x_{f(v)}^{\omega(v)}\right) y^{asc_A(f)} z^{dsc_A(f)} \end{aligned}$$

$$=(yz)\left(B_{(D_{\setminus e},\omega_{\setminus e})}(\mathbf{x};y,z)-\sum_{\substack{f:V\to\mathbb{P}\\ f(u)=f(v)}}\left(\prod_{v\in V}x_{f(v)}^{\omega(v)}\right)y^{asc_{A\setminus e}(f)}z^{dsc_{A\setminus e}(f)}\right)$$

$$+\sum_{\substack{f:V\to\mathbb{P}\\ f(u)=f(v)}}\left(\prod_{v\in V}x_{f(v)}^{\omega(v)}\right)y^{asc_{A\setminus e}(f)}z^{dsc_{A\setminus e}(f)}$$

$$=(yz)B_{(D_{\setminus e},\omega_{\setminus e})}(\mathbf{x};y,z)+(1-yz)\sum_{\substack{f:V\to\mathbb{P}\\ f(u)=f(v)}}\left(\prod_{v\in V}x_{f(v)}^{\omega(v)}\right)y^{asc_{A\setminus e}(f)}z^{dsc_{A\setminus e}(f)}$$

$$=(yz)B_{(D_{\setminus e},\omega_{\setminus e})}(\mathbf{x};y,z)+(1-yz)B_{(D_{/e},\omega_{/e})}(\mathbf{x};y,z)$$

■

We now define the isomorphism between weighted digraphs.

Definition 6.3. Any two weighted digraphs (D,ω) and (D',ω') are *isomorphic* if there exists a digraph isomorphism $\varphi\colon D\to D'$ satisfying $\varphi(\omega(v))=\omega'(\varphi(v))$, for all $v\in V(D)$.

Observe that (6.3) enables us to construct digraphs with equal vertex-weighted quasisymmetric functions as follows: we can exhibit two non-isomorphic digraphs (D,ω) and (D',ω') such that there exist symmetric edges $e\in A(D)$ and $e'\in A(D')$ satisfying

$$(D\setminus e,\omega\setminus e)\simeq(D'\setminus e',\omega'\setminus e')\text{ and }(D/e,\omega/e)\simeq(D'/e',\omega'/e').$$

In particular, if ω and ω' map vertices identically to 1, then the above argument implies that D and D' share the same quasisymmetric B-functions.

In [1], Aliste-Prieto et al. presented the non-isomorphic graphs with the same Tutte symmetric function (see Figure 6.1).

Based on the graphs in Figure 6.1 and (6.3), we claim that the digraphs in Figure 6.2 share the same quasisymmetric B-function.

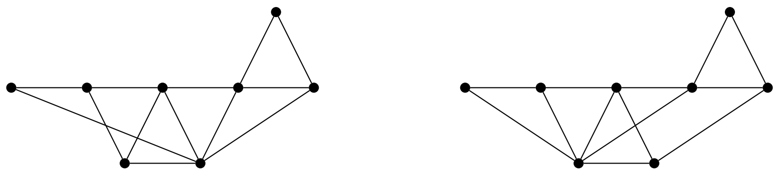
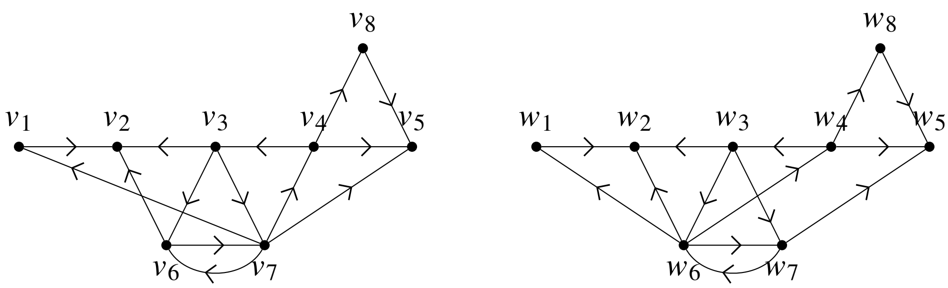


Figure 6.1: Non-isomorphic graphs with equal Tutte symmetric functions.



