A Representation of Chemical Reactions by Labeled Graphs

Héctor Hevia
Western Michigan University

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A REPRESENTATION OF CHEMICAL REACTIONS
BY LABELED GRAPHS

by
Héctor Hevia

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A REPRESENTATION OF CHEMICAL REACTIONS
BY LABELED GRAPHS

Héctor Hevia, Ph.D.

Western Michigan University, 1991

Graphs can be used to represent the atomic structure of chemical compounds where the vertices of the graph represent the individual atoms and the edges of the graph represent the valence bonds between a pair of atoms. M. A. Johnson (1991) introduced a graph-theoretic way to represent structural changes in chemical compounds. Thus, certain labelings of graphs called transitional labelings can be thought as representing chemical equations. Associated with these labelings, we introduce a new invariant of a graph $G$ called the transitional value of $G$. The transitional value of a graph $G$ gives an indication of how dramatic a structural change occurs in a chemical reaction represented by a transitional labeling of $G$.

Although the problem of determining the transitional value of an arbitrary graph is open, the transitional values of some families of graphs are determined in Chapters II and III. Chapter II is mainly devoted to the study of the existence of optimal transitional labelings of complete graphs.

Transitional labelings of graphs can be classified as polarizations or quasipolarizations. Complete graphs are the only graphs that do not accept polarizations. Thus, the value of a complete graph is achieved only by means of quasipolarizations. In Chapter III we show the existence of noncomplete graphs whose transitional values are achieved only by quasipolarizations. Using an algorithm, we prove that the situation for trees is the opposite, that is, for any tree $T$, it is always
possible to find an optimal transitional labeling of $T$ that is a polarization. Therefore, graphs are divided into two classes, one containing the trees and the other containing the complete graphs. Another consequence of the aforementioned algorithm is a lower bound for the transitional value of a tree.

Given a transitional labeling $t$ of a graph $G$, three graphs are naturally defined. They are the negative graph of $t$, the positive graph of $t$, and the linking graph of $t$. We begin Chapter IV with a discussion about the existence of transitional labelings with prescribed negative graph, positive graph, and linking graph.

Johnson (1991) introduced a formalism to represent chemical reactions pathways. The main goal of Chapter IV is to present this formalism from another point of view. A particular type of transitional labeling plays a fundamental role in the modeling introduced by Johnson. They are called transforms. We characterize transforms by proving that the concepts of transforms and quasipolarizations are equivalent.

Motivated by ideas developed in Chapter IV, we introduce the concepts of cores and induced cores of a graph in Chapter V and present properties and some related ideas.
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A representation of chemical reactions by labeled graphs

Hevia, Héctor, Ph.D.
Western Michigan University, 1991
To my children
Rocío, Margarita and Héctor
who enlightened my working days
with their joys and love
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Héctor Hevia
# TABLE OF CONTENTS

**ACKNOWLEDGMENTS** ................................................................................................. ii  

**LIST OF TABLES** ........................................................................................................ vi  

**CHAPTER**

I. **INTRODUCTION** ....................................................................................................... 1  
   1.1 Graphs and Chemical Reactions ............................................................................. 1  
   1.2 Basic Definitions and an Introduction to Reaction Digraphs ................................. 7  

II. **TRANSITIONAL VALUES OF GRAPHS** ................................................................. 12  
   2.1 Transitional Values of Complete Graphs ................................................................. 12  
   2.2 An Exceptional Family of Complete Graphs ......................................................... 25  
   2.3 An Additional Result Concerning Optimal Labelings of Complete Graphs .......... 34  

III. **FURTHER RESULTS ON TRANSITIONAL VALUES OF GRAPHS** ....................... 46  
    3.1 Bounds for the Values of Transitional Labelings of Graphs ................................. 46  
    3.2 Transitional Values of Trees ................................................................................. 65  

IV. **A CHEMICAL REACTIONS PATHWAY MODEL** ..................................................... 86  
   4.1 On the Existence of Transitional Labeling With Prescribed Related Graphs .......... 86  
   4.2 Modeling Chemical Reactions Pathways ............................................................... 99  
   4.3 A Characterization of Transforms ......................................................................... 110  

V. **CORES OF GRAPHS** ............................................................................................... 114  
   5.1 Basic Definitions and Results ................................................................................. 114  
   5.2 Core Sequences of Graphs ..................................................................................... 118  

**REFERENCES** ............................................................................................................. 133
LIST OF TABLES

2.1 The Twenty-Five Values of \( p \) for Which \( \mathbb{K}_p \) Has an Optimal Transitional Labeling \( s \) Such That Exactly \( 6 - 1 \) Vertices Are Labeled 0 by \( s \) .......................................................... 33

3.1 Possible Values of \( \kappa(G) \) and \( p \) If \( G \neq \mathbb{K}_p \) Is a Connected Graph for Which \( v_G > v_G^{\ast} \) and \( |G| \leq 66 \) ......................................................... 57
CHAPTER I

INTRODUCTION

1.1 Graphs and Chemical Reactions

The interaction between graph theory and chemistry has been active and fruitful during the past two centuries. One of the earliest applications of graph theory in chemistry (see [2] and [4]) concerns the representation of individual molecules by graphs, where the vertices of the graph are the atoms of the molecule and the edges of the graph represent the valence bonds between a pair of atoms. For example, the methane molecule has the formula \( \text{CH}_4 \). Since carbon atoms and hydrogen atoms have valence +4 and −1, respectively, a methane molecule can be represented by the graph of Figure 1.1, where the central vertex is the carbon atom and the other vertices are the hydrogen atoms.

![Figure 1.1](image)

With this representation, it is possible to show that compounds with the same molecular formula can differ structurally. Compounds having this property are called isomeric compounds. For example, dimethyl ether and ethyl alcohol have the atomic
formula \( C_2H_6O \), even though they have dissimilar chemical properties. The chemical graphs of these compounds are shown in Figure 1.2, where the vertices of degree 2 represent oxygen atoms.

![Chemical graphs of ethyl alcohol and dimethyl ether](image)

Figure 1.2

In [5], Johnson introduced a graph-theoretic way to represent structural changes in chemical compounds. For instance, common salt (NaCl) may be formed by reacting metallic sodium (Na) directly with hydrochloric acid (HCl). This reaction has the atomic equation

\[
2\text{HCl} + 2\text{Na} \rightarrow 2\text{NaCl} + \text{H}_2. \tag{1.1}
\]

The (labeled) chemical graph \( N \) that represents two molecules of HCl and two sodium atoms is shown in Figure 1.3(a). The (labeled) chemical graph \( P \) in Figure 1.3(b) represents two molecules of NaCl and one molecule of H\(_2\). Here we may think of \( N \) representing chemical compounds prior to the reaction (1.1) and \( P \) the resulting chemical compounds following this reaction.

We may interpret the chemical reaction given by the atomic equation (1.1) as a process of deletion and addition of certain vertices and edges in the graph \( N \) in order to produce the graph \( P \). Let us consider the common (labeled) supergraph \( G \) of \( N \).
and $P$ shown in Figure 1.4(a). We label the elements (that is, the vertices and edges) of $G$ in the following way:

(i) elements of $G$ that are common elements of $N$ and $P$ are labeled 0;

(ii) elements of $N$ that are deleted from $N$ to produce $P$ are labeled $-1$; and

(iii) elements of $P$ that are added to $N$ to produce $P$ are labeled 1.

The labeled graph $G$ so obtained (see Figure 1.4(b)) is a graph-theoretic representation of the chemical reaction given by (1.1).

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Another example of representing a chemical reaction by means of a labeled graph is now presented. The hydrocarbon ethylene ($\text{C}_2\text{H}_4$) is a product of the breakdown, or "cracking," of larger hydrocarbon molecules during petroleum refining. Ethylene has many uses in industry and agriculture, but it is also a starting point for a variety of other chemicals with widely different applications. For example, ethylene and water react under suitable chemical conditions producing diethyl ether ($\text{C}_2\text{H}_5\text{OC}_2\text{H}_5$), which is commonly referred to simply as ether. This reaction can be represented by the atomic equation

$$2 \text{C}_2\text{H}_4 + \text{H}_2\text{O} \rightarrow \text{C}_2\text{H}_5\text{OC}_2\text{H}_5. \quad (1.2)$$

In Figure 1.5(a) we show the (labeled) chemical graph $N$ that represents two molecules of ethylene and one molecule of water. The (labeled) chemical graph $P$ shown in Figure 1.5(b) represents one molecule of ether. We observe that the nature of bonds holding carbon atoms together is different in ethylene and ether, even though we simplify them to a single representation.

In order to represent the chemical reaction (1.2), we consider the common (labeled) supergraph $G$ of $N$ and $P$ shown in Figure 1.6(a). As we have previously described, the elements of $N$ that are deleted from $N$ to produce $P$ are labeled $-1$ while the elements of $P$ that are added to $N$ to produce $P$ are labeled $1$. Elements of $G$ that are common elements of $N$ and $P$ are labeled $0$. Thus, we obtain the labeling of $G$ shown in Figure 1.6(b), which is a representation then of the chemical reaction (1.2).

In certain representations of a chemical reaction (called nonstoichiometric representations), some atoms on one side of the chemical equation may not be explicitly represented on the other side of the equation. Thus, under the assumption that atoms from molecules of water do not participate in the atomic balance of the corresponding
Figure 1.5

Figure 1.6

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chemical equation, we may obtain another modeling for this chemical reaction between ethylene and water. In this case we have

\[2 \text{C}_2\text{H}_4 \rightarrow \text{C}_2\text{H}_5\text{OC}_2\text{H}_5.\]  

(1.3)
Here we obtain the (labeled) chemical graphs $N'$ and $P'$ of Figures 1.7(a) and 1.7(b). By using the (labeled) common supergraph $G'$ of $N'$ and $P'$ shown in Figure 1.7(c), we obtain the labeling of $G'$ shown in Figure 1.7(d). This labeling may be considered as a representation of the chemical reaction described by (1.3).

Thus, from these considerations, it is clear that if we have a labeled graph $G$ representing a certain chemical reaction as described above, then edges labeled 0 are incident only with vertices labeled 0. Since additional edges cannot be incident with deleted vertices, and deleted edges cannot be incident with any added vertices, we conclude that negative edges (that is, edges labeled $-1$) are incident only with nonpositive vertices and positive edges are incident only with nonnegative edges.

An important conclusion from the above observations is that the subgraph of $G$ formed by the nonpositive elements of $G$ and the subgraph of $G$ formed by the nonnegative elements of $G$ are well-defined. Actually, these two subgraphs are, respectively, the chemical graphs of the involved compounds before and after the chemical reaction under consideration is realized. In the given examples, these are the graphs $N$ and $P$.

1.2 Basic Definitions and an Introduction to Reaction Digraphs

The basic concepts and terminology in graph theory are taken from [3]. A few more basic definitions are now presented. The cardinality $|G|$ of a graph $G$ is the total number of vertices and edges of $G$. For example, the graphs $G_1$ and $G_2$ shown in Figure 1.8 have cardinality 8 and 9, respectively.

If a graph $H$ is isomorphic to a subgraph of two given graphs $G_1$ and $G_2$, then $H$ is called a common subgraph of $G_1$ and $G_2$. For the graphs $G_1$ and $G_2$ of Figure 1.8, some common subgraphs of $G_1$ and $G_2$ are $K_1$, $K_2$, $4K_1$, $P_3$, $P_4$, and
A maximum common subgraph of two graphs $G_1$ and $G_2$ is a common subgraph of $G_1$ and $G_2$ of maximum cardinality (see [6]). For the graphs $G_1$ and $G_2$ of Figure 1.8, there are exactly two maximum common subgraphs of $G_1$ and $G_2$, namely, $K_{1,3}$ and $P_4$.

![Figure 1.8]

When a chemical reaction is represented by means of a labeled graph $G$ (as we did in the previous section), the graph $L$ formed by the zero elements of $G$ is a common subgraph of the graph $N$ (formed by the nonpositive elements of $G$) and of the graph $P$ (formed by the nonnegative elements of $G$). For example, as we have previously seen, the chemical reaction given by equation (1.2) can be represented by the labeled graph $G$ given in Figure 1.6(b). For this labeling, we show in Figure 1.9 the unlabeled graphs corresponding to the graphs $N, P$, and $L$. It turns out that $L$ is a maximum common subgraph of the graphs $N$ and $P$.

A graph $G$ is a common supergraph of two given graphs $G_1$ and $G_2$ if $G$ contains a subgraph isomorphic to $G_1$ and a subgraph isomorphic to $G_2$. A minimum common supergraph of $G_1$ and $G_2$ is a common supergraph of $G_1$ and $G_2$ having
minimum cardinality. For the graphs $G_1$ and $G_2$ of Figure 1.8, there are exactly two minimum common supergraphs, namely, the graphs shown in Figure 1.10.

Given two subgraphs $G_1$ and $G_2$ of a graph $G$, the union $G_1 \cup G_2$ is the subgraph of $G$ with $V(G_1 \cup G_2) = V(G_1) \cup V(G_2)$ and $E(G_1 \cup G_2) = E(G_1) \cup E(G_2)$. If we further assume that $V(G_1) \cap V(G_2) \neq \emptyset$, we define the intersection $G_1 \cap G_2$ as the subgraph of $G$ with $V(G_1 \cap G_2) = V(G_1) \cap V(G_2)$ and
Figure 1.10

\[ E(G_1 \cap G_2) = E(G_1) \cap E(G_2). \]

Observe that if \( G \) is a minimum common supergraph of the subgraphs \( G_1 \) and \( G_2 \) of \( G \), then the graph \( G_1 \cap G_2 \) is well defined.

In Section 1.1 we described how ether is produced by reacting ethylene and water. Depending on the amount of water that reacts with the ethylene, either ether or ethanol (\( C_2H_5OH \)) can be formed. Indeed, the reaction with water can take place in two stages, namely,

\[ 2C_2H_4 + H_2O \rightarrow C_2H_5OC_2H_5 \] \hspace{1cm} (1.4)

and

\[ C_2H_5OC_2H_5 + H_2O \rightarrow 2C_2H_5OH. \] \hspace{1cm} (1.5)

We may represent these two consecutive reactions by a "reaction digraph" in which the vertices represent chemical compounds and the arcs represent chemical reactions involving these compounds. The first reaction digraphs were proposed by Balaban, Farcasiu and Bûnică in 1966. (See [1].) For example, if \( C_1 \rightarrow C_2 \) and \( C_2 \rightarrow C_3 \) symbolize the chemical equations (1.4) and (1.5), respectively, then the reaction digraph in Figure 1.11 represents the chemical process involved in reacting ethylene and water. Systems of chemical compounds and reactions such as the one described by
(1.4) and (1.5) are called chemical reaction pathways. To simplify the modeling of chemical reaction pathways, we may assume that chemical compounds are represented by unlabeled graphs. Thus, the vertices of the corresponding reaction digraph can be identified by means of unlabeled graphs.

\[ \text{Figure 1.11} \]
CHAPTER II

TRANSITIONAL VALUES OF GRAPHS

2.1 Transitional Values of Complete Graphs

In the previous chapter we have shown a way to describe a chemical reaction by labeling each vertex and edge of a graph $G$ with one of integers $-1, 0, 1$. The labeling of $G$ so obtained satisfies certain basic conditions which will be used to give a formal definition of a transitional labeling of $G$. The value of a transitional labeling of $G$ is defined as the minimum of the number of negative elements of $G$ and the number of positive elements of $G$. Thus, we introduce a new invariant of a graph $G$ called the transitional value of $G$, defined as the maximum value among all the values of the transitional labelings of $G$. We determine the transitional value of the complete graphs.

A labeling of the vertices and edges of a graph with elements of the set $\{-1, 0, 1\}$ is called transitional if

1. each edge labeled $0$ is incident only with vertices labeled $0$,
2. edges labeled $1$ are not incident with vertices labeled $-1$, and
3. edges labeled $-1$ are not incident with vertices labeled $1$.

Conditions (1), (2), and (3) can be replaced by the following single condition:

Whenever the labels of an edge and an incident vertex are different, then the label of the vertex is $0$.

An example of a graph $H$ and a transitional labeling of $H$ is shown in Figure 2.1. To simplify the drawing of a graph $H$ that shows a transitional labeling $t$ of $H$, we represent the edges of $H$ labeled $-1$ by $t$ by means of dashed lines. The edges of $H$ labeled $0$ by $t$ are represented by dotted lines and the edges of $H$ labeled $1$
by $t$ are represented by solid lines. For example, in Figure 2.2 we show a drawing of the graph $H$ that represents the transitional labeling of $H$ of Figure 2.1.
Unless stated otherwise we shall assume that all transitional labelings are nonconstant. (There is no loss of generality with this assumption since transitional labelings were introduced to model chemical reactions and a constant transitional labeling indicates that no reaction has taken place.)

Let $t$ be a transitional labeling of a graph $H$. The subgraph consisting of the elements of $H$ labeled 0 or $-1$ is called the *negative graph* of $t$ and the subgraph consisting of the elements of $H$ labeled 0 or 1 is called the *positive graph* of $t$. If at least one vertex of $H$ is labeled 0 by $t$, then the subgraph consisting of the zero elements of $H$ (the elements of $H$ labeled 0) is called the *linking graph* of $t$. For example, if $t$ is the transitional labeling of the graph $H$ shown in Figure 2.1, then the linking graph $L$ of $t$, the negative graph $N$ of $t$ and the positive graph $P$ of $t$ are shown in Figure 2.3.

![Diagram of graphs](image)

*Figure 2.3*
The cardinality $|G|$ of a graph $G$ is defined by

$$|G| = |V(G)| + |E(G)|.$$ 

Let $t$ be a transitional labeling of a given graph $G$ with linking graph $L$, negative graph $N$ and positive graph $P$. Then the number of zero elements of $G$ is $|L|$. We denote the number of negative elements of $G$ and the number of positive elements of $G$ by $m_t^-$ and $m_t^+$, respectively. Thus,

$$m_t^- = |N| - |L|$$

and

$$m_t^+ = |P| - |L|.$$ 

We define the value $v_t$ of a transitional labeling $t$ of a graph $G$ as the minimum of $m_t^-$ and $m_t^+$, that is,

$$v_t = \min \{m_t^-, m_t^+\}.$$ 

The maximum value among all the transitional labelings of $G$ is an invariant of $G$, called the transitional value of $G$, and is denoted by $v_G$. Therefore

$$v_G = \max \{v_t \mid t \text{ is a transitional labeling of } G\}.$$ 

Observe that for any transitional labeling $t$ of a graph $G$, $m_t^- + m_t^+ \leq |G|$. Therefore,

$$v_t = \min \{m_t^-, m_t^+\} \leq \left\lfloor \frac{|G|}{2} \right\rfloor$$

so that

$$v_G \leq \left\lfloor \frac{|G|}{2} \right\rfloor.$$ 

For each graph $G$ of order $p$ and size $q$, there exists a transitional labeling $t$ of $G$ such that (i) $L \cong K_p$, (ii) $m_t^- = |E(N)| \geq \left\lfloor \frac{q}{2} \right\rfloor$, and (iii) $m_t^+ = |E(P)| \geq \left\lfloor \frac{q}{2} \right\rfloor$. Therefore, $v_t = \min(m_t^-, m_t^+) \geq \left\lfloor \frac{q}{2} \right\rfloor$ and hence

$$v_G \geq v_t \geq \left\lfloor \frac{q}{2} \right\rfloor.$$
For a connected graph $G$ and a transitional labeling $t$ of $G$ we say that a vertex $v$ of $G$ is a pole of $G$ (with respect to $t$) if the label of $v$ is not 0. In particular, $v$ is a positive pole if the label of $v$ is 1 and $v$ is a negative pole if the label of $v$ is $-1$. If $G$ has positive and negative poles, we say that $t$ is a polarization; otherwise, $t$ is called a quasipolarization. Since a positive pole cannot be adjacent to a negative pole, the complete graph $K_p$ has no polarization. The maximum value among all the polarizations of a graph $G \neq K_p$ is denoted by $v_G^*$. Clearly,

$$v_G^* = \max \{v_t \mid t \text{ is a polarization of } G\} \leq v_G.$$ 

If $G$ is not complete, then $v_G^* > 0$. To see this, suppose that $G$ has two nonadjacent vertices, say $u$ and $v$. Let $Z = V(G) - \{u, v\}$ and denote by $t$ the polarization of $G$ whose linking graph, negative graph, and positive graph are $\langle Z \rangle$, $\langle Z \cup \{u\} \rangle$ and $\langle Z \cup \{v\} \rangle$, respectively. Then each of $m_t^+$ and $m_t^-$ are at least one and $v_G^* \geq v_t \geq 1$.

Suppose that $t$ is a transitional labeling of a graph $G$ that is a quasipolarization. Without loss of generality, we may assume that no vertex of $G$ is labeled 1 by $t$. Let $Z_t$ denote the set of vertices labeled 0 by $t$ and let $z_t$ be the cardinality of $Z_t$. With this notation, the number of negative vertices labeled by $t$ is $p - z_t$. Since there is no vertex labeled 1 by $t$, any positive edges belong to $\langle Z_t \rangle$ and any other edge that does not belong to $\langle Z_t \rangle$ is negative. Hence, we obtain the following lemma.

**Lemma 2.1** If $t$ is a transitional labeling of a graph $G$ that is a quasipolarization, then

$$m_t^- \geq |G| - |\langle Z_t \rangle|$$

and

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The next lemma is a direct consequence of Lemma 2.1.

**Lemma 2.2** If $t$ is a transitional labeling of a graph $G$ that is a quasipolarization, then

$$m_t^- \geq |G| - \frac{z_t(z_t + 1)}{2}$$

and

$$m_t^+ \leq \frac{z_t(z_t - 1)}{2}.$$

Figure 2.4 shows a transitional labeling $t$ of $G \equiv K_6$. Here exactly four vertices of $K_6$ are labeled 0, and the remaining two vertices are labeled −1. Thus, $z_t = 4$ and from Lemma 2.2, $m_t^- \geq 11$ and $m_t^+ \leq 6$. Actually, $m_t^- = 13$ and $m_t^+ = 4$. Hence, $v_t = 4$.

In light of Lemma 2.2, for a graph $G$ of order $p$ and for an integer $z$ with
0 ≤ z ≤ p, we define the parameters α and β by
\[ \alpha = |G| - \frac{z(z+1)}{2} \text{ and } \beta = \frac{z(z-1)}{2}. \]

Note that \( \alpha ≤ \beta \) if and only if \( z ≥ \sqrt{|G|} \). Since \( z \) is an integer, the last inequality is equivalent to
\[ z ≥ \left\lfloor \sqrt{|G|} \right\rfloor. \]

As a matter of convenience, we define the parameter \( \sigma(G) \) by
\[ \sigma(G) = \left\lfloor \sqrt{|G|} \right\rfloor. \]

Thus, we obtain the following lemma.

**Lemma 2.3** Let \( G \) be a graph of order \( p \) and let \( z \) be an integer with \( 0 ≤ z ≤ p \). Then \( \alpha ≤ \beta \) if and only if \( z ≥ \sigma(G) \).