(a) Digraph D (b) Digraph D'

Figure 6.2: Non-isomorphic digraphs with equal quasisymmetric B-functions.

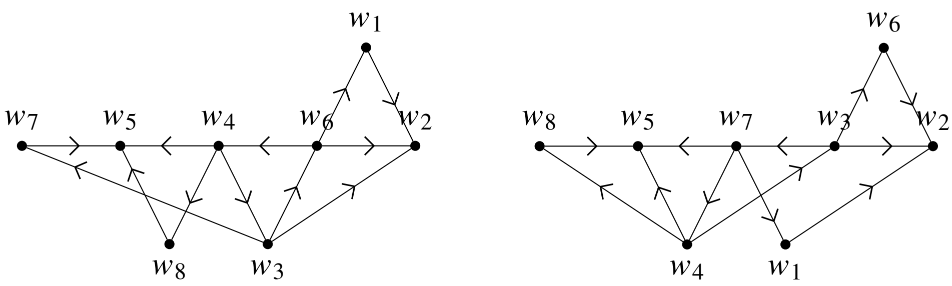
The digraphs D and D' can be considered as weighted digraphs $(D, \mathbf{1})$ and $(D', \mathbf{1})$, respectively, with all vertices assigned weights 1. We prove the equality of their quasisymmetric B-functions by showing that for $e = \{v_6v_7, v_7v_6\}$ and $e' = \{w_6w_7, w_7w_6\}$, the digraphs satisfy $(D \setminus e, \mathbf{1} \setminus e) \simeq (D' \setminus e', \mathbf{1} \setminus e')$ and $(D/e, \mathbf{1}/e) \simeq (D/e', \mathbf{1}/e')$.

It is straightforward to observe that $(D/e, \mathbf{1}/e)$ and $(D/e', \mathbf{1}/e')$ is isomorphic as weighted graphs under the isomorphism $w_i \mapsto v_i$ for all $i = 1, 2, \ldots, 8$. On the other hand, we define a map from $D' \setminus e'$ to $D \setminus e$ as follows:

$$w_1 \mapsto v_8, \qquad w_2 \mapsto v_5, \qquad w_3 \mapsto v_7, \qquad w_4 \mapsto v_3,$$

$$w_5 \mapsto v_2, \qquad w_6 \mapsto v_4, \qquad w_7 \mapsto v_1, \qquad w_8 \mapsto v_6.$$

We illustrate that the map mentioned above is an isomorphism in Figure 6.3 by exhibiting relabeling and redrawing of the graph according to the aforementioned map.



(a) Digraph D with relabeling defined by the isomorphism.

(b) Redrawing the graph D with new labellings.

Figure 6.3: Illustration of isomorphism

Thus, the recurrence relation in Proposition 6.2 can be employed to demonstrate non-isomorphic digraphs with equal quasisymmetric B-functions. Furthermore, (6.3) also provides a subset-sum expansion of the quasisymmetric B-function similar to (4.5).

CHAPTER 7

SUMMARY AND FUTURE DIRECTIONS

While Stanley's tree isomorphism conjecture remains open, our result demonstrates that the ideas presented in [3] can be extended to a more general class of trees that resemble proper caterpillars.