If \( G ≅ K_p \), we write \( \sigma(p) \) for \( \sigma(K_p) \). We now determine \( v_{K_p} \). If \( p = 1 \), then \( v_{K_p} = 0 \). Assume that \( p ≥ 2 \) and let \( \sigma = \sigma(p) \). As we noted earlier, if \( t \) is a transitional labeling of \( K_p \), then \( t \) is a quasipolarization. In the current discussion, let \( z \) be an arbitrary but fixed integer, where \( 0 ≤ z ≤ p \). Let \( T(z) \) denote the set of all transitional labelings \( t \) of \( K_p \) for which \( z_t = z \). Without loss of generality, we may assume that for any \( t \in T(z) \), the set \( Z_t \) formed by the zero vertices is equal to a fixed subset of vertices of \( K_p \), say \( Z \). Now for each such integer \( z \), we construct a transitional labeling \( t^*(z) \in T(z) \) such that
\[ v_{t^*(z)} ≥ v_t \text{ for all } t \in T(z). \]

In order to construct \( t^*(z) \), we first consider the case where \( z < \sigma \). By Lemma 2.3, \( \alpha > \beta \). Let \( t \in T(z) \). Since \( z_t = z \), it follows, by applying Lemma 2.2, that \( m_t^+ ≤ m_t^- \) and hence
Let \( t^*(z) \in T(z) \) be the transitional labeling of \( K_p \) such that each edge of \( \langle Z \rangle \) is labeled 1 by \( t^*(z) \). Then, \( m_{t^*(z)}^+ = \frac{z(z-1)}{2} \) and \( v_{t^*(z)} = \frac{z(z-1)}{2} \). Therefore, \( v_t \leq v_{t^*(z)} \) for all \( t \in T(z) \).

As an illustration, let \( p = 6 \) and \( z = 4 \). In Figure 2.5 we show the transitional labeling \( t^*(4) \) of \( K_6 \). Since \( z < \sigma = 5 \), we have that \( v_t \leq v_{t^*(4)} = 6 \), for all \( t \in T(4) \).

Next we consider the case \( z \geq \sigma \). By Lemma 2.3, \( \alpha \leq \beta \). Note that \( \alpha + \beta + z = |K_p| \). Let \( t \in T(z) \). Then

\[
m_t^+ + m_t^- \leq |K_p| - z = \frac{p(p+1)}{2} - z.
\]

Hence,

\[
v_t \leq \left\lfloor \frac{1}{2} \left( \frac{p(p+1)}{2} - z \right) \right\rfloor.
\]
Let \( t^*(z) \in T(z) \) be a transitional labeling of \( K_p \) that labels exactly \( \alpha + \left\lfloor \frac{\beta - \alpha}{2} \right\rfloor \) edges of \( \langle Z \rangle \) with 1 and that labels all the remaining edges of \( \langle Z \rangle \) with -1.

Thus, since all the elements of \( K_p \) not in \( \langle Z \rangle \) must be labeled -1, we have

\[
m_{t^*(z)}^+ = \alpha + \left\lfloor \frac{\beta - \alpha}{2} \right\rfloor
\]

and

\[
m_{t^*(z)}^- = \alpha + \left( \beta - \left( \alpha + \left\lfloor \frac{\beta - \alpha}{2} \right\rfloor \right) \right) = \beta - \left\lfloor \frac{\beta - \alpha}{2} \right\rfloor.
\]

Clearly, \( m_{t^*(z)}^+ \leq m_{t^*(z)}^- \). Therefore,

\[
v_{t^*(z)} = \min \{ m_{t^*(z)}^-, m_{t^*(z)}^+ \} = m_{t^*(z)}^+ = \alpha + \left\lfloor \frac{\beta - \alpha}{2} \right\rfloor = \frac{\left\lfloor \frac{p(p + 1)}{2} \right\rfloor}{2} - z.
\]

Hence,

\[
v_t \leq v_{t^*(z)} \quad \text{for all } t \in T(z).
\]

For example, let \( p = 6 \) and \( z = 5 \). In Figure 2.6 we show a transitional labeling \( t^*(5) \) of \( K_6 \). Since \( z \geq \sigma = 5 \), it follows that \( v_t \leq v_{t^*(5)} = 8 \) for all \( t \in T(5) \).

![Figure 2.6](image-url)
Thus we have the following result.

**Lemma 2.4** Let \( z \) be an integer with \( 0 \leq z \leq p \) and let \( T(z) \) denote the set of all transitional labelings \( t \) of \( K_p \) for which \( z_t = z \). Let \( t^*(z) \) be the transitional labeling of \( K_p \) defined above. Then

\[
V_t \leq V_{t^*(z)} \quad \text{for all} \quad t \in T(z).
\]

Moreover,

\[
V_{t^*(z)} = \begin{cases} 
\frac{z(z-1)}{2} & \text{if} \quad z < \sigma \\
\left\lfloor \frac{\frac{p(p+1)}{2} - z}{1} \right\rfloor & \text{if} \quad z \geq \sigma
\end{cases}
\]

Note that \( V_{t^*} \) is a nondecreasing function of \( z \) if \( z < \sigma \) and that \( V_{t^*} \) is a nonincreasing function of \( z \) if \( z \geq \sigma \). A further consequence of Lemma 2.4 is that an optimal labeling of \( K_p \) is either \( t^*(\sigma - 1) \) or \( t^*(\sigma) \).

To establish the next theorem, we need a basic lemma.

**Lemma 2.5** \((\sigma - 1)^2 < \frac{p(p+1)}{2}\).

**Proof** Since \( \sigma = \left\lfloor \sqrt{\frac{p(p+1)}{2}} \right\rfloor \), it follows that \( \sigma - 1 < \sqrt{\frac{p(p+1)}{2}} \leq \sigma \). From this, we obtain the desired result. \( \square \)

**Theorem 2.6**

\[
V_{K_p} = \left\lfloor \frac{1}{2} \left( \frac{p(p+1)}{2} - \left\lfloor \sqrt{\frac{p(p+1)}{2}} \right\rfloor \right) \right\rfloor.
\]
Proof Since the result is trivial for $p = 1$, we assume that $p \geq 2$. Let $t_1 = t^* (\sigma - 1)$ and $t_2 = t^* (\sigma)$. From Lemma 2.4 we have

$$v_{t_1} = \frac{(\sigma - 1)(\sigma - 2)}{2} \text{ and } v_{t_2} = \left\lfloor \frac{1}{2} \left( \frac{p(p + 1)}{2} - \sigma \right) \right\rfloor.$$

We prove that $v_{t_1} \leq v_{t_2}$.

Now

$$v_{t_2} = \left\lfloor \frac{1}{2} \left( \frac{p(p + 1)}{2} - \sigma \right) \right\rfloor \geq \frac{p(p + 1)}{2} - \sigma - 1 \geq \frac{1}{2} \left( \frac{p(p + 1)}{2} - \sigma - 2 \right).$$

By Lemma 2.5,

$$v_{t_2} > \frac{1}{2} ((\sigma - 1)^2 - \sigma - 2) = \frac{1}{2} (\sigma^2 - 3\sigma - 1);$$

therefore,

$$v_{t_2} \geq \frac{1}{2} (\sigma^2 - 3\sigma - 1) + 1 = \frac{1}{2} (\sigma - 1)(\sigma - 2) - \frac{1}{2}.$$ 

Since $v_{t_2}$ and $\frac{1}{2} (\sigma - 1)(\sigma - 2)$ are integers, it follows that

$$v_{t_2} \geq \frac{1}{2} (\sigma - 1)(\sigma - 2) = v_{t_1}.$$

Therefore, $t_2 = t^* (\sigma)$ is optimal and

$$v_{K_p} = v_{t_2} = \left\lfloor \frac{1}{2} \left( \frac{p(p + 1)}{2} - \sigma \right) \right\rfloor = \left\lfloor \frac{1}{2} \left( \frac{p(p + 1)}{2} - \sqrt{\frac{p(p + 1)}{2}} \right) \right\rfloor. \quad \Box$$

In the next theorem we present a necessary condition for the existence of an optimal transitional labeling of $K_p$.

Theorem 2.7 Let $s$ be an optimal transitional labeling of $K_p$, where $p \geq 3$. Then

$$\sigma - 1 \leq z_s \leq \sigma + 1.$$

Proof Suppose, to the contrary, that $z_s < \sigma - 1$. Then, by Lemma 2.4

$$v_s \leq v_{t^*(z_s)} \leq v_{t^*(\sigma - 2)}.$$
since \( v_{t^*}(z) \) is a nondecreasing function of \( z \) if \( z \leq \sigma \). We also have from Lemma 2.4 that
\[
v_{t^*}(\sigma-1) - v_{t^*}(\sigma-2) = \frac{(\sigma - 1)(\sigma - 2)}{2} - \frac{(\sigma - 2)(\sigma - 3)}{2} = \sigma - 2 \geq 1,
\]
since \( p \geq 3 \) implies \( \sigma \geq 3 \). Therefore,
\[
v_S \leq v_{t^*}(\sigma-2) \leq v_{t^*}(\sigma-1) - 1 < v_{t^*}(\sigma-1)
\]
which contradicts the optimality of \( s \).

To prove the second inequality, suppose, to the contrary, that \( Z_g > \sigma + 1 \). Then, by Lemma 2.4
\[
v_S \leq v_{t^*}(Z_g) \leq v_{t^*}(\sigma+2),
\]
since \( v_{t^*}(z) \) is a nonincreasing function of \( z \) if \( z \geq \sigma \). Therefore,
\[
v_S \leq \left[ \frac{1}{2} \left( \frac{p(p+1)}{2} - (\sigma + 2) \right) \right] - 1 = v_{K_p} - 1,
\]
which contradicts the optimality of \( s \). \( \Box \)

From Theorem 2.7 we know that if \( s \) is an optimal transitional labeling of \( K_p \), where \( p \geq 3 \), then \( Z_g = \sigma - 1, \sigma \) or \( \sigma + 1 \). In the proof of Theorem 2.6, we have shown that there always exists an optimal transitional labeling \( s \) such that \( Z_g = \sigma \).

Now we proceed to find a necessary and sufficient condition for the existence of an optimal transitional labeling \( s \) of \( K_p \) that satisfies either \( Z_g = \sigma - 1 \) or \( Z_g = \sigma + 1 \).

**Lemma 2.8** Let \( p \geq 5 \). Then there exists an optimal transitional labeling \( s \) of \( K_p \) with \( Z_g = \sigma + 1 \) if and only if \( \frac{p(p+1)}{2} - \sigma \) is odd.
Proof Since \( p \geq 5 \), it follows that \( \sigma + 1 \leq p \). From Lemma 2.4, there is an optimal transitional labeling \( s \) of \( K_p \) with \( z_s = \sigma + 1 \) if and only if

\[
\left| \frac{1}{2}(p(p+1)/2 - \sigma) \right| = \left| \frac{1}{2}(p(p+1)/2 - (\sigma + 1)) \right|
\]

and equality holds in (2.1) if and only if \( \frac{p(p+1)}{2} - \sigma \) is odd. \( \square \)

To characterize the existence of an optimal transitional labeling \( s \) of \( K_p \) with \( z_s = \sigma - 1 \), we present the next lemma.

**Lemma 2.9** There exists an optimal labeling \( s \) of \( K_p (p \geq 2) \) with \( z_s = \sigma - 1 \) if and only if for \( j = 1 \) or \( j = 2 \), the integer \( \frac{p(p+1)}{2} - j \) is a perfect square.

**Proof** By Lemma 2.4 there is an optimal transitional labeling \( s \) of \( K_p \) with \( z_s = \sigma - 1 \) if and only if

\[
\left| \frac{(\sigma-1)(\sigma-2)}{2} \right| = \left| \frac{1}{2}(p(p+1)/2 - \sigma) \right|. \tag{2.2}
\]

Define \( i = 0 \) if \( \frac{p(p+1)}{2} - \sigma \) is even and \( i = 1 \), otherwise. Then, equation (2.2) becomes

\[
\frac{(\sigma-1)(\sigma-2)}{2} = \frac{1}{2}(p(p+1)/2 - \sigma - i).
\]

Simplifying, we get

\[
\sigma^2 - 2\sigma + 2 = \frac{p(p+1)}{2} - i
\]

which is equivalent to

\[
(\sigma - 1)^2 = \frac{p(p+1)}{2} - (i + 1). \quad \square
\]
2.2 An Exceptional Family of Complete Graphs

In this section we determine the values of \( p \) for which there exist optimal transitional labelings of \( K_p \) with \( z_s = \sigma - 1 \), where \( \sigma = \sigma(p) \). From Lemma 2.9, this is equivalent to finding all positive integers \( p \) such that

\[
\frac{p(p + 1)}{2} - j = u^2
\]

(2.3)

for some nonnegative integer \( u \), where \( j = 1 \) or \( j = 2 \). Multiplying (2.3) by 8, we obtain

\[
(2p + 1)^2 - 8u^2 = 8j + 1.
\]

Define \( x = 2p + 1 \) and \( y = 2u \). Solving the diophantine equation (2.3) is equivalent to solving the diophantine equation

\[
x^2 - 2y^2 = 8j + 1.
\]

Thus,

\[
x^2 - 2y^2 = 9
\]

(2.4)

if \( j = 1 \), and

\[
x^2 - 2y^2 = 17
\]

(2.5)

if \( j = 2 \).

In [7, Chap. VI, sections 56, 58] a simple process for determining all the solutions of this type of diophantine equations is described. We follow this process to solve equations (2.4) and (2.5). First, it is required to solve the so-called "Fermat equation"

\[
u^2 - 2v^2 = 1
\]

(2.6)

for positive integers \( u \) and \( v \). Let \( u_i \) and \( v_i \) be positive integers such that \( u_i^2 - 2v_i^2 = 1 \). We say, for simplicity, that \( u_i + v_i\sqrt{2} \) is a solution of (2.6). Among all solutions \( u_i + v_i\sqrt{2} \) of (2.6), define the fundamental solution of (2.6) as that
solution for which \( u_1 + v_1\sqrt{2} \) achieves the least positive value. It is straightforward to verify that the fundamental solution of (2.6) is \( 3 + 2\sqrt{2} \).

The following result [7, p. 197] is helpful for finding the solutions of (2.6).

**Theorem A**  Let \( D \) be a positive integer that is not a perfect square. The set of all solutions \( x + y\sqrt{D} \) of the diophantine equation

\[
x^2 - Dy^2 = 1
\]  

(2.7)

for positive integers \( x \) and \( y \) is \( \{(x_1 + y_1\sqrt{D})^n \mid n = 1, 2, \ldots\} \), where \( x_1 + y_1\sqrt{D} \) is the fundamental solution of (2.7).

With the aid of Theorem A, we see that each solution \( u_n + v_n\sqrt{2} \) of (2.6), where \( u_n \) and \( v_n \) are nonnegative integers, is given by

\[
u_n + v_n\sqrt{2} = (3 + 2\sqrt{2})^n, \quad n = 0, 1, 2, \ldots
\]

Now we look for solutions of equation (2.4). In this case, we have classes of solutions and fundamental solutions defined for each class. In particular, two solutions \( x + y\sqrt{2} \) and \( x' + y'\sqrt{2} \) of (2.4) belong to the same class if there exists a solution \( u + v\sqrt{2} \) of (2.6) such that \( x' + y'\sqrt{2} = (u + v\sqrt{2})(x + y\sqrt{2}) \). Among all the solutions \( x + y\sqrt{2} \) of a class \( K \) of solutions of (2.4), we denote by \( y^* \) the least nonnegative value that \( y \) can assume. At most two solutions of \( K \) achieve this minimum value of \( y \). If exactly one solution of \( K \) achieves this minimum value, then this solution is defined as the fundamental solution of \( K \). If \( K \) contains two distinct solutions \( x + y^*\sqrt{2} \) and \( x' + y'^*\sqrt{2} \), then \( x = -x' \) and in this case, the fundamental solution \( x^* + y^*\sqrt{2} \) is defined for \( x^* = \max\{x, x'\} \). The next theorem [7, p. 205] will help us find fundamental solutions for each class.
Theorem B If $x^* + y^* \sqrt{D}$ is the fundamental solution of the class $K$ of solutions of the equation $x^2 - Dy^2 = N$ and if $u_1 + v_1 \sqrt{D}$ is the fundamental solution of equation (2.7), then

i) $0 \leq y^* \leq \frac{\sqrt{N}}{\sqrt{2}(u_1 + 1)}$

and

ii) $0 < |x^*| \leq \sqrt{\frac{1}{2}(u_1 + 1)N}$.

Assume that $x^* + y^* \sqrt{2}$ is the fundamental solution of a class $K$ of solutions of equation (2.4). Then, from Theorem B, we have that

$0 \leq y^* \leq \frac{2}{\sqrt{2}(3 + 1)} \sqrt{9} = \frac{3}{2} \sqrt{2} = 2.12...$

and

$0 \leq |x^*| \leq \sqrt{\frac{1}{2}(3 + 1)9} = 3\sqrt{2} = 4.24...$

Consequently, $y^* \in \{0, 1, 2\}$ and $x^* \in \{0, \pm1, \pm2, \pm3, \pm4\}$. Since $y^*$ is the least nonnegative value of $y_1$ among all solutions $x_1 + y_1 \sqrt{2}$ of the class $K$, we conclude that $y^* = 0$ and $x^* \in \{3, -3\}$. Observe that the solutions $3 + 0 \cdot \sqrt{2}$ and $-3 + 0 \cdot \sqrt{2}$ belong to the same class. Therefore, we choose $x^* = 3$. Thus, there is exactly one class of solutions for equation (2.4) and only one fundamental solution, namely, $3 + 0 \cdot \sqrt{2} = 3$. The next result [7, p. 207] allows us to find the solutions of (2.4).

Theorem C Let $D$ and $N$ be positive integers, where $D$ is not a perfect square. If $x^* + y^* \sqrt{D}$ is the fundamental solution of a class $K$ of solutions of the diophantine equation
\[ x^2 - Dy^2 = N, \]

then

\[ K = \{(x^* + y^* \sqrt{D})(u_n + v_n \sqrt{D}) \mid u_n + v_n \sqrt{D} \text{ is a solution of } u^2 - Dv^2 = 1\}. \]

By Theorem C, each solution \( x_i + y_i \sqrt{2} \) of (2.4), where \( x_i \) and \( y_i \) are nonnegative integers, is given by

\[ x_i + y_i \sqrt{2} = 3(3 + 2\sqrt{2})^n, \quad n = 0, 1, \ldots \quad (2.7) \]

From (2.7) we obtain a recurrence relation for the values of \( x_i \). First we note that

(2.7) implies

\[ (x_{n-1} + y_{n-1} \sqrt{2})(3 + 2\sqrt{2}) = x_n + y_n \sqrt{2} \quad \text{for } n = 1, 2, \ldots \]

Therefore,

\[ 3x_{n-1} + 4y_{n-1} = x_n \]

and

\[ 2x_{n-1} + 3y_{n-1} = y_n, \quad n \geq 1. \]

Solving this system for \( x_{n-1} \), we obtain

\[ x_{n-1} = 3x_n - 4y_n, \quad n \geq 1. \]

Hence,

\[ 4y_{n-1} = 3x_{n-1} - x_{n-2}, \quad n \geq 2. \]

Combining this equation with the first equation of the above system to eliminate \( y_{n-1} \), we have

\[ x_n = 6x_{n-1} - x_{n-2}, \quad n \geq 2. \]

From (2.7) we find that \( x_0 = 3 \) and \( x_1 = 9 \). Thus, we have the following recurrence relation for the values of \( x_i \) given in (2.7):
Recalling that the corresponding values of \( p \) in which we are interested are given by \( p_i = \frac{x_i - 1}{2} \), we obtain a recurrence relation for these values:

\[
\begin{align*}
  p_0 &= 1 \\
  p_1 &= 4 \\
  p_n &= 6p_{n-1} - p_{n-2} + 3, \quad n \geq 2.
\end{align*}
\]

Since the recurrence relation (2.7') found for \( x_n \) is simpler than that found for \( p_n \), we choose (2.7') to obtain a closed formula for \( x_n \) and hence for \( p_n \). But first we find all solutions \( x_i + y_i \sqrt{2} \) of equation (2.5).

Denote the fundamental solution of a class of solutions of equation (2.5) by \( x^* + y^* \sqrt{2} \). In a similar way, we find that

\[
0 \leq y^* \leq \frac{2}{\sqrt{2}(3 + 1)} \cdot \sqrt{17} = \frac{\sqrt{34}}{2} = 2.91...
\]

and

\[
0 \leq |x^*| \leq \sqrt{\frac{1}{2} (3 + 1) \cdot 17} = \sqrt{34} = 5.83...
\]

In this case we find two classes of solutions where the corresponding fundamental solutions are \( 5 + 2 \sqrt{2} \) and \( -5 + 2 \sqrt{2} \). It turns out that the solutions \( x^{(i)}_n + y^{(i)}_n \sqrt{2} \) of equation (2.5), where \( x^{(i)}_n, y^{(i)}_n \) are nonnegative, are given by

\[
x'_n + y'_n \sqrt{2} = (5 + 2 \sqrt{2})(3 + 2 \sqrt{2})^n, \quad n = 0, 1, 2, \ldots \tag{2.8}
\]

and

\[
x''_n + y''_n \sqrt{2} = (5 - 2 \sqrt{2})(3 + 2 \sqrt{2})^n, \quad n = 0, 1, 2, \ldots \tag{2.9}
\]

For the values \( x'_n \) and \( x''_n \) given in (2.8) and (2.9), we obtain the recurrence relations
Thus far, we have found that the nonnegative values of \( x \) corresponding to the solutions of equations (2.4) and (2.5) form three different families that can be described using the recurrence relations (2.7'), (2.8') and (2.9'). Now, a closed formula for these values of \( x \) is found. We illustrate the procedure with the aid of (2.7').

Assume that \( F(t) \) is the generating function of the sequence \( \{x_n\} \), where \( x_n \) is defined in (2.7'). So

\[
F(t) = x_0 + x_1t + x_2t^2 + \ldots + x_{n-1}t^{n-1} + x_nt^n + \ldots
\]

Then,

\[
6F(t) - tF(t) = 6x_0 + (6x_1 - x_0)t + (6x_2 - x_1)t^2 + \ldots + 6(x_n - x_{n-1})t^n + \ldots.
\]

Hence,

\[
6F(t) - tF(t) = 6x_0 + x_2t + x_3t^2 + \ldots + x_{n+1}t^n + \ldots
\]

or

\[
6F(t) - tF(t) = 6x_0 + \frac{F(t) - x_0 - x_1t}{t}.
\]

Solving the last equation for \( F(t) \), we have

\[
F(t) = \frac{(x_1 - 6x_0)t + x_0}{t^2 - 6t + 1}.
\]

Note that the solutions \( \phi_1 \) and \( \phi_2 \) of \( t^2 - 6t + 1 = 0 \) are

\[
\phi_1 = 3 - 2\sqrt{2}
\]
and

\[ \phi_2 = 3 + 2\sqrt{2}. \]

Therefore \( \phi_1 \phi_2 = 1 \) and

\[
F(t) = \frac{t(x_1 - 6x_0) + x_0}{\phi_1 \phi_2 \left( \frac{1}{\phi_1} \left( \frac{1}{\phi_1} - \frac{1}{\phi_2} \right) \right)}
\]
or

\[
F(t) = \frac{t(x_1 - 6x_0) + x_0}{(1 - \phi_2 t)(1 - \phi_1 t)}.
\]

(2.10)

Since \( x_0 = 3 \) and \( x_1 = 9 \), it follows that

\[
F(t) = \frac{-9t + 3}{(1 - \phi_2 t)(1 - \phi_1 t)}.
\]

This equation can also be expressed by

\[
F(t) = \frac{3}{2} \left( \frac{1}{1 - \phi_1 t} + \frac{1}{1 - \phi_2 t} \right).
\]

Thus,

\[
F(t) = \frac{3}{2} \left( (1 + \phi_1 t + \phi_1^2 t^2 + \ldots + \phi_1^n t^n + \ldots) + (1 + \phi_2 t + \phi_2^2 t^2 + \ldots + \phi_2^n t^n + \ldots) \right)
\]

\[
= \frac{3}{2} \left( 2 + (\phi_1 + \phi_2) t + (\phi_1^2 + \phi_2^2) t^2 + \ldots + (\phi_1^n + \phi_2^n) t^n + \ldots \right).
\]

Therefore,

\[
x_n = \frac{3}{2} \left( \phi_1^n + \phi_2^n \right), \quad n \geq 0.
\]

(2.7)

For the recurrence relations (2.8') and (2.9'), we may use (2.10) to obtain the corresponding closed formulas (2.8'') and (2.9''):

\[
x_n' = \frac{5 - 2\sqrt{2}}{2} \phi_1^n + \frac{5 + 2\sqrt{2}}{2} \phi_2^n, \quad n \geq 0
\]

(2.8'')

\[
x_n'' = \frac{7 - 4\sqrt{2}}{2} \phi_1^n + \frac{7 + 4\sqrt{2}}{2} \phi_2^n, \quad n \geq 0.
\]

(2.9'')

Moreover, (2.7''), (2.8'') and (2.9'') can be combined to obtain
\[
x^{(i)}_n = \frac{(2i + 3) - 2i\sqrt{2}}{2} \phi_1^n + \frac{(2i + 3) + 2i\sqrt{2}}{2} \phi_2^n
\]
(2.11)

for \( n \geq 0, i = 0, 1, 2, \) and where \( \phi_1 = 3 - 2\sqrt{2} \) and \( \phi_2 = 3 + 2\sqrt{2} \).

Observe that \( \phi_1 = 3 - 2\sqrt{2} = 0.17157... \). Therefore, if \( n \) is sufficiently large, formula (2.11) can be simplified. Indeed if \( n \geq 1 \), or if \( n = 0 \) and \( i = 2 \), then

\[
\frac{(2i + 3) - 2i\sqrt{2}}{2} \phi_1^n < 1,
\]

and, consequently, for these values of \( n \) and \( i \),

\[
x^{(i)}_n = \left[ \frac{(2i + 3) + 2i\sqrt{2}}{2} (3 + 2\sqrt{2})^n \right].
\]

Hence, the corresponding values of \( p \) can be given as follows:

\[
p^{(i)}_n = \begin{cases} 
1 & \text{if } n = 0, i = 0 \\
2 & \text{if } n = 0, i = 1 \\
\frac{1}{2} \left( \frac{(2i + 3) + 2i\sqrt{2}}{2} (3 + 2\sqrt{2})^n \right) & \text{otherwise}
\end{cases}
\]

Table 2.1 shows the only twenty-five values of \( p \leq 1,000,000 \) for which \( K_p \) has an optimal transitional labeling \( s \) such that exactly \( \sigma - 1 \) vertices are labeled 0 by \( s \) (that is, \( z_s = \sigma - 1 \)). The next value of \( p \) is the solution \( p^{(1)}_8 = 2,606,306 \). Actually, it is straightforward to prove that the probability of choosing a solution \( p \) to the equation (2.3) among the first \( N \) integers approaches 0 as \( N \) approaches infinity.
Table 2.1

The Twenty-Five Values of $p$ for Which $K_p$ Has an Optimal Transitional Labeling $s$ Such That Exactly $\sigma - 1$ Vertices Are Labeled 0 by $s$

<table>
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<th>$n$</th>
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<th>$p = p^{(i)}_n$</th>
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2.3 An Additional Result Concerning Optimal Labelings of Complete Graphs

Let \( \sigma = \sigma(p) \). We already know that optimal transitional labelings \( s \) of \( K_p \) for which \( z_s = \sigma - 1 \) occur for extremely rare values of \( p \). We consider now the problem of determining those values of \( p \) for which there exists an optimal transitional labeling \( s \) of \( K_p \) such that \( z_s = \sigma + 1 \).

From Lemma 2.8 we know that if \( p > 5 \), then there exists an optimal transitional labeling \( s \) of \( K_p \) with \( z_s = \sigma + 1 \) if and only if

\[
P\left(\frac{p(p+1)}{2}\right) - \sigma \equiv 1 \pmod{2},
\]  

(2.12)

where \( \sigma = \sigma(p) = \left\lfloor \sqrt{\frac{p(p+1)}{2}} \right\rfloor \).

Next, we study the probability that a solution \( p (\geq 5) \) to the congruence (2.12) exists among the first \( N \) integers. Denote by \( f \) the integer-valued function defined by the left side of (2.12), that is,

\[
f(p) = P\left(\frac{p(p+1)}{2}\right) - \sigma(p), \quad p \geq 5.
\]

Note that \( f(p) \) is odd if and only if \( \frac{p(p+1)}{2} \) and \( \sigma(p) \) are of opposite parity. For \( p = 5, 6, \ldots \) define

\[
u_p = \begin{cases} 
0 & \text{if } \frac{p(p+1)}{2} \text{ is even} \\
1 & \text{if } \frac{p(p+1)}{2} \text{ is odd}
\end{cases}
\]

Then, the sequence \( \{u_p\} \) is \( 1, 1, 0, 0, 1, 1, 0, 0, 1, 1, 0, 0, \ldots \). On the other hand, in Figure 2.7 we show the first 31 terms of the sequence \( \{\sigma(p)\} \). Observe that this sequence consists of consecutive numbers that appear in blocks having three or four terms. (See Figure 2.7 where we also show the blocks \( B_i \), \( i = 1, 2, \ldots, 9 \) corresponding to those first 31 terms.) In fact, we will prove that \( \{\sigma(p)\} \) is the
<table>
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Figure 2.7

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juxtaposition of sequences with three or four terms consisting of consecutive integers. An immediate consequence of this is that among the values of p forming a block of three consecutive numbers in \( \{ \sigma(p) \} \), there is at least one value of p for which f(p) is odd, and for the values of p forming a block of four consecutive numbers in \( \{ \sigma(p) \} \), there are exactly two distinct values of p for which f(p) is odd. Moreover, we will prove that in \( \{ \sigma(p) \} \) two consecutive blocks each with three terms, are followed by a block that has four terms. From this it will follow that the probability of choosing p \( \leq N \) so that we have an odd value of f(p) is at least 0.4\( (1 - g(N)) \) where g(N) is a function of N such that \( \lim_{N \to \infty} g(N) = 0 \).

It is convenient to define a real function \( \sigma^*(x) \) for each positive real number x as

\[
\sigma^*(x) = \sqrt{\frac{x(x+1)}{2}}, \quad x > 0.
\]

So, for each positive integer p, \( \sigma(p) = \left\lfloor \sigma^*(p) \right\rfloor \).

**Lemma 2.10** For the function \( \sigma^* \) described above

\[
\lim_{p \to \infty} (\sigma^*(p+1) - \sigma(p)) = \frac{\sqrt{2}}{2}.
\]

**Proof** Observe that

\[
\sigma^*(p+1) - \sigma^*(p) = \sqrt{\frac{(p+1)(p+2)}{2}} - \sqrt{\frac{p(p+1)}{2}}
\]

\[
= \frac{(p+1)(p+2) - p(p+1)}{2 \sqrt{\frac{(p+1)(p+2)}{2}} + \sqrt{\frac{p(p+1)}{2}}}
\]
Thus, \( \lim_{p \to \infty} (\sigma^*(p+1) - \sigma^*(p)) = \frac{\sqrt{2}}{2} \). □

An immediate consequence of Lemma 2.10 is that for sufficiently large \( p \),

\[ \sigma(p + 1) \leq \sigma(p) + 1. \]

Let \( \epsilon = \frac{\sqrt{2}}{2} \). The next corollary is a useful consequence of the above lemma.

**Corollary 2.11** Let \( n \) be a positive integer. For sufficiently large \( p \), if

\[ r_1 < \sigma^*(p) + n \epsilon < r_2, \]

then

\[ r_1 < \sigma^*(p + n) < r_2. \]

Now we prove some basic properties of the sequence \( \{\sigma(p)\} \).

**Lemma 2.12** For sufficiently large \( p \), if \( \sigma(p) = \sigma(p + 1) \), then \( \sigma(p + 3) = \sigma(p + 2) \), which implies that the integers \( \sigma(p + 1), \sigma(p + 2), \sigma(p + 3) \) are consecutive.
Proof Since \( \sigma(p) = \sigma(p + 1) \) for sufficiently large \( p \), \( \sigma^*(p) \) is not an integer and \( \sigma^*(p) + \varepsilon \leq \sigma(p) \). Also, \( \sigma(p) - 1 \leq \sigma^*(p) \). Then,

\[
\sigma(p) - 1 \leq \sigma^*(p) \leq \sigma(p) - \varepsilon.
\]

So,

\[
\sigma(p) + 1.12... \leq \sigma^*(p) + 3\varepsilon \leq \sigma(p) + 1.41...
\]

Therefore, from Corollary 2.11, if \( p \) is sufficiently large, we have

\[
\sigma(p) + 1.1 < \sigma^*(p + 3) < \sigma(p) + 1.5.
\]

Hence, \( \sigma(p + 3) = \lceil \sigma^*(p + 3) \rceil = \sigma(p) + 2 \). \( \square \)

**Lemma 2.13** For sufficiently large \( p \), if \( \sigma(p), \sigma(p + 1), \sigma(p + 2), \sigma(p + 3) \) are consecutive integers, then \( \sigma(p + 4) = \sigma(p + 3) \).

Proof For sufficiently large \( p \) we have

\[
\sigma^*(p + 3) - \sigma^*(p) < 3\varepsilon + 0.1.
\]

Since \( \sigma(p), \sigma(p + 1), \sigma(p + 2) \) are consecutive integers we also have

\[
\sigma(p + 2) - \sigma(p) = 2.
\]

Therefore, subtracting the above relations we obtain

\[
(\sigma(p) - \sigma^*(p)) + (\sigma^*(p + 3) - \sigma(p + 2)) < 3\varepsilon + 0.1 - 2 < 0.23.
\]

Observe that \( \sigma(p) - \sigma^*(p) \) is nonnegative. Moreover, \( \sigma^*(p + 3) - \sigma(p + 2) \) is also nonnegative. (If \( \sigma^*(p + 3) < \sigma(p + 2) \), then \( \sigma(p + 3) \leq \sigma(p + 2) \), which implies that \( \sigma(p + 3) = \sigma(p + 2) \).) Thus,

\[
\sigma^*(p + 3) - \sigma(p + 2) < 0.23.
\]

Therefore,

\[
\sigma^*(p + 3) + \varepsilon < \sigma(p + 2) + \varepsilon + .23 < \sigma(p + 2) + 0.94.
\]

Thus, using Corollary 2.11 for sufficiently large \( p \), we have
\( \sigma^*(p + 4) < \sigma(p + 2) + 0.94. \)

Hence, \( \sigma(p + 4) \leq \sigma(p + 2) + 1 = \sigma(p + 3). \) \( \square \)

Define a block to be any subsequence of consecutive terms of the sequence \( \{ \sigma(p) \} \) that are consecutive integers. Then Lemma 2.12 assures us that \( \{ \sigma(p) \} \) is the juxtaposition of those blocks having a maximum number of terms (maximal blocks). Moreover, Lemma 2.13 implies that every maximal block has either three or four terms. Define a 3-block (4-block) to be any maximal block with exactly three terms (four terms). The next lemma describes how maximal blocks may appear in the sequence \( \{ \sigma(p) \} \).

**Lemma 2.14** Let \( B_1 \) and \( B_2 \) be two adjacent 3-blocks of \( \{ \sigma(p) \} \), where \( B_1 \) precedes \( B_2 \). Then, for sufficiently large \( p \), the maximal block that immediately follows \( B_2 \) is a 4-block.

**Proof** Assume that \( \sigma(p) = \sigma(p + 1), \sigma(p + 3) = \sigma(p + 4) \) and \( \sigma(p + 6) = \sigma(p + 7) \). Thus,

\[ B_1: \sigma(p + 1), \sigma(p + 2), \sigma(p + 3) = \sigma(p + 4) \]

and

\[ B_2: \sigma(p + 4), \sigma(p + 5), \sigma(p + 6) = \sigma(p + 7). \]

From Lemma 2.12, we know that \( \sigma(p + 7), \sigma(p + 8), \) and \( \sigma(p + 9) \) are consecutive integers. We need only prove that \( \sigma(p + 10) = \sigma(p + 9) + 1 \) to conclude that the block immediately following \( B_2 \) is a 4-block.

Since \( \sigma(p) - 1 < \sigma^*(p) \), we have

\[ \sigma(p) + 9\varepsilon - 1 < \sigma^*(p) + 9\varepsilon. \]
Therefore, if \( p \) is sufficiently large, then
\[
\sigma(p) + 9\varepsilon - 1 < \sigma^*(p + 9).
\]
Since \( \sigma(p + 1), \sigma(p + 2), \sigma(p + 4), \sigma(p + 5), \sigma(p + 7), \sigma(p + 8), \sigma(p + 9) \) are seven consecutive integers, we have
\[
\sigma(p + 9) = \sigma(p) + 6.
\]
Therefore,
\[
\sigma(p + 9) - \sigma^*(p + 9) < 7 - 9\varepsilon < \varepsilon
\]
and so
\[
\sigma(p + 9) < \sigma^*(p + 9) + \varepsilon.
\]
Therefore, if \( p \) is large enough, we conclude (by Corollary 2.11) that
\[
\sigma(p + 9) < \sigma^*(p + 10).
\]
Hence, \( \sigma(p + 10) = \sigma(p + 9) + 1. \]

We are now prepared to present our final result of this chapter.

**Theorem 2.15** Let \( P \) be the probability of choosing a number \( p \), with \( p \leq N \), such that there exists an optimal transitional labeling \( s \) of \( K_p \) with \( z_s = \sigma + 1 \). Let \( \delta > 0 \). Then for sufficiently large \( N \),
\[
0.4 - \delta < P < 0.6 + \delta.
\]

**Proof** By Lemma 2.8, we know that the complete graph \( K_p \) has an optimal transitional labeling \( t \) such that \( z_t = \sigma + 1 \) if and only if \( f(p) = \frac{p(p + 1)}{2} - \sigma(p) \) is odd. Recall that \( u_p = 0 \) if \( \frac{p(p + 1)}{2} \) is even and \( u_p = 1 \) if \( \frac{p(p + 1)}{2} \) is odd. Since the sequence \( \{u(p)\} \) is \( 1, 1, 0, 0, 1, 1, 0, 1, 0, 1, 0, 0, \ldots \), there is at least one value of \( p \) among the values of \( p \) that form a 3-block in \( \{\sigma(p)\} \) for which \( f(p) \) is odd. For the values of \( p \) that form a 4-block there are exactly two different values of \( p \) for
which \( f(p) \) is odd. Lemma 2.14 assures us that if \( p \) is large enough, then \( \{\sigma(p)\} \) cannot have more than two consecutive 3-blocks. Therefore, \( P \) cannot be less than the probability we obtain by assuming that the sequence \( \{\sigma(p)\} \) for \( p = M, M+1, \ldots \) is formed by two consecutive 3-blocks followed by a 4-block and so on, for some integer \( M \geq 5 \).

Thus, if \( N \geq M \),

\[
P \geq \frac{4\left\lfloor \frac{N-M}{10} \right\rfloor}{N-4} \geq \frac{4(N-M-10)}{10(N-4)} = 0.4 - \frac{2(M+6)}{5(N-4)}.
\]

Hence, taking \( N \) such that

\[
N > \frac{2(M+6)}{5\delta} + 4,
\]

we have \( \frac{2(M+6)}{5(N-4)} < \delta \) and then \( P > 0.4 - \delta \).

To prove the second inequality, we remark that among the values of \( p \) that form a 3-block in \( \{\sigma(p)\} \) there are at most two values of \( p \) for which \( f(p) \) is odd. Therefore, \( P \) cannot be larger than the probability we obtain by assuming that the sequence \( \{\sigma(p)\}, p = M, M+1, \ldots \) is formed by two consecutive 3-blocks followed by a 4-block and so on, for some integer \( M \geq 5 \). Thus, if \( N \geq M \),

\[
P \leq \frac{M-4 + 6\left\lfloor \frac{N-M}{10} \right\rfloor}{N-4} \leq \frac{10(M-4) + 6(N-M) + 60}{10(N-4)} \leq 0.6 + \frac{2(M+11)}{5(N-4)}.
\]

Hence, taking \( N \) such that

\[
N > \frac{2(M+11)}{5\delta} + 4,
\]

we have that \( \frac{2(M+11)}{5(N-4)} < \delta \) and so, \( P < 0.6 + \delta \). □
Conjecture  For $P$ defined above,

$$\lim_{N \to \infty} P = 0.5.$$  

For $p = 6$, we show $t^*(z)$ in Figure 2.8 for $z = \sigma - 1, \sigma, \sigma + 1$. For this value of $p$, note that if $s$ is an optimal transitional labeling of $K_p$ then $z_s = \sigma = 5$. The case $p = 11$ is the smallest value of $p$ for which there exists an optimal transitional labeling $s$ satisfying $z_s = z$ for $z = \sigma - 1, \sigma, \sigma + 1, \sigma = 9$. See Figures 2.9, 2.10, and 2.11.

![Graphs showing transitional labeling for $p=6$, $p=5$, and $p=6$]

Figure 2.8
\[ s_1 = t^*(8) \]

\[ v_{s_1} = 28 \quad z_{s_1} = \sigma - 1 = 8 \]

Figure 2.9
$s_2 = t^*(9)$

$v_{s_2} = 28 \quad z_{s_2} = \sigma = 9$

Figure 2.10
\[ s_3 = t^*(10) \]

\[ v_{s_3} = 28 \quad z_{s_3} = \sigma + 1 = 10 \]

Figure 2.11
CHAPTER III

FURTHER RESULTS ON TRANSITIONAL VALUES OF GRAPHS

3.1 Bounds for the Values of Transitional Labelings of Graphs

Recall that a labeling \( t \) of the vertices and edges of a graph \( G \) with elements of the set \( \{-1, 0, 1\} \) is a transitional labeling if

1. each edge labeled \( 0 \) is incident only to vertices labeled \( 0 \),
2. edges labeled \( 1 \) are not incident with vertices labeled \( -1 \), and
3. edges labeled \( 1 \) are not incident with vertices labeled \( 1 \).

The number of negative elements of \( G \) and the number of positive elements of \( G \) are denoted by \( m^- \) and \( m^+ \), respectively. The value \( v_t \) of the transitional labeling \( t \) is defined as that minimum of \( m^- \) and \( m^+ \).

As we previously noted,

\[
v_G \leq \left\lfloor \frac{|G|}{2} \right\rfloor.
\]

If \( G \cong P_n \), then \( |G| = 2n - 1 \). Also

\[
v_{P_n} = \begin{cases} 
  n - 1 & \text{if } n \text{ is odd} \\
  n - 2 & \text{if } n \text{ is even}.
\end{cases}
\]

Thus, paths of odd order show that the above bound is sharp.

For a transitional labeling \( t \) of a graph \( G \), recall that a vertex \( v \) of \( G \) is a pole if the label of \( G \) is not \( 0 \). In particular, \( v \) is a positive pole if the label of \( v \) is \( 1 \) and \( v \) is a negative pole if the label of \( v \) is \( -1 \). If \( G \) has positive and negative poles, we say that \( t \) is a polarization. The maximum value among all the polarizations of a graph \( G \cong K_p \) is denoted by \( v^*_G \). Suppose that \( t \) is a polarization of a connected graph \( G \). Then at least one vertex of \( G \) is labeled \( 0 \) by \( t \) and, moreover, the removal of all
zero vertices results in a disconnected graph. Therefore, at least \( \kappa(G) \) vertices of \( G \) are labeled 0 by \( t \) and, so, at most \( |G| - \kappa(G) \) elements of \( G \) can be labeled 1 or -1 by \( t \). Therefore, for a connected graph \( G \),

\[
v_G^* \leq \left\lfloor \frac{|G| - \kappa(G)}{2} \right\rfloor.
\]

(3.1)

Another bound for \( v_G^* \) is presented in the next lemma.

**Lemma 3.1** If \( G \) is a connected noncomplete graph of order \( p \), then

\[
v_G^* \leq \left\lfloor \frac{p^2 - p + 2}{4} \right\rfloor.
\]

**Proof** Assume that \( G \) is a connected graph of order \( p \) and let \( t \) denote a polarization of \( G \) in which exactly \( z \) vertices of \( G \) are labeled 0. Since at most \( |G| - z \) elements of \( G \) are labeled -1 or 1 by \( t \), it follows that

\[
v_t \leq \frac{|G| - z}{2}.
\]

(3.2)

Suppose that \( x \) vertices of \( G \) are labeled -1 by the transitional labeling \( t \) and \( y \) vertices of \( G \) are labeled 1. Then

\[
x + y + z = p,
\]

(3.3)

\[1 \leq x, y, z \leq p - 2,\]

and

\[
|G| \leq \frac{p(p + 1)}{2} - xy.
\]

(3.4)

Combining (3.2), (3.3) and (3.4), we have

\[
v_t \leq \frac{1}{2} \left( x - xy + y + \frac{p(p - 1)}{2} \right).
\]

(3.5)
Assume now that $x$ and $y$ are real variables and let $f = f(x, y)$ denote the real-valued function defined as the right side of (3.5), where $1 \leq x, y \leq p - 2$. Then the maximum value of $f$ is achieved at $x = y = 1$. (Actually, this maximum value is achieved at any point $(x, y)$ for which $x = 1$ or $y = 1$.) Thus,

$$v_t \leq \frac{1}{2} \left( 1 + \frac{p(p - 1)}{2} \right) = \frac{p^2 - p + 2}{4}.$$  

Hence,

$$v_t \leq \left\lfloor \frac{p^2 - p + 2}{4} \right\rfloor.$$

The *cyclomatic number* $v(G)$ of a graph $G$ is the minimum number of edges whose removal from $G$ results in an acyclic graph. Thus,

$$v(G) = q(G) - p(G) + k(G),$$

where $k(G)$ is the number of components of $G$. Using this relation we can prove the following lemma.

**Lemma 3.2** If $H$ is an induced subgraph of a graph $G$, then

$$v(H) \leq v(G).$$

Recall that a quasipolarization $t$ of a graph $G$ is a transitional labeling of $G$ that is not a polarization. Now we present a bound for the value of a quasipolarization of a connected graph $G$.

**Theorem 3.3** If $t$ is a quasipolarization of a connected graph $G$ of size $q$, then

$$v_t \leq \left\lfloor \frac{2q}{3} \right\rfloor.$$
Proof. We may assume that $G$ has no positive pole. Let $Z$ be the set of zero vertices of $G$ and let $z = |Z|$. From Lemma 2.1 we have

$$m_t^- \geq |G| - |H|$$

and

$$m_t^+ \leq |E(H)|,$$

where $H = \langle Z \rangle$. Since $|G| = 2p + v(G) - 1$ and $|H| = 2z + v(H) - k(H)$, it follows that

$$m_t^- \geq 2(p - z) + (v(G) - v(H)) + (k(H) - 1)$$

and

$$m_t^+ \leq z + v(H) - k(H).$$

Since every graph has at least one component, we obtain by Lemma 3.2

$$m_t^- \geq 2(p - z)$$

and

$$m_t^+ \leq z + v(G) - 1.$$

We now divide the remainder of the proof into two cases.