Along this line, we call a tree $T(V, E)$ as a *generalized caterpillar* if the trunk of the tree forms a path. Further, a *generalized proper caterpillar* is a generalized caterpillar in which every vertex of the trunk has degree at least 3. Equivalently, a tree is a generalized proper caterpillar if and only if it satisfies $|T^\circ| = |V| - \delta_1 - \delta_2$, where T° represents the trunk of the tree and δ_i denotes the number of vertices of degree i in T. We believe that further generalizations of Lemma 3.16 might hold for generalized proper caterpillars. In particular, we propose the following question:

Question 7.1. *Do the U-polynomials of generalized proper caterpillars relate to the $\mathcal{L}$-polynomials of the associated integer compositions?*

For instance, consider a tree T obtained from a proper q-caterpillar S by gluing an additional twig of length $q + 1$ at i^{th} vertex of the spine. Let $\varphi'(T)$ be the integer composition obtained from $\varphi(S)$ by replacing the i^{th} component $\varphi(S)_i$ with $\varphi(S)_i + (q+1)$. Then, it can be seen that

$$U_T(\underbrace{0, 0 \ldots, 0}_{q}, x_{q+1}, \ldots) = \mathcal{L}(\varphi'(T); \mathbf{x}) + x_{q+1}\mathcal{L}(\varphi(S); \mathbf{x}).$$

Observe that the U-polynomial of T is expressed as the sum of the $\mathcal{L}$-polynomials of $\varphi(S)$ and $\varphi'(T)$. It turns out that in such cases, Theorem 3.13 cannot be applied directly. Nevertheless, we do believe that distinguishing such trees by U-polynomial is feasible.

For digraphs, we demonstrated that certain orientations of proper q-caterpillars can be distinguished by their quasisymmetric B-functions. Furthermore, for $q = 1$, our methods demonstrate that these orientations can be reconstructed. To the best of our knowledge, the orientations of trees in Theorem 5.11 mark the first instance of trees containing induced 'N' that can be distinguished by their quasisymmetric functions. Since the method primarily relies on the integer compositions associated with the trees, it shows promise for applications to other trees, such as generalized proper caterpillars.

We conclude with the following questions regarding digraphs with equal quasisymmetric B-functions.

Question 7.2. *Does there exist*

(a) infinitely many pairs of non-isomorphic digraph containing a unique directed 2*-cycle and equal quasisymmetric B-function?*

(b) pair of non-isomorphic digraphs without containing a 2*-cycle and equal quasisymmetric B-function?*

APPENDIX A

COMPUTATION USING SAGEMATH

We present the Sagemath code for computing the quasisymmetric B-function in its monomial quasisymmetric basis. The code is primarily derived from the Sagemath code of chromatic quasisymmetric function [47].

Input: A digraph $D(V, A)$

Output: Quasisymmetric B-function of D in monomial quasisymmetric functions.

Code:

```
def quasisymmetric_B_function(D, z=None, y=None, R=None):
# Import QuasisymmetricFunctions and OrderedSetPartitions from the
                                    repository.
    from sage.combinat.ncsf_qsym.qsym import QuasiSymmetricFunctions
    from sage.combinat.set_partition_ordered import
                                        OrderedSetPartitions
# Defining the ring of bivariate polynomials over rational numbers.
    if y is None and z is None and R is None:
        R, (y, z) = PolynomialRing(RationalField(), 2, 'yz').objgens
                                            ()
# Defining ring of quasisymmetric functions over $Q[y,z]$ with family
                                     of monomial quasisymmetric
                                    functions basis.
    M = QuasiSymmetricFunctions(R).M()
    ret = M.zero()
    V = D.vertices()
    A = list(D.edges(labels=False))
# Defining ascents and descents with respect to an ordered partition.
    def asc(sigma):
        stat = 0
        for i, s in enumerate(sigma):
```

```
            for u in s:
                stat += sum(A.count((u,v)) for p in sigma[i+1:] for v in p
                            if D.has_edge(u,v))
        return stat
    def dsc(sigma):
        stat = 0
        for i, s in enumerate(sigma):
            for u in s:
                stat += sum(A.count((v,u)) for p in sigma[i+1:] for v in p
                            if D.has_edge(v,u))
        return stat
# Associating the monomials of ascents and descents of an ordered partition to its corresponding monomial quasisymmetric basis.
    for sigma in OrderedSetPartitions(V):
        ret += M.term(sigma.to_composition(), (y**asc(sigma))*(z**dsc(sigma)))
    return ret
```

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