Case 1. Assume $z \leq \frac{2p - v(G) + 1}{3}$.

Since $z \leq \frac{2p - v(G) + 1}{3}$ is equivalent to $z + v(G) - 1 \leq 2(p - z)$, we have $m_t^+ \leq m_t^-$. Therefore,

$$v_t = \min \{ m_t^-, m_t^+ \} = m_t^- \leq z + v(G) - 1 \leq \frac{2p - v(G) + 1}{3} + v(G) - 1.$$
\[ \leq \frac{2}{3} (p + v(G) + 1) \]
\[ \leq \frac{2}{3} q. \]

Case 2 Assume \( z > \frac{2p - v(G) + 1}{3} \).

Since \( |G| - z \) elements of \( G \) are labeled \(-1\) or \(1\) by \( t \),

\[
v_t \leq \frac{|G| - z}{2} < \frac{1}{2} \left( (2p + v(G) - 1) - \frac{2p - v(G) + 1}{3} \right) \]
\[ < \frac{2}{3} (p + v(G) - 1) \]
\[ < \frac{2}{3} q. \quad \Box \]

The upper bound given in Theorem 3.3 is sharp since this bound is attained by paths, as we next show. In Figure 3.1 we present a transitional labeling \( t \) of \( P_{3k+r} \), where \( k \) is a positive integer and \( r \) is an integer with \( 0 \leq r \leq 2 \). This transitional labeling is a quasipolarization and its value is

\[
v_t = \left\{ \begin{array}{ll}
2k - 1 & \text{if } r = 0 \\
2k & \text{otherwise,}
\end{array} \right.
\]

that is,

\[
v_t = \left\lfloor \frac{2}{3} (3k + r - 1) \right\rfloor.
\]

We will soon show that \( v_G \leq v_{K_p} \) for every connected graph \( G \) of order \( p \). Toward this goal, we present the following lemma.

Lemma 3.4 If \( p \geq 5 \), then \( \sigma(p) \leq p - 1 \).

Proof If \( p = 5, 6, 7 \), then \( \sigma(p) = 4, 5, 6 \), respectively. Assume \( p \geq 8 \). Then
\[ m_t^- = 2k \]

\[ m_t^+ = 2k + r - 1 \]

Figure 3.1

9p \leq p^2 + 8. So

\[ \frac{p^2 + p}{2} \leq p^2 - 4p + 4. \]

Then

\[ \sqrt{\frac{p(p + 1)}{2}} + 1 \leq p - 1. \]

Finally,

\[ \sigma(p) = \left\lfloor \sqrt{\frac{p(p + 1)}{2}} \right\rfloor \leq p - 1. \]

We are now prepared to present the aforementioned bound for \( v_G \).

**Theorem 3.5** If \( G \) is a connected graph of order \( p(\neq 3) \), then

\[ v_G \leq v_{K_p}. \]

**Proof** Let \( t \) be a transitional labeling of a connected graph \( G \) of order \( p \). We consider two cases.

**Case 1** Assume \( t \) is a polarization of \( G \). In this case \( p \geq 4 \). We prove that the bound for \( v_t \) given in the proof of Lemma 3.1 is at most \( v_{K_p} \). If \( p = 4 \), then
If \( p \geq 5 \), then, by Lemma 3.4, \( \sigma(p) \leq p - 1 \). A simple computation shows that this inequality is equivalent to

\[
\frac{p^2 - p + 2}{4} \leq \frac{1}{2} \left( \frac{p(p + 1)}{2} - \sigma(p) \right).
\]

Therefore,

\[
\left| \frac{p^2 - p + 2}{4} \right| = \frac{1}{2} \left( \frac{p(p + 1)}{2} - \sigma(p) \right) = v_{K_p}.
\]

**Case 2** Assume \( t \) is a quasipolarization of \( G \). In this case, we may assume that there is no vertex in \( G \) labeled 1 by \( t \). From \( t \), we construct a transitional labeling \( s \) of \( K_p \) as follows.

Start with the graph \( G \) labeled by \( t \). Now, suppose that \( u \) and \( v \) are nonadjacent vertices of \( G \). Then, if at least one of these vertices has a nonzero label, we add the edge \( uv \) labeled \(-1\) to \( G \); otherwise, we add the edge \( uv \) labeled \( 0 \).

Repeating the above procedure for each pair \( u, v \) of nonadjacent vertices in \( G \), we obtain a transitional labeling \( s \) of \( K_p \).

Note that \( m^{-}_{t} \leq m^{-}_{s} \) and \( m^{+}_{t} \leq m^{+}_{s} \). Therefore,

\[
v_{t} = \min \{ m^{-}_{t}, m^{+}_{t} \} \leq \min \{ m^{-}_{s}, m^{+}_{s} \} = v_{s} \leq v_{K_p}.
\]

From Cases 1 and 2 we have that if \( p \neq 3 \), then \( v_{t} \leq v_{K_p} \) for any transitional labeling \( t \) of \( G \). Hence,

\[
v_{G} \leq v_{K_p}
\]

for every \( p \neq 3 \). \( \square \)

For a connected graph \( G \) of order \( p \) having a relatively large number of edges, the bound \( v_{G} \leq v_{K_p} \) is smaller than the bound.
With respect to Theorem 3.5, observe that if \( p = 3 \) and \( G \equiv P_3 \), then \( V_G = 2 \) and \( v_{K_p} = 1 \). This exceptional situation also shows that it is not true that \( V_H \leq V_F \) for a subgraph \( H \) of a connected graph \( F \).

Next we present an infinite family \( \{G_k\} \) of graphs such that for each positive integer \( k \), the graph \( G_k \) contains a subgraph \( H_k \) with \( V_{H_k} > V_{G_k} \). Let \( H_k \) be the graph obtained by the identification of the central vertex of a path \( P_{2k+1} \) with an end-vertex of another copy of \( P_{2k+1} \). The graph \( G_k \) is obtained by joining two vertices \( u \) and \( v \) of \( H_k \) such that \( d(u,v) = 3k \). In Figure 3.2 we show the graphs \( H_k \) and \( G_k \) for \( k = 2 \).

![Figure 3.2](image.png)

We show that \( V_{H_k} = 4k \). Since the order of \( H_k \) is \( 4k + 1 \),

\[
|H_k| = 8k + 1 \quad \text{and} \quad V_{H_k} \leq \left\lfloor \frac{|H_k|}{2} \right\rfloor = 4k.
\]

Since there exists a transitional labeling of \( H_k \) whose value is \( 4k \), it follows that \( V_{H_k} = 4k \). Now we show that \( V_{G_k} < 4k \). The order and the size of \( G_k \) are equal to \( 4k + 1 \). Therefore, \( |G_k| = 8k + 2 \). Suppose that \( t \) is a transitional labeling of \( G_k \). If \( t \) is a quasipolarization of \( G_k \), then by Lemma 3.3, we have \( V_t \leq \left\lfloor \frac{2(4k + 1)}{3} \right\rfloor < 4k \).
Assume that \( t \) is a polarization of \( G_k \). If the unique cycle \( C \) of \( G_k \) is either a subgraph of the negative graph of \( t \) or of the positive graph of \( t \), then \( v_t \leq 2k \). Thus, we may assume that \( t \) restricted to \( C \) is a polarization of \( C \). Hence \( z_t \geq 2 \). If \( z_t > 2 \), then the number of nonzero elements of \( t \) is at most \( |G_k| - 3 = 8k - 1 \). Therefore, \( v_t \leq \left\lfloor \frac{8k - 1}{2} \right\rfloor = 4k - 1 \). If \( z_t = 2 \), then \( v_t \leq 4k \) and, moreover, \( v_t = 4k \) implies that \( m_t^+ = m_t^- = 4k \). Suppose, to the contrary, that there exists such a polarization \( t \) of \( G_k \) satisfying \( z_t = 2 \) and \( v_t = 4k \). Then, it turns out that \( m_t^+ \) and \( m_t^- \) must be odd. This contradiction shows that \( v_t < 4k \) in this case as well.

If \( H \) is an induced subgraph of \( G \), then we have the following result.

**Theorem 3.6** If \( H \) is an induced subgraph of a graph \( G \), then

\[
v_H \leq v_G.
\]

**Proof** Let \( F \) be an induced subgraph of a graph \( G \). Suppose first that \( p(F) = p(G) - 1 \). Let \( v \) denote the unique vertex of \( G \) that is not in \( F \), and let \( t \) be a transitional labeling of \( F \). We extend \( t \) to a transitional labeling \( t' \) of \( G \) as follows:

\[
\begin{align*}
t'(v) &= 0 \\
t'(vx) &= t(x) & \text{if } vx \in E(G) \\
t'(z) &= t(z) & \text{if } z \in V(F) \cup E(F).
\end{align*}
\]

Then \( m_t^+ \leq m_t^- \) and \( m_t^- \leq m_t^+ \). Hence, if \( t \) is also an optimal transitional labeling of \( F \), we have

\[
v_H = v_t = \min\{m_t^-, m_t^+\} \leq \min\{m_t^-, m_t^+\} = v_t' \leq v_G.
\]

Now by proceeding inductively, we see that for every induced graph \( H \) of \( G \), we have \( v_H \leq v_G \). \( \square \)
Since complete graphs have no polarizations, $v_{K_p}$ is achieved by means of transitional labelings that are quasipolarizations. A natural question arises. Does there exist a connected noncomplete graph $G$ such that $v_G$ is achieved only by means of transitional labelings that are quasipolarizations? Or, equivalently, does there exist such a graph $G$ for which $v_G > v_G^*$? In order to answer this question, it is convenient to define, for a connected, noncomplete graph $G$,

$$d = \left\lfloor \frac{|G| - \kappa(G)}{2} \right\rfloor - v_G^*.$$

Because of the bound (3.1), it follows that $d \geq 0$. Assume now that $G$ is a connected and noncomplete graph for which $v_G > v_G^*$. Assume that $t$ is an optimal transitional labeling of $G$ such that no vertex of $G$ is labeled 1 by $t$. We claim that

$$z_t < \kappa(G) + 2d; \quad (3.6)$$

for suppose, to the contrary, that $z_t \geq \kappa(G) + 2d$. Then since

$$v_G \leq \left\lfloor \frac{|G| - z_t}{2} \right\rfloor,$$

it follows that

$$v_G \leq \left\lfloor \frac{|G| - \kappa(G) - 2d}{2} \right\rfloor = v_G^*,$$

which contradicts our assumption.

We also claim that

$$m^-_t - m^+_t < \kappa(G) + 2d - z_t. \quad (3.7)$$

If this were not the case, then $m^-_t - m^+_t \geq \kappa(G) + 2d - z_t > 0$ by (3.6), which implies that

$$v_G = v_t \leq \left\lfloor \frac{|G| - m^-_t - m^+_t - z_t}{2} \right\rfloor \leq \left\lfloor \frac{|G| - \kappa(G)}{2} \right\rfloor - d = v_G^*,$$

again producing a contradiction.
Next we apply Lemma 2.2 and obtain
\[ m_t^- \geq |G| - \frac{(\kappa(G) + 2d - 1)(\kappa(G) + 2d)}{2} = a, \]
\[ m_t^+ \leq \frac{(\kappa(G) + 2d - 1)(\kappa(G) + 2d - 2)}{2} = b, \]
and
\[ m_t^- - m_t^+ \geq a - b = |G| - (\kappa(G) + 2d - 1)^2. \quad (3.8) \]

Combining (3.7) and (3.8), we obtain the following lemma.

**Lemma 3.7** Let \( G \) be a connected noncomplete graph for which \( v_G > v_G^* \).
Moreover, suppose that \( t \) is an optimal transitional labeling of \( G \). Then
\[ \kappa(G) + 2d - z_t + (\kappa(G) + 2d - 1)^2 > |G| \cdot \quad (3.9) \]

In particular, if \( G \) has an optimal transitional labeling \( t \) such that \( z_t = \kappa(G) + 2d - 1 \), then (3.9) becomes
\[ \kappa(G) + 2d - 1 \geq \sqrt{|G|} \]
which is equivalent to
\[ \kappa(G) + 2d > \sigma(G). \]
If we further assume that \( d = 0 \), then
\[ \kappa(G) > \sigma(G). \quad (3.10) \]

Once again, assume that \( G \) is a connected, noncomplete graph of order \( p \) and size \( q \) for which \( v_G > v_G^* \). Suppose now that \( d = 0 \) and that \( G \) has an optimal transitional labeling \( t \) with \( z_t = \kappa(G) + 2d - 1 \). Then
(i) \( \kappa(G) > \sigma(G), \)
(ii) \( \frac{p(p + 1)}{2} \geq |G| \), and

(iii) \( p \leq \frac{2|G|}{\kappa(G) + 2} \).

Inequality (iii) can be obtained from the fact that

\[
|G| = p + q \geq p + \frac{\delta(G)p}{2} \geq p + \frac{\kappa(G)p}{2}.
\]

By assigning values to \(|G|\), we can use inequalities (i), (ii) and (iii) to search for possible values of \( \kappa(G) \) and \( p \). We did this by means of a computer program that finds those values of \( \kappa(G) \) and \( p \) for \( 1 \leq |G| \leq m \), for a given positive integer \( m \). Table 3.1 shows the outcome for \( m = 66 \), which is the cardinality of \( K_{11} \).

Table 3.1

| \( |G| \) | \( \kappa(G) \) | \( p \) |
|---|---|---|
| 61 | 9 | 11 |
| 62 | 9 | 11 |
| 63 | 9 | 11 |
| 64 | 9 | 11 |

If \( G \) satisfies the first outcome of Table 3.1, then \( G \) is isomorphic to \( K_{11} - F \) where \( F \) is a maximum matching. It is straightforward to find a polarization of \( G \) to prove that \( d = 0 \). So

\[
v_G^* = \left\lfloor \frac{|G| - \kappa(G)}{2} \right\rfloor = 26.
\]
On the other hand, $\kappa(G) = 9$ and hence $z_t = 8$. Therefore,

$$v_G^* < v_G = v_t \leq \left\lfloor \frac{|G| - z_t}{2} \right\rfloor = 26.$$  

This contradiction shows that there is no such graph $G$ that satisfies the first outcome.

For the second outcome of Table 3.1, it turns out that $G$ is isomorphic to $K_{11} - F$ where $F$ is a matching with four edges. Similar to the first case, we can see that $d = 0$; so $v_G^* = 26$. In Figure 3.3 we show a transitional labeling $t$ of $G$ such that $z_t = 8$ and $v_t = 27$. Therefore, we have found a connected, noncomplete graph $G$ for which $v_G > v_G^*$. 

![Figure 3.3](image.png)
From the above we conclude that if there exists a connected graph \( G \neq K_p \) for which \( v_G > v^*_G \) and \( |G| < 62 \), then \( d > 0 \) or \( G \) has an optimal transitional labeling \( t \) such that \( z_t < \kappa(G) + 2d - 1 \). The problem of finding the smallest cardinality among all those graphs for which \( v_G > v^*_G \) remains open. A weaker form of Lemma 3.7 is now given.

**Corollary 3.8** If \( G \) is a connected, noncomplete graph with \( v_G > v^*_G \), then

\[
\kappa(G) + 2d - 3 + (\kappa(G) + 2d - 1)^2 > |G|.
\]

**Proof** By Lemma 3.7, it suffices to show that if \( t \) is an optimal transitional labeling of \( G \), then \( z_t \geq 3 \). Note that the order of \( G \) is at least 3 and since \( G \) is not complete, \( v^*_G \geq 1 \). Suppose, to the contrary, that \( G \) has an optimal transitional labeling \( t \) such that \( z_t < 3 \). Then, Lemma 2.2 implies that \( v_t \leq m^+ \leq 1 \), contradicting the fact that \( v_t = v_G > v^*_G \geq 1 \). \( \square \)

We now illustrate the last two results. Consider the complete bipartite graph \( K_{m,n} \) where \( m \leq n \) and \( n \geq 2 \). In Figures 3.4, 3.5, and 3.6 we exhibit a polarization \( t \) of \( K_{m,n} \) such that

\[
v_t = \left\lfloor \frac{mn}{2} \right\rfloor + \left\lceil \frac{n}{2} \right\rceil.
\]

(3.11)

Figure 3.4 illustrates the situation where \( n \) is even. Figure 3.5 shows the situation when \( n \) is odd and \( m \) is even, and in Figure 3.6, \( n \) and \( m \) are both odd.

Note that

\[
d \leq \left\lfloor \frac{|K_{m,n}| - \kappa(K_{m,n})}{2} \right\rfloor - v_t
\]

\[
\leq \left\lfloor \frac{mn + n}{2} \right\rfloor - \left( \left\lfloor \frac{mn}{2} \right\rfloor + \left\lceil \frac{n}{2} \right\rceil \right) = \begin{cases} 0 & \text{if } mn \text{ is even} \\ 1 & \text{otherwise.} \end{cases}
\]
Therefore, for \( G \equiv K_{m,n} \)

\[
\kappa(G) + 2d - 3 + (\kappa(G) + 2d - 1)^2 \leq x = \begin{cases} 
  m^2 - m - 2 & \text{if } mn \text{ is even} \\
  m^2 + 3m & \text{otherwise.}
\end{cases}
\]

Now \(|G| = mn + m + n \geq x\) if \( mn \) is even or if \( m < n \). Therefore, for these values of \( m \) and \( n \),

\[
|G| \geq \kappa(G) + 2d - 3 + (\kappa(G) + 2d - 1)^2.
\]  \( (3.12) \)

Consequently, by Corollary 3.8, \( v_G \leq v_G^* \), so that

\[
v_G = v_G^*.
\]

If neither \( mn \) is even nor \( m < n \), then \( m \) is odd and \( m = n \). In this case we claim that (3.12) also holds. Thus, let us assume that \( m \) is odd and \( m = n \), and suppose, to the contrary, that \( v_G > v_G^* \).
Let $s$ be an optimal transitional labeling of $G$ that has no positive pole. From (3.11) we have

$$m_s^+ \geq \nu_s = \nu_G > \nu_G^* \geq \left\lfloor \frac{m^2}{2} \right\rfloor + \left\lfloor \frac{m}{2} \right\rfloor = \frac{m(m + 1)}{2} - 1.$$  

So

$$m_s^+ \geq \frac{m(m + 1)}{2}.$$ 

Observe that each positive edge of $s$ is an edge of the subgraph $(Z_s)$ induced by the zero vertices of $s$. Since $m_s^+ > 0$, the subgraph $(Z_s)$ is not empty, which implies that $(Z_s)$ is isomorphic to a complete bipartite graph, say $K_{a,b}$. Moreover,

$$q((Z_s)) = ab \geq m_s^+ \geq \frac{m(m + 1)}{2}.$$
Assume now that $a$ and $b$ denote real variables, where $a, b > 0$. It is straightforward to prove that

$$a + b \geq 2\sqrt{\frac{m(m + 1)}{2}}.$$

Hence, for integers $a$ and $b$ we have

$$z_s = a + b \geq \begin{cases} m + 3 & \text{if } m \geq 5 \\ 5 & \text{if } m = 3. \end{cases}$$

If $m = 3$, then

$$v_G = v_s \leq \left\lfloor \frac{|K_{3,3}| - z_s}{2} \right\rfloor \leq 5 = v_t \leq v_G^*.$$
where $t$ is the polarization of $G$ whose value is given by (3.11). This contradiction completes the case $m = 3$.

Assume now that $m \geq 5$. Since $d \leq 1,$

$$\kappa(G) + 2d - z_s + (\kappa(G) + 2d - 1)^2 \leq m^2 + 2m.$$  

But $|G| = |K_{m,n}| = m^2 + 2m$. Therefore, by Lemma 3.7, we obtain the contradiction

$$m^2 + 2m \geq \kappa(G) + 2d - z_s + (\kappa(G) + 2d - 1)^2 > |G| = m^2 + 2m.$$  

We summarize our results as a lemma.

**Lemma 3.9** Let $G \equiv K_{m,n}$ where $m \leq n$ with $n \geq 2$. Then

$$v_G = v_G^*.$$  

The next lemma establishes the transitional value of $K_{m,n}$.

**Lemma 3.10** Let $m \leq n$ where $n \geq 2$. Then

$$v_{K_{m,n}} = \left[ \frac{mn}{2} \right] + \left[ \frac{n}{2} \right].$$  

**Proof** Suppose $G \equiv K_{m,n}$, where the partite sets are $V_1$ and $V_2$, with $|V_1| = m$ and $|V_2| = n$. If $mn$ is even, we know that $d = 0$. Thus,

$$v_G = v_G^* = \left[ \frac{|G| - \kappa(G)}{2} \right] = \left[ \frac{mn + n}{2} \right] = \left[ \frac{mn}{2} \right] + \left[ \frac{n}{2} \right].$$
Assume that \( mn \) is odd. Then \( m \) and \( n \) are odd. We know that \( d \leq 1 \) in this case. Suppose, to the contrary, that \( d = 0 \). Then, there exists an optimal transitional labeling \( s \) of \( G \) such that \( s \) is a polarization and

\[
v_s = \left\lfloor \frac{|G| - \kappa(G)}{2} \right\rfloor = \frac{mn + n}{2} = \frac{mn + n}{2}.
\]

We know that

\[
z_s \geq \kappa(G) = m,
\]

\[
m_s^- \geq v_s = \frac{mn + n}{2}
\]

and

\[
m_s^+ \geq v_s = \frac{mn + n}{2}.
\]

Since \( z_s + m_s^- + m_s^+ \leq |G| = mn + m + n \), it follows that

\[
z_s = m \quad \text{and} \quad m_s^- = m_s^+ = \frac{mn + n}{2}.
\]

Moreover, since \( Z_s \) is a separating set of cardinality \( m \), the set \( Z_s \) must be the partite set \( V_1 \). Assume now that \( x \) vertices of the partite set \( V_2 \) are labeled \(-1\) by \( s \). Then

\[
x + mx = m_s^- = m_s^+ = n - x + m(n - x).
\]

Thus, \( x(1 + m) = (n - x)(1 + m) \) and hence \( n = 2x \), which is a contradiction since \( n \) is odd. Therefore, \( d = 1 \) and

\[
v_G = v_G^* = \left\lfloor \frac{|G| - \kappa(G)}{2} \right\rfloor - 1
\]

\[
= \frac{mn + n}{2} - 1
\]

\[
= \left\lfloor \frac{mn}{2} \right\rfloor + \left\lfloor \frac{n}{2} \right\rfloor.
\]
3.2 Transitional Values of Trees

In this section we will be primarily concerned with trees $T$. We will establish a lower bound for $v^*_T$ and use this to prove that $v_T = v^*_T$, that is, each tree has an optimal transitional labeling that is a polarization. We also extend this result to unicyclic graphs.

Recall that a branch at a vertex $v$ (or rooted at a vertex $v$) of a tree $T$ is a maximal subtree containing $v$ as an end-vertex. Let $B$ be a branch at a vertex $v$ of $T$. Each element of $B$ that is different from $v$ is called a proper element of $B$. Then, the set $\mathcal{P}(B)$ of proper elements of $B$ is

$$\mathcal{P}(B) = V(B) \cup E(B) - \{v\}.$$  

Observe that $|\mathcal{P}(B)| = p(B) + (p(B) - 1) - 1 = 2(p(B) - 1)$, that is, the number of proper elements of $B$ is twice the number of proper vertices of $B$. For example, the tree $T$ of Figure 3.7 has two branches at $v_0$, namely $B_1$ and $B_2$. Note that $|\mathcal{P}(B_1)| = 6$ and $|\mathcal{P}(B_2)| = 36$.

Let $T$ be a tree of order at least 2 and let $M$ be a given positive integer with $M \leq |T| - 2$. Our next result is an algorithm that allows us to construct a transitional labeling $s$ of $T$ for which $M \leq m^+_s \leq M + 1$. Before formally presenting this algorithm, we illustrate it with the tree $T$ of Figure 3.7 for $M = 17$.

Arbitrarily select a vertex $v_0$ of $T$ which we initially label 0. Since $|\mathcal{P}(B_1)| = 6 < M < 42 = |\mathcal{P}(B_1)| + |\mathcal{P}(B_2)|$, we assign the label 1 to all the proper elements of the branch $B_1$ (see Figure 3.8(a)). Next, we assign 0 to the unique vertex $v_1$ of $B_2$ that is adjacent to $v_0$. Note that the vertex $v_0$ can be relabeled 1. We also label the edge $v_0v_1$ by 1. Thus, we obtain the partial labeling of $T$ shown in Figure 3.8(b). Denote the three branches at $v_1$ that do not contain $v_0$ by $B_1', B_2'$ and $B_3'$. These
Figure 3.7

have 6, 12, and 16 proper elements, respectively. Thus far, 8 elements of $T$ have been labeled 1. Observe that $|\phi(B'_1)| = 6 < M - 8 < 18 = |\phi(B'_1)| + |\phi(B'_2)|$.

We then proceed to label all the proper elements of $B'_1$ with the label 1 (see Figure 4(c)).

Next, we label the unique vertex $v_2$ of $B'_2$ adjacent to $v_1$ by 0 and label the edge $v_1v_2$ by 1. This time we retain the label 0 of the vertex $v_1$ in order to have
available the proper elements of $B_3$ to be labeled $-1$. The partial labeling so obtained is shown in Figure 3.8(d).

Let $B_1''$ be the branch at $v_2$ not containing $v_1$ that has four proper elements, and let $B_2''$ be the other such branch. At this step, 15 elements of $T$ have been labeled 1. Note that $0 < M - 15 < 4 = \left| \varphi(B_1'') \right|$. Then, we label the unique vertex $v_3$ of $B_1''$ that is adjacent to $v_2$ by 0 and label the edge $v_2v_3$ by 1 (see Figure 3.8(e)). We retain the label 0 of the vertex $v_2$ in order to have available the proper elements of $B_2''$ to be labeled $-1$.

Denote by $B_1'''$ the unique branch at $v_3$ that does not contain $v_2$, where, then, $\left| \varphi(B_1''') \right| = 2$. At this step, 16 elements of $T$ have been labeled 1. Note that $0 < M - 16 < \left| \varphi(B_1''') \right|$. Then, label the unique vertex $v_4$ of $B_1'''$ that is adjacent to $v_3$ by 0.

Relabel the vertex $v_3$ with 1 and label the edge $v_3v_4$ by 1. Thus, we obtain the partial labeling shown in Figure 3.8(f) which has 18 positive elements. We finally complete the labeling $s$ of $T$ by assigning the label $-1$ to each element of $T$ that has not been previously labeled. The transitional labeling $s$ so obtained is shown in Figure 3.9. Observe that the procedure described above also assures that $s$ can be chosen satisfying $z_s \leq e(v_0)$, where $e(v_0)$ denotes the eccentricity of $v_0$.

A formal presentation of this algorithm is now given.

**Algorithm 3.11** Let $T$ be a given tree of size $q \geq 1$ and $M$ a given positive integer with $M \leq |T| - 2$.

1.1 [An initial root is selected.]

Select an arbitrary vertex $v_0$ of $T$ and define $M_0 = M$.  

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Figure 3.8

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Figure 3.9

1.2 [An integer $k_1$ is selected such that the total number of proper elements of the branches $B_1, B_2, ..., B_k$ at $v_0$ is at least $M_0$.]

Label the branches of $T$ at $v_0$ by $B_j$, where $1 \leq j \leq \deg v_0$, in such a way that $|\varnothing(B_g)| \leq |\varnothing(B_h)|$, if $1 \leq g < h \leq \deg v_0$. Then, there exists a smallest integer $k_1$, with $1 \leq k_1 \leq \deg v_0$, such that

$$\sum_{j=1}^{k_1} |\varnothing(B_j)| \geq M_0.$$ 

(The existence of $k_1$ is guaranteed since $\sum_{j=1}^{\deg v_0} |\varnothing(B_j)| = |T| - 1 > M_0$.)

1.3 [A new root is selected.]

Let $v_1$ be the unique vertex of $B_{k_1}$ that is adjacent to $v_0$.

1.4 [The set $A_1$ of elements of $T$ which will be assigned label 1 is defined.]

Define

$$\Delta = \begin{cases} \{v_0v_1\} & \text{if } k_1 < \deg v_0 \\ \{v_0v_1, v_0\} & \text{if } k_1 = \deg v_0 \end{cases}$$

and
\[ A_1 = \begin{cases} 
\Delta \cup \bigcup_{j=1}^{k_1-1} \emptyset(B_j) & \text{if } k_1 > 1 \\
\Delta & \text{if } k_1 = 1
\end{cases} \]

1.5 [The number \( M_j \) of elements of \( T \) that are left to be labeled 1 is defined.]

Since \( |A_1| \) elements of \( T \) have been selected to assign them the label 1, the number \( M_1 \) of elements of \( T \) that are left to be labeled 1 is

\[ M_1 = M_0 - |A_1|. \]

If \( M_1 \leq 0 \) then define \( I = 1 \) and go to Step 4.

2. Given that \( v_{i-1}, v_i, A_i \) and \( M_i > 0 \) have been obtained for some \( i \), where \( i \geq 1 \), we define \( v_{i+1}, A_{i+1} \) and \( M_{i+1} \) as follows.

2.1 [An integer \( k_i \) is selected such that the total number of proper elements of the branches \( B_1^{(i)}, B_2^{(i)}, \ldots, B_k^{(i)} \) at \( v_i \) is at least \( M_i \).]

Denote by \( B_j^{(i)} \), where \( 1 \leq j \leq \deg v_i - 1 \), the branches of \( T \) at \( v_i \) that do not contain \( v_{i-1} \) in such a way that \( |\emptyset(B_g^{(i)})| \leq |\emptyset(B_h^{(i)})| \) if \( 1 \leq g < h \leq \deg v_i - 1 \). Then there exists a smallest integer \( k_i \), with \( 1 \leq k_i \leq \deg v_i - 1 \) such that

\[ \sum_{j=1}^{k_i} |\emptyset(B_j^{(i)})| \geq M_i. \]

(The existence of such an integer \( k_i \) will be guaranteed by Lemma 12, to follow shortly.)

2.2 [If the total number of proper elements of the branches \( B_1^{(i)}, B_2^{(i)}, \ldots, B_k^{(i)} \) is at most \( M_i + 1 \), then the set \( A_i + 1 \) of elements of \( T \) which will be assigned the label 1 is defined.]
If
\[ \sum_{j=1}^{k_i} |\phi(B_j^{(i)})| \leq M_i + 1, \]
then define
\[ A_{i+1} = \bigcup_{j=1}^{k_i} B_j^{(i)}, \]
and then go to Step 4.

2.3.1 [If the total number of proper elements of the branches \( B_1^{(i)}, B_2^{(i)}, \ldots, B_k^{(i)} \) is greater than \( M_i + 1 \), then a new root \( v_i + 1 \) is selected and the set \( A_i + 1 \) of elements of \( T \) which will be assigned the label 1 is defined.]

If
\[ \sum_{j=1}^{k_i} |\phi(B_j^{(i)})| > M_i + 1, \]
then choose \( v_{i+1} \) as the unique vertex of \( b_{k_i}^{(i)} \) that is adjacent to \( v_i \). Define
\[ \Delta = \begin{cases} \{v_{i}v_{i+1}\} & \text{if } k_i < \deg v_i + 1 \\ \{v_{i}v_{i+1}, v_i\} & \text{if } k_i = \deg v_i + 1 \end{cases} \]
and
\[ A_{i+1} = \begin{cases} \Delta \cup \bigcup_{j=1}^{k_i} \phi(B_j^{(i)}) & \text{if } k_i > 1 \\ \Delta & \text{if } k_i = 1 \end{cases} \]

2.3.2 [The number \( M_{i+1} \) of elements of \( T \) that are left to be labeled 1 is defined.]

Since \( |A_{i+1}| \) elements of \( T \) have been selected to assign them the label 1, the
number \( M_{i+1} \) of elements of \( T \) that are left to be labeled 1 is

\[
M_{i+1} = M_i - |A_{i+1}|
\]

If \( M_{i+1} \leq 0 \), then define \( i = i + 1 \) and go to Step 4.

3. \( \text{[This step updates the value } i.\text{]} \)
   
   Replace \( i \) by \( i + 1 \) and return to Step 2.

4. \( \text{[A labeling of the elements of } T \text{ is defined.]} \)
   
   Let
   \[
   A = \bigcup_{i=1}^{I} A_i.
   \]
   
   Let \( s \) be the labeling of \( T \) such that
   
   (i) each element of \( A \) is labeled 1 by \( s \),
   (ii) \( Z_s = \{ v_0, v_1, \ldots, v_I \} \setminus A \), and
   (iii) the remaining elements of \( T \) are labeled -1 by \( s \).

From the definitions of \( k_i \) and \( M_i \) given in Algorithm 3.11, we obtain the following properties.

**Lemma 3.12** Let \( I \) be a positive integer.

(a) If \( i \) is an integer with \( 1 \leq i \leq I - 1 \), then

\[
\sum_{j=1}^{k_i} |g(B_j^{(i)})| \geq M_i
\]

and

\[
\sum_{j=1}^{k_{i-1}} |g(B_j^{(i)})| \leq M_i - 1.
\]

(b) If \( i \) is an integer with \( 1 \leq i \leq I \), then
The next lemma verifies the existence of $k_i$ in Step 2 of Algorithm 3.11.

**Lemma 3.13** If $M_i > 0$ for some $i \geq 2$, then there exists an integer $k$ with $1 \leq k \leq \deg v_i - 1$, such that

$$\sum_{j=1}^{k} |\varphi(B_j^{(i)})| \geq M_i.$$

**Proof** First we note that

$$\deg v_i - 1 \quad \varphi(B_{k_i-1}^{(i-1)}) = \bigcup_{j=1}^{k_i-1} \varphi(B_j^{(i)}) \cup \{v_i, v_{i-1}, v_i\}, \quad i \geq 2.$$  

Then

$$\sum_{j=1}^{\deg v_i - 1} |\varphi(B_j^{(i)})| = |\varphi(B_{k_i-1}^{(i-1)})| - 2. \quad (3.13)$$

On the other hand, from Lemma 3.12(a),

$$\sum_{j=1}^{k_{i-1}} |\varphi(B_j^{(i-1)})| \geq M_{i-1}.$$

Therefore,

$$|\varphi(B_{k_{i-1}}^{(i-1)})| \geq M_{i-1} - \sum_{j=1}^{k_{i-1}-1} |\varphi(B_j^{(i-1)})|. \quad (3.14)$$

Combining (3.13) and (3.14), we obtain...
Next we present some properties of labelings produced by Algorithm 3.11.

Lemma 3.14 Assume that $T$ is a tree of size $q \geq 2$ and $M$ is a positive integer with $M \leq |T| - 2$. Then, each labeling $s$ of $T$ obtained by applying Algorithm 3.11 to $T$ is a transitional labeling of $T$ such that

1. $M \leq m_s^+ \leq M + 1$, and
2. $z_s \leq c(v_0)$.

Proof We first note that any labeling $s$ obtained by applying the algorithm to $T$ is a transitional labeling of $T$. To prove (1) we consider three cases, depending on which step was performed immediately preceding step 4.

Case 1 Assume Step 1 was applied to $T$ immediately before Step 4. From this assumption we have $I = 1, M_1 \leq 0$ and

$$A_1 = \Delta \cup \bigcup_{j=1}^{k_1-1} B_j.$$ 

Then, using Lemma 3.12(a), we obtain

$$m_s^+ = |A_1| \leq 2 + \sum_{j=1}^{k_1-1} |B_j| \leq 2 + (M - 1) = M + 1.$$ 

Since $M_1 = M - |A_1| \leq 0$,

$$M \leq m_s^+ \leq M + 1.$$
Case 2  Assume Step 2.1 was applied to $T$ immediately before Step 4. From this assumption we have $I > 1$,

$$
\sum_{j=1}^{k_{I-1}} |\varnothing(B_j^{(I-1)})| \leq M_{I-1} + 1
$$

and

$$
A_I = \bigcup_{j=1}^{k_{I-1}} \varnothing(B_j^{(I-1)}).
$$

Using Lemma 3.12(a), we obtain

$$
M_{I-1} \leq |A_I| \leq M_{I-1} + 1. \tag{3.15}
$$

On the other hand, Lemma 3.12(b) implies that

$$
m^+_I = \sum_{i=1}^{I-1} |A_i| + |A_I| = (M - M_{I-1}) + |A_I|.
\tag{3.16}
$$

Combining (3.15) and (3.16) we obtain

$$
M \leq m^+_I \leq M + 1.
$$

Case 3  Assume Step 2.2 was applied to $T$ immediately before Step 4. From this assumption we have $I > 1$, $M_I \leq 0$ and

$$
A_I = \Delta \cup \bigcup_{j=1}^{k_{I-1} - 1} \varnothing(B_j^{(I-1)}).
$$

Using Lemma 3.12(a) we obtain

$$
|A_I| \leq 2 + \sum_{j=1}^{k_{I-1} - 1} \left|\varnothing(B_j^{(I-1)})\right| \leq 2 + (M_{I-1} - 1) = M_{I-1} + 1.
$$

Since $M_I = M_{I-1} - |A_I| \leq 0$, 

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\[ M_{L-1} \leq |A_1| \leq M_{L-1} + 1. \]

As in Case 2, since \[ m_s^+ = M - M_{L-1} + |A_1|, \] we obtain

\[ M \leq m_s^+ \leq M + 1. \]

To prove (2) we first note that \( v_0, v_1, ..., v_I \) is a path of \( T \). Therefore,

\[ z_s \leq I + 1 \leq e(v_0) + 1. \]

Suppose, to the contrary, that \( z_s = e(v_0) + 1 \). Then \( I = e(v_0) \geq 1 \) and \( v_I \) is an end-vertex of \( T \). Moreover, each vertex \( u \) adjacent to \( v_{L-1} \) (where \( u \neq v_{L-2} \) if \( I \geq 2 \)) is an end-vertex of \( T \). This implies that \( |\mathcal{B}(B_j^{(I-1)})| \geq 2 \) for all \( j = 1, 2, ..., \)

\[ \deg v_{L-1} - 1. \]

Observe that \( I = e(v_0) \) also implies that Step 2.2 was immediately applied before Step 4. Then \( M_{L-1} > 0 \) and

\[ \sum_{j=1}^{k_{L-1} - 1} |\mathcal{B}(B_j^{(I-1)})| > M. \]  \hspace{1cm} (3.17)

If \( k_{L-1} > 1 \) we obtain

\[ \sum_{j=1}^{k_{L-1} - 1} |\mathcal{B}(B_j^{(I-1)})| \geq M_{L-1}, \]

which contradicts the definition of \( k_{L-1} \). Therefore, \( k_{L-1} = 1 \) and (3.17) implies that \( M_{L-1} \leq 0. \) From this contradiction,

\[ z_s \leq e(v_0). \]

Now, using Lemma 3.14 we establish a lower bound for \( v_T^* \). Prior to doing this, we present the next lemma.

**Lemma 3.15** Let \( T \) be a tree of size \( q \geq 2 \) and let

\[ M' = q - \left\lfloor \frac{\text{diam} T}{2} \right\rfloor. \]

Then
0 < M' \leq |T| - 2.

**Proof** If $T \equiv P_3$, then $M' = 1 \leq |T| - 2$. Assume $q \geq 3$. Since $2 \leq \text{diam } T \leq q$, we obtain

$$M' \geq q - \frac{\text{diam } T}{2} - 1 \geq \frac{q}{2} - 1$$

and

$$M' \leq q - \frac{\text{diam } T}{2} = \frac{|T| - 1 - \text{diam } T}{2} \leq \frac{|T| - 3}{2} \leq |T| - 2. \quad \Box$$

**Theorem 3.16** If $T$ is a tree of size $q \geq 2$, then

$$v_t^* \geq q - \left\lfloor \frac{\text{diam } T}{2} \right\rfloor.$$

**Proof** Let $v$ be an end-vertex of $T$ and let $M = M'$. By Lemma 3.15, it follows that $0 < M \leq |T| - 2$. Then we may apply Algorithm 3.11 to $T$ for the given value of $M$, where we select $v_0 = v$. Thus, from Lemma 3.14, we obtain a transitional labeling $s$ of $T$ such that (1) $M \leq m_s^- \leq M + 1$, and (2) $z_s \leq \text{diam } T$.

First we prove that $s$ is a polarization of $T$. Observe that in the process of applying Algorithm 3.11 to $T$ to obtain $s$, the value of $k_1$ (described in Step 1) satisfies the inequality $1 \leq k_1 \leq \text{deg } v_0 = 1$, so that $k_1 = 1$. This implies that in Step 1, $v_0 \in \Delta$ and $A_1 = \Delta$. Since $I \geq 1$, we have

$$v_0 \in \Delta = A_1 \subseteq \bigcup_{i=1}^{I} A_i = A.$$

From Step 4 of Algorithm 3.11, it follows that $v_0$ is a positive pole of $s$.

On the other hand, observe that Algorithm 3.11 assures the existence of a negative pole if $s$ satisfies $m_s^- > 0$. Since $T$ has no zero edge, $m_s^- + z_s + m_s^+ = |T| = 2q + 1$. By using (3.13) and (3.14), we have that
\[ m^-_s = |T| - m^+_s - z_s \]
\[ \geq 2q + 1 - (M + 1) - \text{diam } T \]
\[ \geq q - \left( \text{diam } T - \left\lfloor \frac{\text{diam } T}{2} \right\rfloor \right) \]
\[ \geq q - \left\lfloor \frac{\text{diam } T}{2} \right\rfloor \geq M > 0. \]

Therefore, \( s \) is a polarization of \( T \). Moreover, \( m^-_s \geq M \). Thus,

\[ v^*_s = \min\{m^-_s, m^+_s\} \geq M. \]

Consequently,

\[ v^*_T \geq v^*_s \geq M = q - \left\lfloor \frac{\text{diam } T}{2} \right\rfloor. \]

To establish one of the main results of this section we require two lemmas.

**Lemma 3.17** For a positive integer \( q \),

\[ \left\lfloor \frac{2q}{3} \right\rfloor \geq 2 \left\lfloor \frac{q + 1}{3} \right\rfloor \geq \left\lfloor \frac{2q}{3} \right\rfloor. \]

**Lemma 3.18** If \( T \) is a tree of size \( q \geq 2 \), then

\[ v^*_T \geq \left\lfloor \frac{2q}{3} \right\rfloor. \]

**Proof** We divide the proof into two cases.

**Case 1** Assume \( \text{diam } T \leq \frac{2q}{3} \). By Theorem 3.16,

\[ v^*_T \geq q - \left\lfloor \frac{\text{diam } T}{2} \right\rfloor \]
\[ \geq \left( \left\lfloor \frac{2q}{3} \right\rfloor + \left\lfloor \frac{q}{3} \right\rfloor \right) - \left\lfloor \frac{q}{3} \right\rfloor = \left\lfloor \frac{2q}{3} \right\rfloor. \]

**Case 2** Assume \( \text{diam } T > \frac{2q}{3} \). From Lemma 3.17,
diam $T \geq \left\lceil \frac{2q}{3} \right\rceil \geq 2x$, where $x = \left\lceil \frac{q + 1}{3} \right\rceil$.

Let $P: v_0, v_1, \ldots, v_{2x+1}$ be a path of length $2x$ in $T$ and let $t$ be the polarization of $P$ shown in Figure 3.10. Note that $v_t = 2x$. Since $P$ is an induced subgraph of $T$, we can extend $t$ to a polarization $t'$ of $T$ as we did in the proof of Theorem 2.4. Then, applying Lemma 3.17, we obtain

$$v_T^* \geq v_{t'} \geq v_t = 2x \geq \left\lceil \frac{2q}{3} \right\rceil.$$  \hfill \Box

Figure 3.10

**Theorem 3.19** If $T$ is a tree of size at least 2, then

$$v_T = v_T^*.$$  \hfill \Box

**Proof** Let $T$ be a tree of size $q \geq 2$. Then, from Lemma 3.18,

$$v_T^* \geq \left\lceil \frac{2q}{3} \right\rceil.$$  \hfill \Box

On the other hand, if $s$ is a transitional labeling of $T$ that is a quasipolarization, then by Theorem 3.3,

$$v_s \leq \left\lceil \frac{2q}{3} \right\rceil.$$  \hfill \Box

Therefore,

$$v_T = v_T^*.$$  \hfill \Box

Now we proceed to improve the bound given in Theorem 3.16 for the transitional value of a tree $T$. The idea is to apply Algorithm 3.11 to $T$, where $v_0$ is
selected as a central vertex of $T$, in order to obtain a transitional labeling $s$ of $T$ with $z_s \leq \text{rad} T$. The selection of $v_0$ as a central vertex of $T$ does not guarantee that the transitional labeling $s$ so obtained is a polarization of $T$. For example, in Figure 3.11, we show a tree $T$ and the transitional labeling $s$ of $T$ obtained by applying Algorithm 3.11 to $T$ for $M = 2$, choosing the central vertex of $T$ as $v_0$. Since $t$ has no positive pole, $t$ is not a polarization. Nevertheless, for the particular value of $M$ we will use, it is possible to prove that the transitional labeling so obtained is a polarization of $T$. The next lemma assures us that this value of $M$ satisfies the requirements of Algorithm 3.11.

![Figure 3.11](image_url)

**Lemma 3.20** Let $T$ be a tree of size $q \geq 4$ and let

$$M'' = q - \left\lfloor \frac{\text{rad} T}{2} \right\rfloor.$$

Then
Proof Since \( \text{rad } T \leq \text{diam } T \), it follows that \( 0 < M' \leq M'' \). On the other hand, since \( \text{rad } T \geq 1 \),
\[
M'' \leq q - 1 \leq |T| - 2. \quad \square
\]

**Theorem 3.21** If \( T \) is a tree of size at least 4, then
\[
\nu_T^* \geq q - \left\lceil \frac{\text{rad } T}{2} \right\rceil.
\]

**Proof** Let \( v \) be a central vertex of \( T \) and let \( M = M'' \). By Lemma 3.20,
\( 0 < M \leq |T| - 2 \). Then we may apply Algorithm 3.11 to \( T \) for the given value of \( M \), where \( v_0 = v \). Thus, we obtain a transitional labeling \( s \) of \( T \) such that
\[
M \leq m_s^+ \leq M + 1 \tag{3.18}
\]
and
\[
z_s \leq \text{rad } T. \tag{3.19}
\]

Similar to the proof of Theorem 3.16 we obtain \( m_s^- \geq M > 0 \). Since \( m_s^- > 0 \), Algorithm 3.11 assures us that \( s \) has at least one negative pole. Suppose, to the contrary, that \( s \) has no positive pole. Then, we claim that \( k_i = 1 \) for all \( i = 0, 1, ..., I - 1 \); otherwise, if \( k_i > 1 \) for some \( i \), then \( \varphi(B_i^{(i)}) \subseteq A_{i+1} \subseteq A \) and, in particular, at least one vertex \( u \neq v_i \) of the branch \( B_i^{(i)} \) will be labeled \( 1 \) by \( s \). Consequently, the only positive elements of \( s \) are the edges of the path \( v_0, v_1, v_2, ..., v_1 \). Hence, \( M = I \leq \text{rad } T \); indeed, \( M < \text{rad } T \), for otherwise \( M = \text{rad } T \) and then \( v_1 \) is an end-vertex of \( T \) labeled \( 1 \) by \( s \). Therefore,
\[
M = q - \left\lceil \frac{\text{rad } T}{2} \right\rceil < \text{rad } T. \tag{3.20}
\]
Let $j = 0$ or $j = 1$, according to whether $\text{rad } T$ is even or odd, respectively.

Then inequality (3.20) is equivalent to

$$q - \frac{\text{rad } T - j}{2} < \text{rad } T.$$  

Then

$$\frac{2q + j}{3} < \text{rad } T.$$  

Since for any tree $T$ of size $q$

$$\text{rad } T \leq \left\lfloor \frac{q + 1}{2} \right\rfloor,$$  

we obtain

$$\frac{2q + j}{3} < \text{rad } T \leq \frac{q + 1}{2}.$$  

Therefore,

$$q \leq 3 - 2j.$$  

This contradiction shows us that $s$ has a positive pole. Thus, $s$ is a polarization of $T$.

Since

$$v_s \geq \min \{m_s^-, m_s^+\} \geq M,$$  

we obtain

$$v_T^* \geq v_s \geq M = q - \left\lfloor \frac{\text{rad } T}{2} \right\rfloor. \quad \Box$$

Let $T$ be the tree shown in Figure 3.12. Note that $\text{rad } T = 2$. Therefore, from Theorems 3.19 and 3.21, $v_T = v_T^* \geq 5$. Observe that if $t$ is a transitional labeling of $T$ for which $z_t = 1$, then $v_t \leq 4$. Therefore, if $t$ is an optimal transitional labeling of $t$, then $z_t \geq 2$. Hence,

$$v_t \leq \left\lfloor \frac{|T| - z_t}{2} \right\rfloor = 5.$$  

Thus, for the tree $T$ of Figure 3.12, $v_T = 5$.  

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We have mentioned that \( \text{rad} \, T \leq \left[ \frac{q + 1}{2} \right] \) for a tree \( T \) of size \( q \). Therefore, from Theorem 3.21 we obtain

\[
v_T^* \geq q - \left[ \frac{\text{rad} \, T}{2} \right] = q - \left[ \frac{q + 1}{2} \right] = \frac{3q - j}{4},
\]

where \( j = 0, 3, 2, 1 \) if \( q \equiv 0, 1, 2, 3 \) (mod 4), respectively. Therefore,

\[
v_T^* \geq \left[ \frac{3q}{4} \right].
\]

and Lemma 3.18 is obtained as a corollary of Theorem 3.21.

**Corollary 3.22** If \( T \) is a tree of size \( q \), then

\[
v_T \geq \left[ \frac{3q}{4} \right].
\]

Now we present some results that can be obtained from another application of Algorithm 3.11. Let \( G \) be a connected graph and suppose that \( T \) is a spanning tree of \( G \). We may apply Algorithm 3.11 to \( T \) to obtain a transitional labeling \( t \) of \( T \) for which
Now, from $t$ we construct a transitional labeling $t'$ of $G$ as follows. Assume that no edge of $G$ joins two poles of distinct sign of $T$. Then for each $e = xy \in E(G) - E(T)$, we define

$$
t'(e) = \begin{cases} 
t(x) & \text{if } t(x) = t(y) \\
t(y) + t(x) & \text{if } t(x) \neq t(y). 
\end{cases}
$$

Otherwise, let $e_i = x_i y_i$, $i = 1, 2, ..., n$ be the edges of $G - E(T)$ that join poles of distinct sign of $T$, where $1 \leq n \leq v(G)$. Relabel all the vertices $x_1, x_2, ..., x_n, y_1, y_2, ..., y_n$ by 0 and label the edges of the sets $\{e_1, e_2, ..., e_r\}$ and $\{e_{r+1}, e_{r+2}, ..., e_n\}$ by 1 and -1 respectively, where $r = \left\lfloor \frac{n}{2} \right\rfloor$. Let $s$ be the transitional labeling so obtained. Then we can extend $s$ to a transitional labeling $t'$ of $G$ as we did previously.

Observe that, by construction, $t'$ satisfies

$$v_{t'} \geq v_t - v(G) + \left\lfloor \frac{v(G)}{2} \right\rfloor = v_t - \left\lfloor \frac{v(G)}{2} \right\rfloor.$$

Suppose that $G$ has size $q$. Then

$$v_G \geq v_t \geq \frac{3(q - v(G))}{4} - \left\lfloor \frac{v(G)}{2} \right\rfloor \geq \frac{3q}{4} - \left( \frac{5}{4} v(G) + 1 \right).$$

We formalize this result in the following theorem.

**Theorem 3.23** If $G$ is a connected graph of size $q$, then

$$v_G \geq \frac{3q}{4} - \left( \frac{5}{4} v(G) + 1 \right).$$

Observe that if $G$ is a connected graph for which
then, by Theorems 3.3 and 3.23,

$$\frac{3q}{4} - \left(\frac{5}{4} v(G) + 1\right) > \frac{2q}{3}, \quad (3.21)$$

where $t$ is any quasipolarization of $G$. Hence, condition (3.21) assures us that each optimal transitional labeling of $G$ is a polarization of $G$. Since (3.21) is equivalent to

$$v(G) < \frac{q - 12}{15},$$

we obtain the following property.

**Corollary 3.24** If $G$ is a connected graph with $v(G) < \frac{q - 12}{15}$, then each optimal transitional labeling of $G$ is a polarization.

The sufficient condition given in Corollary 3.24 can be expressed in terms of the density $\frac{q}{p}$ of $G$. From (3.21), we obtain

$$q - p + 1 < \frac{q - 12}{15},$$

or, equivalently,

$$\frac{q}{p} < \frac{15}{14} - \frac{27}{14p}.$$

**Corollary 3.25** If $G$ is a unicyclic graph of order $p \geq 28$, then every optimal transitional labeling of $G$ is a polarization of $G$.

**Proof** If $G$ is unicyclic and $p \geq 28$, then

$$\frac{q}{p} = 1 < \frac{15}{14} - \frac{27}{14p}. \quad \Box$$
CHAPTER IV

A CHEMICAL REACTIONS PATHWAY MODEL

4.1 On the Existence of Transitional Labelings With Prescribed Related Graphs

For two graphs $G_1$ and $G_2$, Johnson [5] showed how to construct a graph $G$ and a transitional labeling $t$ of $G$ such that the negative graph of $t$ is isomorphic to $G_1$ and the positive graph of $t$ is isomorphic to $G_2$. We describe this procedure. Let $G'$ be a common supergraph of $G_1$ and $G_2$. Let $H_1$ and $H_2$ be two subgraphs of $G'$ that are isomorphic to $G_1$ and $G_2$, respectively. Define a transitional labeling $t$ of $G = H_1 \cup H_2$ by

$$
t(x) = 
\begin{cases} 
-1 & \text{if } x \text{ is an element of } H_1 \text{ but not of } H_2 \\
1 & \text{if } x \text{ is an element of } H_2 \text{ but not of } H_1 \\
0 & \text{if } x \text{ is a common element of } H_1 \text{ and } H_2.
\end{cases}
$$

As an illustration, if $G_1$ and $G_2$ are the two graphs in Figure 4.1, we choose the common supergraph $G'$ of $G_1$ and $G_2$ and the subgraphs $H_1$ and $H_2$ of $G'$ shown in Figure 4.2. Thus, we obtain the transitional labeling $t$ of $G = H_1 \cup H_2$ shown in Figure 4.3.

Recall that a graph $F$ is a maximum common subgraph of the graphs $G_1$ and $G_2$ if $F$ is a graph of maximum cardinality that is isomorphic to a common subgraph of $G_1$ and $G_2$. A graph $G$ is a minimum common supergraph of $G_1$ and $G_2$ if $G$ is a graph of minimum cardinality that is isomorphic to a common supergraph of $G_1$ and $G_2$. 

86
Let $G$ be a minimum common supergraph of the graphs $G_1$ and $G_2$ and denote by $H_i$ a subgraph of $G$ isomorphic to $G_i$, $i = 1, 2$. Then

$$|G| = |H_1| + |H_2| - |F|$$

and so

$$|G| = |G_1| + |G_2| - |F|,$$

where $F = H_1 \cap H_2$. Note that $F$ is a common subgraph of $G_1$ and $G_2$. Moreover, equation (4.2) shows that $F$ is a maximum common subgraph of $G_1$ and $G_2$.

It follows from this last observation that in constructing the transitional labeling $t$ described in (4.1), if we choose $G'$ as a minimum common supergraph of $G_1$ and $G_2$, then the linking graph of $t$ is a maximum common subgraph of $G_1$ and $G_2$. In Figure 4.4 we show a transitional labeling $s$ whose negative and positive graphs are isomorphic to the graphs $G_1$ and $G_2$ of Figure 4.2, respectively, and where the linking graph of $s$ is a maximum common subgraph of $G_1$ and $G_2$.

A transitional labeling $t$ is said to be of maximum linkage if its linking graph is a maximum common subgraph of the positive and negative graphs of $t$. Thus, the transitional labeling shown in Figure 4.4 is of maximum linkage.
Lemma 4.1 If $t$ is a transitional labeling of maximum linkage of a graph $G$, then $t$ is a quasipolarization of $G$.

Proof If $t$ is a transitional labeling of maximum linkage of a graph $G$, then $G$ is a
minimum common supergraph of the negative graph $N$ and the positive graph $P$ of $t$. Suppose, to the contrary, that $G$ has poles with distinct signs, say $u$ and $v$. Observe that by identifying the vertices $u$ and $v$ in $G$ we obtain a common supergraph of $N$ and $P$ whose cardinality is less than the cardinality of $G$, contradicting the minimality of $G$. □

The converse of Lemma 4.1 is, in general, not true as is illustrated by the quasipolarization shown in Figure 4.5.

![Figure 4.4](image1)

![Figure 4.5](image2)

We already know that given graphs $G_1$ and $G_2$, there exists a transitional labeling such that its negative and positive graphs are isomorphic to $G_1$ and $G_2$, 

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respectively. Next we study those common subgraphs $F$ of $G_1$ and $G_2$ for which there exists such a transitional labeling whose linking graph is isomorphic to $F$. A sufficient condition for this is now presented.

**Lemma 4.2** Let $F_1$ and $F_2$ be isomorphic subgraphs of the given graphs $G_1$ and $G_2$, respectively, such that $F_1$ is induced in $G_1$ or $F_2$ is induced in $G_2$. Then there exists a transitional labeling $t$ of some graph $G$ such that the negative graph of $t$, the positive graph of $t$, and the linking graph of $t$ are isomorphic to $G_1$, $G_2$, and $F$, respectively, where $F_1 \equiv F \equiv F_2$.

**Proof** Without loss of generality, assume that $F_1$ is an induced subgraph of $G_1$. Suppose that $f: V(F_1) \rightarrow V(F_2)$ is an isomorphism of the graphs $F_1$ and $F_2$, where $V(F_1) = \{u_1, u_2, ..., u_k\}$ and $V(F_2) = \{v_1, v_2, ..., v_k\}$, such that $f(u_i) = v_i$ for $i = 1, 2, ..., k$. From $G_1$ and $G_2$ construct a graph $G$ by identifying the vertices $u_i$ and $v_i$ for $i = 1, 2, ..., k$. Thus, $G$ is a common supergraph of $G_1$ and $G_2$ and the set of the common vertices of $G_1$ and $G_2$ in $G$ is $V(F_1) = V(F_2)$. Clearly, the subgraphs $G_1$ and $G_2$ of $G$ share the edges of $F_1$ and $F_2$, and since $F_1$ is induced in $G_1$, no other common edge of $G_1$ and $G_2$ exists. Therefore, the subgraph $G_1 \cap G_2$ of $G$ is isomorphic to $F_1 (\equiv F)$. Using (4.1) for $H_1 = G_1$ and $H_2 = G_2$, we define a transitional labeling $t$ of $G$ that satisfies the required conditions. □

For example, for the graphs $G_1$ and $G_2$ of Figure 4.6, let $F \equiv P_4$. Note that $F$ is a common subgraph of $G_1$ and $G_2$. Moreover, $F$ is isomorphic to the subgraph $F_1$ of $G_1$ induced by the set $\{a, b, c, d\}$ of vertices. Choose any subgraph of $G_2$ isomorphic to $P_4$, say $F_2$, where $V(F_2) = \{f, g, h, i\}$ and $E(F_2) = \{fg, gh, hi\}$. The
Figure 4.6

graph $G$ is obtained by identifying vertices $a$, $b$, $c$, $d$ with $f$, $g$, $h$, $i$, respectively. In Figure 4.7(a), we show the resulting graph $G$. Labeling all the elements of $G$ that are common elements of $G_1$ and $G_2$ by 0, and labeling the remaining elements of $G$ that belong to $G_1$ and $G_2$ by $-1$ and $1$, respectively, we obtain a transitional labeling $t$ of $G$ such that $N \equiv G_1$, $P \equiv G_2$, and $L \equiv F$. We show $t$ in Figure 4.7(b).

The sufficient condition given in Lemma 4.2 is not a necessary condition as we may see by considering the transitional labeling shown in Figure 4.8.

Let $F$ and $G$ be graphs where $F$ is isomorphic to a subgraph of $G$. Among all the subgraphs of $G$ that are isomorphic to $F$, choose one whose vertices induce a subgraph of the smallest size and denote this size by $\tilde{q}_G(F)$. For example, for the graph $F \equiv 4K_1$ and the graphs $G_1$ and $G_2$ of Figure 4.1, we have $\tilde{q}_{G_1}(4K_1) = 2$ and $\tilde{q}_{G_2}(4K_2) = 5$. In the next lemma we present a necessary condition for the existence of a transitional labeling $t$ with a prescribed negative graph, positive graph, and linking graph.
Lemma 4.3  Let $F$ be a common subgraph of the graphs $G_1$ and $G_2$, where the order of $F$ is $p$. If $t$ is a transitional labeling of some graph $G$ whose negative graph $N$, positive graph $P$, and linking graph $L$ are isomorphic to $G_1, G_2$, and $F$, respectively, then

$$\bar{q}_{G_1}(F) + \bar{q}_{G_2}(F) - q(F) \leq \frac{p(p - 1)}{2}$$  \hspace{1cm} (4.2)
Proof Let $Z$ denote the set of vertices of the linking graph $L$ of $t$. Then the set $E((Z)_G) = E((Z)_N) \cup E((Z)_P)$, where $E((Z)_N) \cap E((Z)_P) = E(L)$. So

$q((Z)_G) = q((Z)_N) + q((Z)_P) - q(L)$.

Since $L$ is a subgraph of $(Z)_N$,

$q((Z)_N) \geq \tilde{q}_N(L) = \tilde{q}_{G_1}(F)$

and, similarly,

$q((Z)_P) \geq \tilde{q}_P(L) = \tilde{q}_{G_2}(F)$.

Therefore,

$\tilde{q}_{G_1}(F) + \tilde{q}_{G_2}(F) - q(F) \leq q((Z)_G) \leq \frac{p(p-1)}{2}$. \hfill \square$

To illustrate this lemma consider the graphs $G_1$ and $G_2$ shown in Figure 4.1 and let $F \equiv 4K_1$. We know that $\tilde{q}_{G_1}(4K_1) = 2$ and $\tilde{q}_{G_2}(4K_1) = 5$. Therefore, using Lemma 4.3 we conclude that there is no transitional labeling $t$ whose negative graph, positive graph, and linking graphs are isomorphic to $G_1$, $G_2$ and $F$, respectively.

We observe that the condition presented in Lemma 4.3 is not sufficient as we see by considering the graphs $G_1$ and $G_2$ shown in Figure 4.9 and $F \equiv 4K_1$. Since $\tilde{q}_{G_1}(F) = 2$ and $\tilde{q}_{G_2}(F) = 3$, these graphs satisfy (4.2). On the other hand, suppose, to the contrary, that there exists a transitional labeling $t$ of some graph $G$ such that the negative graph, the positive graph, and the linking graph of $t$ are isomorphic to $G_1$, $G_2$, and $F$, respectively. Then the order of $G$ is 4 and each vertex of $G$ is labeled 0. Therefore, $G_1$ and $G_2$ must be edge-disjoint subgraphs of a graph of order 4, which is impossible. Hence, there is no such transitional labeling $t$.

In view of Lemma 4.2 we present the following definition. The graph $F$ is said
to be a **universal link** if for any supergraphs $G_1$ and $G_2$ of $F$ satisfying (4.2), there exists a transitional labeling $t$ whose negative graph, positive graph, and linking graph are isomorphic to $G_1, G_2,$ and $F,$ respectively. For example, complete graphs are universal links; for if $F$ is a common complete subgraph of the graphs $G_1$ and $G_2,$ then $F$ is an induced subgraph of $G$. An application of Lemma 4.2 provides the existence of the required transitional labeling. On the other hand, if $F$ is complete, (4.2) is satisfied trivially. In Figure 4.10 we present all the noncomplete universal links of order at most 4.

For $F = K_p - E(K_2),$ $p \geq 2,$ let $G_1$ and $G_2$ be two supergraphs of $F$ for which (4.2) holds. It is straightforward to see that $F$ must be an induced subgraph of $G_1$ or $G_2.$ Hence, by Lemma 4.2, the graphs $K_p - E(K_2), p \geq 2$ are universal links.

**Theorem 4.4** The graphs $K_p - E(P_3), p \geq 3,$ and $K_p - E(2K_2), p \geq 4,$ are universal links.

**Proof** Let $F$ be isomorphic to a complete graph with two deleted edges. Let $G_1$ and $G_2$ be two supergraphs of $F$ such that (4.2) holds. If $F$ is either an induced subgraph of $G_1$ or of $G_2,$ then by Lemma 4.2, there exists a transitional labeling whose negative, positive, and linking graphs are isomorphic to $G_1, G_2,$ and $F,$ respectively. Then we may assume that $F$ is neither an induced subgraph of $G_1$ nor $G_2.$ Therefore,
\( p = 2: \)

\[ \begin{array}{c}
\circ \\
\circ \\
\end{array} \]

\( p = 3: \)

\[ \begin{array}{c}
\circ \\
\circ \\
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\end{array} \quad \begin{array}{c}
\circ \\
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\( p = 4: \)

\[ \begin{array}{c}
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Figure 4.10

\[ q_{G_1}(F) < \bar{q}_{G_1}(F) \quad \text{and} \quad q_{G_2}(F) < \bar{q}_{G_2}(F). \]

On the other hand, suppose that \( \bar{q}_{G_1}(F) = \frac{p(p-1)}{2} \). Then (4.2) implies that
\( \overline{q}_{G_2}(F) \leq q(F) \) and hence \( F \) is an induced subgraph of \( G_2 \). Therefore, 
\[
\overline{q}_{G_1}(F) < \frac{p(p - 1)}{2}
\]
and, similarly, 
\[
\overline{q}_{G_2}(F) < \frac{p(p - 1)}{2}.
\]
Then 
\[
\frac{p(p - 1)}{2} - 2 < \overline{q}_{G_i}(F) < \frac{p(p - 1)}{2}
\]
for \( i = 1, 2 \). Thus, 
\[
\overline{q}_{G_1}(F) = \frac{p(p - 1)}{2} - 1,
\]
and then \( G_1 \) and \( G_2 \) contain induced subgraphs isomorphic to \( K_p - E(K_2) \). Let \( H_1 \) and \( H_2 \) be two of these subgraphs of \( G_1 \) and \( G_2 \), respectively. We divide the remainder of the proof into two cases.

**Case 1** Assume \( F \equiv K_p - E(P_3) \), \( p \geq 3 \). Let \( u, v, \) and \( w \) be three distinct vertices of a complete graph \( J \) on \( p \) vertices. We define a transitional labeling \( t_1 \) of \( J \) by 
\[
t_1(y) = \begin{cases} 
-1 & \text{if } y = uv \\
1 & \text{if } y = vw \\
0 & \text{otherwise.}
\end{cases}
\]

Observe that the negative graph \( N \) and the positive graph \( P \) of \( t_1 \) are isomorphic to \( K_p - E(K_2) \) and that the linking graph of \( t_1 \) is isomorphic to \( F \). Recall that \( H_1 \) and \( H_2 \) are induced subgraphs of \( G_1 \) and \( G_2 \), respectively, that are isomorphic to \( K_p - E(K_2) \). Therefore, we can add a convenient number of negative elements and positive elements to the labeled graph \( J \) in order to extend \( t_1 \) to a
transitional labeling $t$ of some graph $G$ with the negative graph isomorphic to $G_1$ and the positive graph isomorphic to $G_2$. The linking graphs of $t$ and $t_1$ coincide. So the linking graph of $t$ is isomorphic to $F$ as required.

Case 2 Assume $F \equiv K_p - E(K_2)$, $p \geq 4$. Let $u$, $v$, $w$, and $x$ be four distinct vertices of a complete graph $J$ on $p$ vertices. We define a transitional labeling $t_2$ of $J$ by

$$t_2(y) = \begin{cases} -1 & \text{if } y = uv \\ 1 & \text{if } y = wx \\ 0 & \text{otherwise.} \end{cases}$$

Similar to Case 1, the negative graph and the positive graph of $t_2$ are isomorphic to $K_p - E(K_2)$ and the linking graph of $t_2$ is isomorphic to $F$. A similar argument to the previous case follows to prove that $t_2$ can be extended to a transitional labeling $t$ of a graph $G$ with the negative graph, positive graph, and linking graph isomorphic to $G_1$, $G_2$, and $F$, respectively. □

We illustrate Theorem 4.4 and its proof. Let $G_1$ and $G_2$ be the graphs shown in Figure 4.11. Observe that the universal link $C_4 \equiv K_4 - E(2K_2)$ is a subgraph of $G_1$ and $G_2$. Since $\bar{q}_{G_1}(C_4) = 5$ and $\bar{q}_{G_2}(C_4) = 5$, condition (4.2) is satisfied for $F \equiv C_4$. In Figure 4.12(a) we show a transitional labeling $t_2$ of the complete graph $J$ on four vertices. In Figure 4.12(b) we show a transitional labeling $t$ of a graph $G$ obtained by applying the construction given in the proof of Theorem 4.4.

The problem of characterizing those common subgraphs $F$ of two given graphs $G_1$ and $G_2$ for which there exists a transitional labeling $t$ of a graph $G$ such
that $N \equiv G_1$, $P \equiv G_2$, and $L \equiv F$ remains open, as does the problem of characterizing universal links.

Figure 4.11

Figure 4.12

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4.2 Modeling Chemical Reactions Pathways

A major part of this section is devoted to developing the chemical reactions pathways model introduced by Johnson in [5] from a somewhat different point of view. Assume that \( t_1 \) is a transitional labeling of a graph \( G_1 \) (\( i = 1, 2 \)). We say that \( t_1 \) is isomorphic to \( t_2 \) if there exists an isomorphism \( \phi \) between \( G_1 \) and \( G_2 \) such that the diagram of Figure 4.13 is commutative, that is,

\[
t_1 = t_2 \circ \bar{\phi},
\]

where \( \bar{\phi} \) is the extension of \( \phi \) to the edge sets of \( G_1 \) and \( G_2 \).

![Diagram](image)

For example, in Figure 4.14 we show two graphs \( G_1 \) and \( G_2 \) and the corresponding transitional labelings \( t_1 \) and \( t_2 \). If \( \phi: V(G_1) \rightarrow V(G_2) \) is the isomorphism of graphs defined by \( \phi(u_i) = v_i, i = 1, 2, 3, 4 \), then, \( t_1 = t_2 \circ \bar{\phi} \) and hence \( t_1 \) is isomorphic to \( t_2 \). It is straightforward to see that the relation "is isomorphic to" is an equivalence relation on any set of transitional labelings.

A transitional labeling \( t \) of a graph \( G \) is called trivial if all the elements of \( G \) are labeled 0 by \( t \). Let \( t \) be a nontrivial transitional labeling of a graph \( G \). The core
Figure 4.14

t_c of t is the restriction of t to the subgraph obtained from G by deleting all the zero edges and all the zero vertices that are not incident with a nonzero edge. For example, in Figure 4.15 we show a transitional labeling t of $K_1 \cup K_2 \cup P_3$ and the core $t_c$ of t.

From its definition, we can see that $t_c$ is the restriction of t to the subgraph H of G induced by the nonzero edges and the isolated vertices of G that are poles of G. Thus, $t_c$ is a transitional labeling of H. Two transitional labelings t and $t'$ are said to have the same core if $t_c \equiv t'_c$. This relation is an equivalence relation on any set of transitional labelings.
Let \( t \) and \( t' \) be transitional labelings of the graphs \( G \) and \( G' \), respectively. We write \( t \leq t' \) if \( t \) is isomorphic to a restriction of \( t' \). Observe that \( t \leq t' \) if and only if we can construct a transitional labeling from \( t \) that is isomorphic to \( t' \) by adding certain zero elements to the labeled graph \( G \). Thus, if \( t \leq t' \), then \( t_c \equiv t'_c \). If \( t \leq t' \) we say that \( t \) is a restriction of \( t' \) or that \( t' \) is an extension of \( t \). If \( t \leq t' \) but \( t \not= t' \), then we say that \( t' \) is a proper extension of \( t \). Observe that the relation \( \leq \) partially orders any set \( T \) of transitional labelings. Clearly, the relation \( \leq \) is reflexive and transitive. To see that \( \leq \) is also antisymmetric, suppose that \( t \) and \( t' \) are transitional labelings of the graphs \( G \) and \( G' \), respectively, such that \( t \leq t' \) and \( t' \leq t \). Then, \( t \) and \( t' \) must have an equal number of zero elements and, consequently, \( t \equiv t' \).

For example, consider the set \( T \) whose elements are the transitional labelings \( t_1, t_2, \ldots, t_9 \) shown in Figure 4.16. Note that these transitional labelings have isomorphic cores. Thus, \( T \) is partially ordered by the relation \( \leq \), and \( T \) ordered by \( \leq \) may be represented by the Hasse diagram in Figure 4.16. With respect to this example, an extension \( t \) of \( t_1 \) is of maximum linkage if and only if the negative graph and the positive graph of \( t \) are not isomorphic.

A transitional labeling \( t \) is called a transform if there exists an extension \( t' \) of \( t \) that is of maximum linkage, that is, the linking graph of \( t' \) is a maximum common subgraph of the negative and positive graphs of \( t' \). Thus, every transitional labeling of maximum linkage is a transform. Transforms have been introduced and utilized by Johnson [5] to model chemical reaction pathways. In Figure 4.17 we show the transitional labelings \( t_1 \) and \( t_3 \) of the previous example together with their corresponding negative and positive graphs. Since \( t_3 \) is of maximum linkage and \( t_1 \leq t_3 \), it follows that \( t_1 \) (and, of course, \( t_3 \) as well) is a transform. In this example observe that the linking graph of \( t_1 \) is not a maximum common subgraph of the
negative graph $N_1$ and the positive graph $P_1$ of $t_1$. So $t_1$ is not of maximum linkage.
In Figure 4.18 we present a transitional labeling \( t \) that is not a transform. To see this, first observe that for any extension \( s \) of \( t \), the linking graph \( L \) of \( s \) is a proper subgraph of the negative graph \( N \) of \( s \). On the other hand, observe that \( N \) and the positive graph \( P \) of \( s \) are isomorphic graphs and, hence, the maximum common subgraph of \( N \) and \( P \) is isomorphic to \( N \). From these two observations, we conclude that for every extension \( s \) of \( t \), the linking graph of \( s \) is not a maximum common subgraph of the negative graph \( N \) and the positive graph \( P \) of \( s \). Hence, \( t \) is not a transform.

Let \( t \) be a transform. An ordered pair \( (G_1, G_2) \) of unlabeled graphs is called an action of \( t \) if there exists an extension \( t' \) of maximum linkage of \( t \) such that the negative graph of \( t' \) is isomorphic to \( G_1 \) and the positive graph of \( t' \) is isomorphic to \( G_2 \). It follows from this definition that \((N, P)\) is an action of \( t \) whenever \( t \) is of
maximum linkage with negative graph $N$ and positive graph $P$. For example, if $t_1$ is the transform shown in Figure 4.17, then the pair $(N_3, P_3)$ formed by the graphs $N_3$ and $P_3$ shown in Figure 4.17 is an action of $t_1$ and of $t_3$.

Recall that a chemical reaction pathway can be represented by means of a digraph $D$ where each vertex of $D$ corresponds to an unlabeled graph and where it is assumed that this correspondence is one-to-one. Johnson [5] defined a metadigraph $M = (D, g)$ as a (possibly infinite) digraph $D = (V, E)$ together with an injective function $g: V \rightarrow \Gamma$, where $\Gamma$ is a set of unlabeled graphs. Thus, representations of chemical reaction pathways determine metadigraphs.

Let $M_1 = (D_1, g_1)$ and $M_2 = (D_2, g_2)$ be two metadigraphs where $D_1 = (V_1, E_1)$ and $D_2 = (V_2, E_2)$. Then $M_1$ is isomorphic to $M_2$ if there exists an isomorphism $\phi: V_1 \rightarrow V_2$ of the digraphs $D_1$ and $D_2$ such that $g_1(u) = g_2(\phi(u))$ for all $u \in V_1$.

A transform kit $K$ is an ordered pair $(T_g, T_b)$ of sets of transforms. The elements of $T_g$ are called the generating transforms of $K$ and the elements of $T_b$ are called the blocking transforms of $K$. Let $K = (T_g, T_b)$ be a transform kit and let $t \in T_g$ and $t' \in T_b$. Then an action $(G_1, G_2)$ of $t$ is blocked by $t'$ if

(i) $(G_1, G_2)$ is an action of $t'$ and
(ii) $t \leq t'$, that is, $t'$ is an extension of $t$.

For example, consider the set $T$ whose elements are those transitional labelings shown in Figure 4.16 and let $K = (T_g, T_b)$ with $T_g = \{t_1\}$ and $T_b = \{t_3\}$. As previously seen, $a_1 = (N_3, P_3)$ is an action of $t_1$ and $t_3$, where $N_3$ and $P_3$ are the graphs shown in Figure 4.17. Since $t_1 \leq t_3$, the action $a_1$ of $t_1$ is blocked by $t_3$. On the other hand, if $N_8$ and $P_8$ denote the negative and positive graphs of $t_8$ (see Figure 4.19), then $a_2 = (N_8, P_8)$ is an action of $t_1$ that is not blocked by $t_3$. If, on
the other hand, $a_2$ is blocked by $t_3$, then $a_2$ is an action of $t_3$. Therefore, there exists an extension of $t_3$ whose negative graph $N$ is isomorphic to $N_8$. Since $N$ contains the negative graph $N_3$ of $t_3$, the graph $N_8$ has a triangle, and a contradiction is obtained. For the transform kit $K' = (T_8', T_{b'})$, with $T_{b'} = \{t_2\}$, the actions $a_1$ and $a_2$ of $t_1$ are both blocked by the transform $t_2$.

![Diagram](image.png)

**Figure 4.19**

The actions of a transform kit $K$ are the actions of the generating transforms of $K$ that are not blocked by any blocking transform of $K$. Thus, in the corresponding previous example, $a_2$ is an action of $K$. Given a nonempty set $\Delta$ of unlabeled graphs and a transform kit $K$, we can associate with $\Delta$ and $K$ a metadigraph $A(\Delta, K)$ as follows. Each vertex of $A(\Delta, K)$ corresponds to an unlabeled graph of $\Delta$. Let $u$ and $v$ be vertices of $A(\Delta, K)$ with corresponding graphs $G_1$ and $G_2$, respectively. Then the vertex $v$ is adjacent from $u$ if $(G_1, G_2)$ is an action of $K$. For example, let $\Delta = \{G_1, G_2, G_3\}$ and $K = \{(t, r), (s)\}$, where $G_1, G_2, G_3$ and $r, s, t$ are the graphs and transitional labelings, respectively, shown in Figure 4.20.

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Observe that the extension $r'$ of $r$ is of maximum linkage and its negative and positive graphs are isomorphic to $G_1$ and $G_2$, respectively. Therefore, $(G_1, G_2)$ is an action of $r$ and of $r'$. A similar argument involving $r''$ proves that $(G_2, G_1)$ is an action of $r'' = t$ and $r$. So, $(G_2, G_1)$ is blocked by $t$. On the other hand, $(G_1, G_2)$ is not blocked by $t$. Thus, $(G_1, G_2)$ is an action of $K$ and $(G_2, G_1)$ is not. Moreover, $(G_2, G_3)$ and $(G_3, G_2)$ are actions of $s$ (to see this, consider the extensions $s'$ and $s''$ of $s$) that cannot be blocked by $t$ since $s$ and $t$ have distinct cores. Then $(G_2, G_3)$ and $(G_3, G_2)$ are actions of $K$. Finally, $G_1$ and $G_3$ have a unique maximum common subgraph, namely $P_4$. Then if $x$ is a transitional labeling of maximum linkage whose negative and positive graphs are isomorphic to $G_1$ and $G_3$, or to $G_3$ and $G_1$, respectively, then $x$ has a core distinct from the cores of $r$ and $s$. This shows that $(G_1, G_3)$ and $(G_3, G_1)$ are not actions of $r$ and $s$, and, consequently, are not actions of $K$. The resulting metadigraph $A(\Delta, K)$ is shown in Figure 4.20.

Suppose that the metadigraph $M$ is isomorphic to the metadigraph $A(\Delta, K)$ for some set $\Delta$ of unlabeled graphs and for a transform kit $K$. Then we say $(\Delta, K)$ is a specification for $M$. Our next goal is to present a theorem due to Johnson [5] that establishes the existence of a specification $(\Delta, K)$, for any given metadigraph $M$.

Recall that a transitional labeling $t$ of maximum linkage is itself a transform. If $N$ and $P$ are the negative and positive graphs of $t$, respectively, then $(N, P)$ is an action of $t$. The next lemma concerns this situation.

**Lemma 4.5** Let $t$ be a transitional labeling of maximum linkage of a graph $G$. Let $N$ and $P$ denote the negative and positive graphs of $t$, respectively. Then, there exists no transform $t'$ such that $t'$ is a proper extension of $t$ and $(N, P)$ is an action of $t'$. 

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Figure 4.20

$G_1$: $\quad G_2$: $\quad G_3$:  

$\quad r: -1 \quad r': -1 \quad t = r'': -1$  

$s: \quad s': \quad s'':$  

$K = \{(r, s), \{t\}\}$  

$\Delta = \{G_1, G_2, G_3\}$  

$A(\Delta, K)$:
Proof Suppose, to the contrary, that there exists a transform \( t' \) such that \( t' \) is a proper extension of \( t \) and \((N, P)\) is an action of \( t' \). Since \((N, P)\) is an action of \( t' \), there exists a transitional labeling \( t'' \) of some graph \( G'' \) that is of maximum linkage and whose negative graph and positive graph are isomorphic to \( N \) and \( P \), respectively. Thus, \( G \) and \( G'' \) are minimum common supergraphs of \( N \) and \( P \) and so \( |G| = |G''| \). On the other hand, \( t'' \) is a proper extension of \( t \). Thus, \( |G| < |G''| \) and a contradiction is obtained. □

Corollary 4.6 If \( K = (T_g, T_b) \) is a transform kit and the transform \( t \in T_g - T_b \) is of maximum linkage, then \((N, P)\) is an action of \( K \), where \( N \) and \( P \) are the negative and positive graphs of \( t \), respectively.

Proof Since \( t \in T_g - T_b \) it follows that any extension \( t' \) of \( t \) in \( T_b \) is a proper extension of \( t \). By Lemma 4.5, \((N, P)\) is not an action of \( t' \) for any \( t' \in T_b \). So, \((N, P)\) is an action of \( K \). □

For the given graphs \( G_1 \) and \( G_2 \), let \( t_m(G_1, G_2) \) denote the set of all the transitional labelings of maximum linkage whose negative and positive graphs are isomorphic to \( G_1 \) and \( G_2 \), respectively. For example, for the graphs \( G_1 \) and \( G_2 \) of Figure 4.20 we have \( t_m(G_1, G_2) = \{t_1, t_2\} \), where \( t_1 \) and \( t_2 \) are the transitional labelings shown in Figure 4.21.

Lemma 4.7 Let \( K = (T_g, T_b) \) be a transform kit. If \( G_1 \) and \( G_2 \) are graphs such that \( t_m(G_1, G_2) \subseteq T_b \), then \((G_1, G_2)\) is not an action of \( K \).

Proof Assume that \((G_1, G_2)\) is an action of some transform \( t \in T_g \). Then there exists a transitional labeling \( t' \) of maximum linkage such that \( t \leq t' \) and the negative graph and positive graph of \( t' \) are isomorphic to \( G_1 \) and \( G_2 \), respectively. Since
(G_1, G_2) is an action of t' and t' \in t_m(G_1, G_2) \subseteq T_b, we conclude that (G_1, G_2) is blocked by t'. Then (G_1, G_2) is not an action of K. □

Now we are prepared to prove the aforementioned result of Johnson [5].

**Theorem 4.8** For every metadigraph M, there exists a specification (\Delta, K) such that M \equiv A(\Delta, K).

**Proof** Let M = (D, g) be a metadigraph with D = (V, E) and g = V \rightarrow \Gamma. Let \Delta = g(V). For each arc e = (u, v) in E construct a transitional labeling t_e of maximum linkage whose negative graph and positive graph are isomorphic to the graphs g(u) and g(v), respectively. Let \( T_g = \{ t_e \mid e \in D \} \) and \( T_b = T_g' \), where \( T_g' \) is the complement of \( T_g \) with respect to the set of all transforms. We claim that (\Delta, K) with K = (T_g, T_b) is a specification for M.

To prove the claim, assume first that e = (u, v) is an arc of D. Then the transform \( t_e \in T_g - T_b \). By Corollary 4.6, (g(u), g(v)) is an action of K and so the
vertex of $A(\Delta, K)$ corresponding to $g(v)$ is adjacent from the vertex of $A(\Delta, K)$ corresponding to $g(u)$.

Second, suppose that $e = (u, v)$ is not an arc of $D$. Observe that in this case $t_m(g(u), g(v)) \leq T_b$. By Lemma 4.7, $(g(u), g(v))'$ is not an action of $K$ and so the vertex of $A(\Delta, K)$ corresponding to $g(v)$ is not adjacent from the vertex of $A(\Delta, K)$ corresponding to $g(u)$.

Therefore, the restriction $g'$ of $g$, $g': V \to \Delta$ is an isomorphism of the metadigraph $M$ and $A(\Delta, K)$. □

4.3 A Characterization of Transforms

In the previous section we have seen how to describe any metadigraph $M$ using a specification for $M$. Transforms play an important role in these descriptions. The main goal of this section is to present a characterization of transforms.

Let $G_1$ and $G_2$ be graphs with $p(G_1) \geq p(G_2) = z$, and let $f: V(G_2) \to V(G_1)$ be a one-to-one function. Suppose that $V(G_2) = \{v_1, v_2, \ldots, v_z\}$ and let $f(v_i) = u_i$, for $i = 1, 2, \ldots, z$. Then we can associate with $f$ a quasipolarization of a graph $G$, as we next describe. Construct a common supergraph $G$ of $G_1$ and $G_2$ by identifying the vertices $u_1, u_2, \ldots, u_z$ of $G_1$ with the corresponding vertices $v_1, v_2, \ldots, v_z$ of $G_2$. Denote by $H_1$ and $H_2$ the copies of $G_1$ and $G_2$ in $G$, respectively, and define $t$ using (4.1).

It is straightforward to see that every quasipolarization with negative graph isomorphic to $G_1$ and positive graph isomorphic to $G_2$ can be thought of as associated with some one-to-one function from $V(G_2)$ into $V(G_1)$. We use these ideas in the proof of the main result of this section.
Theorem 4.9  Let \( t \) be a transitional labeling of a graph \( G \). Then \( t \) is a transform if and only if \( t \) is a quasipolarization.

Proof  Suppose that \( t \) is a transform. Then there exists an extension \( t' \) of \( t \) of maximum linkage. Therefore, by Lemma 4.1, \( t' \) is a quasipolarization. Since \( t \leq t' \), the labelings \( t \) and \( t' \) have the same core; so \( t \) is a quasipolarization as well.

To prove the converse, assume that \( t \) is a quasipolarization of \( G \). Without loss of generality, suppose that \( G \) has no positive pole. Let \( \{ w_1, w_2, \ldots, w_z \} \) be the set of zero vertices of \( G \), which is also the set of vertices of the positive graph of \( t \). We extend \( t \) to a quasipolarization \( t' \) of a graph \( G' \) by adding some zero elements to the labeled graph \( G \). In particular, we attach \( b_i \) end-vertices to the vertex \( w_i \), for each \( i = 1, 2, \ldots, z \), where \( b \) is some fixed integer for which

\[
 b \geq \max\{2, 2|G| - z\}.
\]

We claim that \( t' \) is a transitional labeling of \( G' \) of maximum linkage.

Let \( G_1 \) and \( G_2 \) be graphs isomorphic to the negative graph and positive graph of \( t' \), respectively. Since \( t' \) is a quasipolarization, \( p(G_1) \geq p(G_2) = z \). Let \( L \) be the linking graph of \( t' \). We prove the claim by showing that for each one-to-one function \( f: V(G_2) \to V(G_1) \) we have \( |F| \leq |L| \), where \( F \) is the linking graph of the quasipolarization \( s \) of the graph \( G'' \) that is associated with \( f \).

Let \( V(G_2) = \{ v_1, v_2, \ldots, v_z, v_{z+1}, \ldots, v_{z'} \} \), where the vertex \( v_i \) corresponds to the vertex \( w_i \), for \( i = 1, 2, \ldots, z \), and where the vertices \( v_{z+1}, v_{z+2}, \ldots, v_{z'} \) correspond to the end-vertices added to \( G \) in order to obtain \( G' \). Thus,

\[
z' = z + \sum_{i=1}^{z} b_i
\]

and

\[
 \deg v_i = b_i + \deg_{G} w_i,
\]
for $i = 1, 2, ..., z$.

Let $f(v_i) = u_i$ for $i = 1, 2, ..., z'$. Denote the vertices of $G_1$ corresponding to $w_1, w_2, ..., w_z$ by $x_1, x_2, ..., x_z$. We divide the remainder of the proof into two cases.

Case 1 Assume $u_j \neq x_j$ for some $j$, $1 \leq j \leq z$. We know that

$$\deg v_j = b^j + \deg_{G} w_j.$$ 

Moreover,

$$\deg u_j \leq |G| - 1 \text{ if } u_j \neq x_i \text{ for all } i = 1, 2, ..., z$$

and

$$\deg u_j = b^k + \deg_{G} w_k \text{ if } u_j = x_k \text{ for some } k \neq j, 1 \leq k \leq z.$$ 

Hence,

$$|\deg u_j - \deg v_j| \geq b - |G| + 1.$$ 

Therefore, at least $b - |G| + 1$ edges of $G''$ have nonzero label. Then

$$|F| \leq |G''| - (b - |G| + 1).$$

Since

$$|G''| = |G| + 2 \sum_{i=1}^{z} b^i,$$

it follows that

$$|F| \leq |G| + 2 \sum_{i=1}^{z} b^i - (b - |G| + 1)$$

$$\leq z + 2 \sum_{i=1}^{z} b^i - 1 - (b - 2|G| + z).$$

From the definition of $b$, we have $b - 2|G| + z \geq 0$. Then
\[ |F| < z + 2 \sum_{i=1}^{z} b^i \leq |L|. \]

**Case 2** Assume \( f(v_i) = u_i = x_i \) for all \( i = 1, 2, \ldots, z \). In this case, it is straightforward to see that \( F \) has cardinality at most \( |L| \). Therefore, \( L \) is a maximum common subgraph of \( G_1 \) and \( G_2 \) and, hence, \( t' \) is a transitional labeling of \( G' \) of maximum linkage. Since \( t' \) is an extension of \( t \), the labeling \( t \) is a transform. \( \square \)

As an illustration, in Figure 4.22 we show a quasipolarization \( t \) of the graph \( P_3 \) and an extension \( t' \) of \( t \) of maximum linkage. The extension \( t' \) was obtained by applying to \( t \) the construction given in the proof of Theorem 4.9. In this example, \( z = 2 \) and we have chosen \( b = 8 \).

![Diagram](image-url)
CHAPTER V
CORES OF GRAPHS

5.1 Basic Definitions and Results

Recall that a transitional labeling $t$ of a graph $G$ can be reconstructed from its core by adding certain zero elements to it. In such a reconstruction, the core of $t$ remains as a unique (labeled) subgraph of $G$. On the other hand, if $H$ is a subgraph of a graph $G$, we can reconstruct $G$ by adding certain edges and, possibly, vertices to $H$. In this process, we may, eventually, produce another copy of $H$. Indeed, this will occur if $G$ contains another copy of $H$. Therefore, if $H$ is a connected subgraph of $G$ of minimum size that is unique in the sense that no subgraph of $G$ distinct from $H$ is isomorphic to $H$ then, $H$ may be considered as a sort of "corner stone" of the graph $G$. This suggests a new concept, which we investigate in this chapter.

A core of a connected graph $G$ is a connected subgraph $C$ of minimum size such that whenever $C'$ is a subgraph of $G$ with $C' \cong C$, then $C' = C$. In Figure 5.1 the graph $G_1$ has exactly two cores, namely, $K_3$ and $K_{1,3}$, while the graphs $G_2$ and $G_3$ have a unique core. The core of $G_2$ is $C_4$ and the core of $G_3$ is $G_3$ itself.

![Figure 5.1](image_url)

Figure 5.1

114

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For a connected graph $G$, the \textit{induced core} of $G$ is an induced connected subgraph $C$ of minimum size such that whenever $C'$ is an induced subgraph of $G$ with $C' \cong C$, then $C' = C$. Each of the graphs $G_1$, $G_2$, and $G_3$ of Figure 5.1 has a unique induced core. They are $K_3$, $G_2$, and $G_3$, respectively.

The \textit{core set} $C(G)$ of a graph $G$ is the set consisting of all cores of $G$. If $G$ has a unique core $C$, then we write $C(G) = C$. In particular, a graph $G$ is said to be a \textit{self-core graph} if $C(G) = G$. In a similar manner, the \textit{induced core set} $IC(G)$ of a graph $G$ is defined.

The size of a core of a graph $G$ never exceeds the size of an induced core of $G$. The core and the induced core of the graph $G_2$ of Figure 5.1 have distinct sizes.

\textbf{Lemma 5.1} Let $C$ be a subgraph that is either a core or an induced core of a connected graph $G$, and let $u$ and $v$ be similar vertices of $G$. If $u$ belongs to $C$, so does $v$.

\textbf{Proof} Let $u$ and $v$ be similar vertices of $G$, and suppose, to the contrary, that $u \in V(C)$ and $v \notin V(C)$. Let $h$ be an automorphism of $G$ such that $h(u) = v$ and let $h(C)$ denote the subgraph of $G$ with vertex set $h(V(C))$ and edge set $h(E(C)) = \{h(x)h(y) \mid xy \in E(C)\}$. Clearly, $h(C)$ is isomorphic to $C$ and $v$ is a vertex of $h(C)$. Since $v$ is not a vertex of $C$, the isomorphic subgraphs $C$ and $h(C)$ of $G$ are distinct, contradicting the uniqueness of $C$. $\Box$

\textbf{Corollary 5.2} Let $C$ be a subgraph that is either a core or an induced core of a connected graph $G$. Denote the set of the orbits of $G$ by $\mathcal{A}$. Then for some subset $\mathcal{A}'$ of $\mathcal{A}$,

$$V(C) = \bigcup_{A \in \mathcal{A}'} A.$$
The next two corollaries deal with induced cores.

**Corollary 5.3** If $G$ is a connected vertex-transitive graph, then $G$ is a self-induced core graph. Thus, complete graphs and cycles are self-induced core graphs.

**Corollary 5.4** Assume that a connected graph $G$ has exactly two orbits that induce corresponding subgraphs $G_1$ and $G_2$. If neither $G_1$ nor $G_2$ are unique subgraphs of $G$, then $G$ is a self-induced core graph.

In particular, we obtain the following consequences.

**Corollary 5.4a** Let $G$ be a graph of order at least 3, containing exactly two orbits $A_1$ and $A_2$ which induce subgraphs $G_1$ and $G_2$. If either $G_1$ is disconnected or $p(G_i) \leq 2$, for some $i = 1, 2$, then $G$ is a self-induced core graph.

**Proof** Neither a disconnected subgraph of $G$ nor a subgraph of order 1 or 2 can be an induced core of $G$. By Corollary 5.2, if $C$ is an induced core of $G$, then $V(C) = A_1 \cup A_2 = V(G)$; so $C = G$. □

As a result of this, the complete bipartite graph $K_{m,n}$, where $m \leq n$, is a self-induced core graph, as we next show. If $m = n$, then $K_{m,m}$ is vertex-transitive and by Corollary 5.3, $K_{m,m}$ is a self-induced core graph. If $m < n$, then $K_{m,n}$ has exactly two orbits, each of which induces a disconnected graph. The result follows from Corollary 5.4a.

The graphs $G_1$ and $G_2$ shown in Figure 5.2 are self-induced core graphs, as can be seen from Corollary 5.4a.

Corollary 5.2 may be applied in searching for the core set or the induced core...
set of a given graph $G$. For example, the graph $G$ of Figure 5.3 has three orbits, namely, $A_1 = \{v_0\}$, $A_2 = \{v_1, v_2, v_3\}$ and $A_3 = \{v_4, v_5, v_6, v_7, v_8, v_9\}$. Let $C$ be a core of $G$. Since the sets $A_2$, $A_3$, $A_1 \cup A_2$ and $A_2 \cup A_3$ induce disconnected graphs, $V(C)$ is one of the sets $A_1$, $A_1 \cup A_2$ and $V(G)$. Clearly, then, $V(C) = V(G)$. It turns out that $G$ is a self-induced core graph. The core $C$ of $G$ is shown in Figure 5.3.
5.2 Core Sequences of Graphs

Trees can be characterized as those connected graphs for which each connected subgraph is induced. Thus, for a tree, the concepts of core and induced core are equivalent. In this section we are primarily concerned with trees.

A peripheral vertex of a graph $G$ is a vertex of $G$ whose eccentricity is $\text{diam } G$. Let $u$ and $v$ be vertices of a graph $G$. A shortest $u$-$v$ path in $G$ is called a \textit{geodesic}. A \textit{diametrical path} of $G$ is a longest geodesic of $G$. Thus, if a $u$-$v$ path is a diametrical path of $G$, then $d(u,v) = \text{diam } G$ and $u$ and $v$ are said to be \textit{antipodal vertices}. For example, the graph shown in Figure 5.4 has exactly two diametrical paths and two pairs of antipodal vertices.

![Figure 5.4](image)

The \textit{trunk} $t(T)$ of a tree $T$ is defined as the subgraph of $T$ induced by all those vertices lying on some diametrical path. Observe that if $P$ and $P'$ are two distinct diametrical paths of a tree $T$, then $P$ and $P'$ share a central vertex of $T$. Therefore, the trunk of $T$ is a connected subgraph of $T$, that is, a subtree of $T$. For example, in Figure 5.4 we show trees $T_1$ and $T_2$ and their corresponding trunks.
For a tree $T$,

$$\text{diam } T = \text{diam } t(T).$$

Moreover, $T$ and $t(T)$ have in common all their geodesics of length $\text{diam } T$.

**Lemma 5.5** Let $T$ be a tree and suppose that $S$ is a subtree of $T$ isomorphic to $t(T)$. Then $S = t(T)$.

**Proof** Assume that the subtree $S$ of $T$ is isomorphic to $t(T)$. Let $v \in V(S)$. Then $v$ belongs to a $u$-$w$ path $P$ in $T$ of length $\text{diam } T$. Since $T$ is a tree, this $u$-$w$ path is unique. Hence, $e_T(u) = e_T(w) = \text{diam } T$. Therefore, $P$ is a diametrical path of $T$ which implies that $v \in V(t(T))$. Thus, $V(S) \subseteq V(t(T))$ and since $S \subseteq t(T)$, it follows that $V(S) = V(t(T))$. \(\square\)
Corollary 5.6  If $C$ is a core of the tree $T$, then $q(C) \leq q(t(T))$.

Proof  By Lemma 5.5 the subgraph $t(T)$ of $T$ is unique. □

For the trees $T_1$ and $T_2$ of Figure 5.4, we notice that $T_1$ has unique core $C_1 = t(T_1)$. The tree $T_2$ also has unique core isomorphic to $K_{1,6}$.

Observe that $K_1$, $K_2$ and $P_3$ are the only graphs with core size equal to 0, 1, 2, respectively. Therefore, if the order of a connected graph $G$ is at least 4, then the core size of $G$ is at least 3.

Theorem 5.7  For every pair $m$, $n$ of integers with $3 \leq m \leq n$, there exists a tree $T$ with a core $C$ such that $q(C) = m$ and $q(t(T)) = n$.

Proof  If $m = n$, then $T \cong K_{1,m}$ has the desired property. If $m < n$, then we construct a tree $T$ by identifying an end-vertex of a path $P_{n-m+1}$ with an end-vertex of the star $K_{1,m}$. Then $C(T) \cong K_{1,m}$ and $t(T) \cong T$. Hence, $q(C) = m$ and $q(t(T)) = m + (n - m + 1) - 1 = n$. □

Corollary 5.8  For every pair $m$, $n$ of integers with $3 \leq m \leq n$, there exists a tree $T$ with a core $C$ such that $q(C) = m$ and $q(T) = n$.

Let $T$ be a tree and suppose that a path $P$ is obtained by the deletion of all the end-vertices of $T$. Then $T$ is called a caterpillar and $P$ is called the spine of $T$. Let $P: v_1, v_2, ..., v_k$ be the spine of a tree $T$, where $\deg v_i = s_i$ for $i = 1, 2, ..., k$. Since the numbers $s_1, s_2, ..., s_k$ characterize $T$, we denote $T$ by $S_{n_1, n_2, ..., n_k}$. In particular, if $k = 1$ then $S_{n_1} = K_{1,n_1}$. If $k = 2$, then $S_{n_1, n_2}$ is called a double star.

We next characterize those trees that are trunks of trees.
**Theorem 5.9** A tree $S$ is the trunk of some tree $T$ if and only if every end-vertex of $S$ is a peripheral vertex of $S$.

**Proof** Let $S$ be the trunk of a tree $T$, and let $v$ be an end-vertex of $S$. Then $v$ belongs to a geodesic $P$ of $S$ having length $\text{diam } S$. Since $v$ is an end-vertex of $S$, it follows that $v$ is one of the end-vertices of $P$. Therefore, $e(v) = \text{diam } S$.

For the converse, assume that every end-vertex of a tree $S$ is a peripheral vertex of $S$. We prove that every vertex $v$ of $S$ belongs to a geodesic of $S$ of length $\text{diam } S$. This result is clear if $v$ is an end-vertex of $S$. Assume then that $\deg v \geq 2$ and suppose, to the contrary, that $v$ does not belong to a geodesic of $S$. Consider the tree $S$ rooted at $v$. Observe that each branch of $S$ contains a geodesic of length $\text{diam } S$. Since $\deg v \geq 2$, $S$ contains two disjoint geodesics of length $\text{diam } S$. This contradiction shows that the vertex $v$ belongs to a geodesic of $S$ of length $\text{diam } S$. Therefore, $V(S) \subseteq V(t(S))$ and hence $S = t(S)$. □

If $S$ is a tree for which every end-vertex is a peripheral vertex, then Theorem 5.9 guarantees the existence of a tree $T$ such that $t(T) = S$. If we further require that $T \neq S$, then we obtain the following result.

**Corollary 5.10** A tree $S$ is the trunk of some tree $T$, where $S \neq T$, if and only if every end-vertex of $S$ is an antipodal vertex and $S$ is not isomorphic to a star or a double star.

Recall that a graph $G$ is a self-core graph if $C(G) = G$. We next present a necessary condition for a tree to be a self-core tree.

**Theorem 5.11** If $T$ is a self-core tree, then $t(T) = T$. 

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Proof  By Corollary 5.6,
\[ q(T) \leq q(t(T)) \leq q(T). \]
Therefore, \( q(t(T)) = q(T) \) and hence \( t(T) = T \). □

Corollary 5.12  If \( T \) is a self-core tree, then all the end-vertices of \( T \) are peripheral.

The converse of Corollary 5.12 is not true as we may see from the tree of Figure 5.5, whose core is \( K_{1,3} \).

![Figure 5.5](image)

Not every connected graph is a core, as we show next.

Theorem 5.13  The double star \( S_{2,n} \), with \( n \geq 3 \), is not a core of any connected graph \( G \).

Proof  Suppose, to the contrary, that there exists a graph \( G \) with core \( C \equiv S_{2,n} \), where \( n \geq 3 \). Then there are two distinct copies \( S \) and \( S' \) of a star \( K_{1,n} \) in \( G \). Let \( u \) and \( v \) be the central vertices of these two stars and let \( P \) be a \( u-v \) path in \( G \). If
u ≠ v, the subgraph induced by the vertices of S, P and S' contains two distinct copies of C. Therefore, u = v and since S ≠ S', deg u > n. Thus, G contains at least n + 1 distinct copies of S_{2,n}, contradicting the uniqueness of C. □

With respect to Theorem 5.13 we observe that the double star S_{2,4} is an induced core of the graph shown in Figure 5.6.

![Figure 5.6](image_url)

It is clear that all stars and the double stars S_{n,n} are self-core trees. An infinite family of caterpillars that are cores of caterpillars is now presented.

**Theorem 5.14** Let S_{n_1, n_2, ..., n_k} be a caterpillar such that k ≥ 2 and n_1, n_k ≥ 3. Then there exists a caterpillar L such that C(L) = S_{n_1, n_2, ..., n_k}.

**Proof** Let v_1', v_2', ..., v_f' be the vertices of the spine of S' = S_{n_1, n_2, ..., n_k} that have degree at least 3. Note that f ≥ 2. For each 1 = 1, 2, ..., f, let x_i be an end-vertex of S adjacent to v_i' and let H_{2i-1} and H_{2i} be two copies of S - x_i. Let H_0 = S and H_{2f+1} = H_{2f}. Observe that the graphs H_j, 0 ≤ j ≤ 2f + 1, are caterpillars whose spines have length k. Now, for each of these caterpillars H_j, 0 ≤ j ≤ 2f + 1, select two vertices u_j and w_j such that d(u_j, w_j) = diam H_j (= diam S). As a matter of
convenience, we assume that the vertices \( u_{2i-1} \) and \( u_{2i} \) are corresponding vertices via an isomorphism of \( H_{2i-1} \) and \( H_{2i} \), for \( i = 1, 2, \ldots, f \). We make the same assumption for the vertices \( u_{2f} \) and \( u_{2f+1} \).

From the graphs \( H_j, 0 \leq j \leq 2f + 1 \), we construct a caterpillar \( L \) by connecting the vertices \( u_{j+1} \) and \( w_j \) by a path \( p^{(j+1)} \) of length \( q \) for each \( j \) \((0 \leq j \leq 2f)\), where \( q \) is the size of \( H_0 \). We prove that \( H_0 \) is a core of \( L \).

Let \( T \) be a subtree of \( L \) whose size is less than \( q \). It is clear that if \( T \) is a path, then \( L \) contains more than one copy of \( T \). If \( T \) is a subtree of \( H_0 \), then \( T \) is isomorphic to a subtree of \( H_{2i-1} \), for some \( 1 \leq i \leq f \). So \( L \) has at least two distinct copies of \( T \). Assume that \( T \) is neither a path nor a subgraph of \( H_0 \). We consider three cases.

**Case 1** Assume \( T \subset H_{2i-1} \cup P^{(2i)} \) for some \( 1 \leq i \leq f \). In this case, there is a distinct copy of \( T \) in \( H_{2i} \cup P^{(2i+1)} \).

**Case 2** Assume \( T \subset P^{(2i+1)} \cup H_{2i-1} \) for some \( 1 \leq i \leq f \). In this case, there is a distinct copy of \( T \) in \( P^{(2i)} \cup H_{2i} \).

**Case 3** Assume \( T \subset H_0 \cup P_f \). Since \( T \) is not a path, \( p(T \cap H_0) \geq 4 \). In any case, \( T \cap H_0 \) is a subtree of \( H_{2i-1} \), for some \( 1 \leq i \leq f \). Therefore, there is a distinct copy of \( T \) in \( H_{2i-1} \cup P^{(2i)} \).

From above, if \( C \) is a core of \( L \), then \( q(S) \geq q \). Since \( n_1, n_3 \geq 3 \), there is no copy of \( S \) distinct from \( H_0 \) in \( L \). Thus, \( H_0 \) is a core of \( L \). Moreover, by construction, \( H_0 \) is the unique core of \( L \). Therefore, \( C(L) = H_0 \). \( \Box \)

For the caterpillar \( S \) in Figure 5.7 we show some steps in constructing a caterpillar \( L \) such that \( C(L) = S \).
Figure 5.7

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Given a connected graph $G$, a **core sequence** of $G$ is a sequence \( \{R_i \mid i = 0, 1, \ldots \} \) of subgraphs of $G$ such that $R_0 = G$ and $R_{i+1}$ is a core of $R_i$, for $i = 0, 1, \ldots$. For example, the graphs $G = R_0$, $R_1$ and $R_2$ shown in Figure 5.8 form a core sequence \( \{R_i \} \) of $G$, where $R_{i+1} = R_i$ for $i \geq 2$. We obtain another core sequence \( \{R'_i \} \) of $G$ by taking $R'_0 = G$, $R'_1 = P_7$ and $R'_{i+1} = R'_i$ for $i \geq 1$. Thus, a graph need not have a unique core sequence. Of course, this is not surprising since a graph may very well have more than one core.

Let $G$ be a connected graph and suppose that \( \{R_i \} \) is a core sequence of $G$. A subgraph $H$ of $G$ is said to be the **limit** of \( \{R_i \} \) if there exists an integer $N$ such that $R_i = H$ for all $i \geq N$. It is straightforward to see that every core sequence has a limit. The number of distinct subgraphs of $G$ that belong to the core sequence \( \{R_i \} \) of $G$ is said to be the **length** of the core sequence \( \{R_i \} \).

For example, the core sequence \( \{R_i \} \) of the graph $G$ shown in Figure 5.8 has length 3 and its limit is $R_2$. We notice that two core sequences of the same graph may have distinct lengths, as can be seen from the core sequences \( \{R_i \} \) and \( \{R'_i \} \) of the graph $G$ shown in Figure 5.8.

**Theorem 5.15** For every positive integer $n$, there exists a graph $G$ with a core sequence of length $n$.

**Proof** If $n = 1$ then we may take $G$ to be any self-core graph, such as $P_4$. For $n \geq 2$, let $G = S_{n+1}$. By Theorem 5.14 there exists a caterpillar $L_1$ such that $C(L_1) \equiv G$. Observe that the two end-vertices of the spine of $L_1$ have degree at least $n$. Thus, if $n \geq 3$ we may apply Theorem 5.14 to $L_1$ and obtain a caterpillar $L_2$ such that $C(L_2) = L_1$. Continuing in this way, we can obtain at least $n - 1$ caterpillars $L_1, L_2, \ldots, L_{n-1}$ such that $C(L_i) \equiv L_{i-1}$ for $1 \leq i \leq n - 1$, where $L_0 \equiv G$. 

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Therefore, defining $R_0 = L_{n-1}$ and $R_i = C(R_{i-1})$ for $i = 1, 2, \ldots$ we obtain

\begin{align*}
R_0 &= L_{n-1} \\
R_1 &= C(R_0) = C(L_{n-1}) = L_{n-2} \\
R_2 &= C(R_1) = C(L_{n-2}) = L_{n-3} \\
&\quad \vdots \\
R_{n-2} &= C(R_{n-3}) = C(L_2) = L_1 \\
R_{n-1} &= C(R_{n-2}) = C(L_1) = G \\
R_n &= C(R_{n-1}) = C(G) = G.
\end{align*}

Thus, $\{R_i\}$ is a core sequence of $L_{n-1}$ having length $n$. □
It is clear that the limit of a core sequence of a graph $G$ must be a self-core graph. We now characterize those caterpillars that are self-core graphs.

**Theorem 5.16** If $T$ is a self-core caterpillar, then $T$ is isomorphic to $K_{1,n}$, $n \geq 2$, to $S_{m,n}$, $2 \leq m \leq n$, or to $S_{m,1,\ldots,1,n}$, $1 \leq m \leq n$.

**Proof** Let $T$ be a self-core caterpillar. Then, by Corollary 5.12, $T$ must be isomorphic to $K_{1,n}$, $n \geq 2$, or $S_{m,n}$, $2 \leq m \leq n$, or $S_{m,1,\ldots,1,n}$, $1 \leq m \leq n$. It is straightforward to see that all of these graphs are self-core trees. □

The next theorems are concerned with determining the core set of some special families of caterpillars.

Let $H$ be a connected subgraph of a connected graph $G$, and suppose that $H$ can be embedded in $G$ by a mapping that has no fixed vertex. Then no subgraph of $H$ is a core of $G$. For example, consider the caterpillars $G$ and $H$ of Figure 5.9. Observe that $H$ can be embedded in $G$ by the mapping $f$ defined by $v^{(i)}_j \rightarrow v^{(i)}_{j-1}$ for $j = 1, 2, 3, 4$ if $i = 0$, and for $j = 2, 3$ if $i = 1, 2$. Since $f$ has no fixed vertex, no subgraph of $H$ can be a core of $G$.

![Figure 5.9](image-url)
Theorem 5.17 If the caterpillar $T \equiv S_{n_1,n_2,\ldots,n_k}$, where $n_1 = n_k \geq n_2 = \ldots = n_{k-1}$, with $k \geq 3$, then $C(T) = t(T)$.

Proof Let $C$ be a core of $T$ and let $v_i$ denote the vertex of the spine of $T$ with $\deg v_i = n_i$, $i = 1, 2, \ldots, k$. Let $H$ be the subtree obtained from $T$ by deleting the end-vertices adjacent to $v_1$ and to $v_k$. Observe that $H$ can be embedded into the subtree of $T$ isomorphic to $S_{n_1,n_2,\ldots,n_{k-2}}$ by a mapping that has no fixed vertex. Then no subgraph of $H$ can be a core of $T$. Hence, $C$ must contain one end-vertex $v$ adjacent to $v_1$ or $v_k$. Since all the end-vertices adjacent to $v_1$ or $v_k$ are similar to $v$, it follows by Lemma 5.1, that $C$ must contain $t(T)$. Therefore, $C(T) = t(T)$. □

In Figure 5.10 we show a caterpillar $T$ (together with its core $C$) that satisfies the hypothesis of Theorem 5.17.

![Figure 5.10](image-url)
Theorem 5.18  Let $T \cong S_{n_1,n_2,\ldots,n_k}$ be a caterpillar with $n_1 = n_k = m < n = n_2 = \ldots = n_{k-1}$, $k \geq 3$. Then

1. $C(T) = t(T)$ if $n > 2m$, $k = 3$ or $n > m + 1$, $k \geq 4$;
2. $C(T) = F$ if $n < 2m$, $k = 3$;
3. $C(T) = \{t(T), F\}$ if $n = 2m$, $k = 3$ or $n = m + 1$, $k \geq 4$,

where

(a) $F \cong S_{n_1',n_2',\ldots,n_{k-2}'}$ with $n_1' = n_{k-2}' = n$, $n_2' = \ldots = n_{k-3}' = 2$, if $k \geq 5$,
(b) $F \cong S_{n,n}$ if $k = 4$ and
(c) $F \cong K_{1,n}$ if $k = 3$.

Proof  Let $C$ be a core of $T$ and let $v_i$ denote the vertex of the spine of $T$ with $\deg v_i = n_i$ ($i = 1, 2, \ldots, k$). Let $H$ be the subtree obtained from $T$ by deleting the end-vertices adjacent to $v_1, v_2, v_{k-1},$ and $v_k$. Observe that $H$ can be embedded into the subtree of $T$ isomorphic to $S_{n_1,n_2,\ldots,n_{k-2},1}$ by a mapping that has no fixed vertex. Then $C$ must contain the end-vertices adjacent to $v_1$ and $v_k$, or the end-vertices adjacent to $v_2$ and $v_{k-1}$. In the latter case, the vertices $v_1$ and $v_k$ must also be in $C$. Therefore, $t(T) \subseteq C$ or $F \subseteq C$, where $F \cong S_{n_1',n_2',\ldots,n_{k-2}'}$, with $n_1' = n_{k-2}' = n$ and $n_2' = \ldots = n_{k-3}' = 2$.

We know that there is a unique copy of $t(T)$ in $T$. It is straightforward to see that this is true for the subtree $F$. Therefore, to obtain the core set of $T$ we need only compare the sizes of $t(T)$ and $F$. Since these sizes are

$q(t(T)) = k + 2m - 3$,

and

\[\text{...}\]
\[ q(F) = \begin{cases} 
  n & \text{if } k = 3 \\
  k + 2n - 5 & \text{if } k \geq 4,
\end{cases} \]

the desired result follows. \( \square \)

To illustrate Theorem 5.18, in Figure 5.11 we show caterpillars \( T_1, T_2 \) and \( T_3 \) and their cores. The core set of \( T_3 \) is \( \{C, C'\} \).
Figure 5.11
REFERENCES


