Contents

Chapter 1

Introduction and Preliminaries

This thesis is devoted to a study of topics in graph theory: Near Automorphisms and Chaotic Mappings. We start with an introduction of terminologies in graph theory.

1.1 Basic Notions of Graphs

A *graph* G is a triple consisting of a *vertex set* $V(G)$, an *edge set* $E(G)$, and a relation that associates with each edge two vertices (not necessarily distinct) called its *endpoints*. A *loop* is an edge whose endpoints are equal. *Multiple edges* are edges having the same pair of endpoints.

A *simple graph* is a graph having no loops or multiple edges. We specify a simple graph by its vertex set and edge set, treating the edge set as a set of unordered pairs of vertices and writing $e = uv$ (or $e = vu$) for an edge e with endpoints u and v. When u and v are the endpoints of an edge e, they are *adjacent* and are *neighbors*, and we say they are *incident* to e. We write $u \leftrightarrow v$ for "u is adjacent to v".

The degree of vertex v (in a loopless graph) is the number of incident edges. In many important applications, loops and multiple edges do not arise, and we restrict our attention to simple graphs. Thus in a simple graph we view an edge as an unordered pair of vertices and can ignore the formality of the relation associating endpoints to edges. This study emphasizes simple graphs.

A graph is *finite* if its vertex set and edge set are finite. We adopt the convention that every graph mentioned in this study is finite, unless explicitly constructed otherwise. An *independent set* (or *stable set*) in a graph is a set of pairwise nonadjacent vertices. A graph G is *bipartite* if $V(G)$ is the union of two disjoint independent sets called *partite sets* of G. A graph G is k-partite if $V(G)$ can be expressed as the union of k independent sets. A *path* is a simple graph whose vertices can be ordered so that two vertices are adjacent if and only if they are consecutive in the list. A *cycle* is a graph with an equal number of vertices and edges whose vertices can be placed around a circle so that two vertices are adjacent if and only if they appear consecutively along the circle.

A *subgraph* of a graph G is a graph H such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$ and the assignment of endpoints to edges in H is the same as in G. We then write $H \subseteq G$ and say that "G contains H". A graph G is *connected* if each pair of vertices in G belongs to a path; otherwise, G is *disconnected*. An *isomorphism* from a simple graph G to a simple graph H is a *bijection (one to one correspondence)* $f : V(G) \rightarrow V(H)$ such that $uv \in E(G)$ if and only if $f(u)f(v) \in E(H)$. We say "G is *isomorphic to* H", written $G \cong H$, if there is an isomorphism from G to H. The (unlabeled) path and cycle with n vertices are denoted P_n and C_n, respectively; an n-*cycle* is a cycle with n vertices. A *complete graph* is a simple graph whose vertices are pairwise adjacent, the (unlabeled) complete graph with n vertices is denoted K_n. A complete bipartite graph (or *biclique*) is a simple bipartite graph such that two vertices are adjacent if and only if they are in different partite sets. When the sets have sizes r and s, the (unlabeled) complete bipartite graph is denoted $K_{r,s}$.

The structural properties of a graph are determined by its adjacency relation and hence are preserved by isomorphism. An *automorphism* of G is an isomorphism from G to G. A graph G is *vertex-transitive* if for every pair $u, v \in V(G)$ there is an automorphism that maps u to v. The *components* of a graph G are its maximal connected subgraphs of G. A component (or graph) is *trivial* if it has no edges; otherwise it is *nontrivial*. An *isolated vertex* is a vertex of degree 0. A *cut-edge* or *cut-vertex* of a graph is an edge or vertex whose deletion increase the number of components. We write $G - e$ or $G - M$ for the subgraph of G obtained by deleting an edge e or set of edges M. We write $G - v$ or $G - S$ for the subgraph obtained by deleting a vertex v or set of vertices S, and its or their incident edges.

A *directed graph* or *digraph* G is a triple consisting of a *vertex set* $V(G)$, an *arc set* $A(G)$, and a function assigning each direct-edge an ordered pair of vertices. The first vertex of the ordered is the *tail* of the direct-edge, and the second is the *head*; together, they are the *endpoints*. We say that an direct-edge is an direct-edge *from* its tail *to* its head. The terms "head" and "tail" come from the arrows used to draw digraphs. As with graphs, we assign each vertex a point in the plane and each edge a curve joining its endpoints. When drawing a digraph, we give the curve a direction from the tail to the head. In a digraph, a *loop* is an edge whose endpoints are equal. *Multiple direct-edges* are direct-edges having the same ordered pair of endpoints. A digraph is *simple* if each ordered pair is the head and tail of at most one direct-edge; one loop may be present at each vertex.

A digraph is a *path* if it is a simple digraph whose vertices can be linearly ordered so that there is an direct-edge with tail u and head v if and only if v immediately follows u in the vertex ordering. A *cycle* is defined similarly using of the vertices on the circle. A graph with no cycle is *acyclic*. A *forest* is an acyclic graph. A *tree* is a connected acyclic graph. A leaf (or pendent vertex) is a vertex of degree 1. Paths are trees. A tree is a path if and only if its maximum degree is 2. A *star* is a tree consisting of one vertex adjacent to all the others. The n-vertex star is the biclique $K_{1,n-1}$ (or S_{n-1}). If G has u,v-path, then the *distance* from u to v, written $d_G(u,v)$ or simply $d(u,v)$, is the least length of a u,v-path. If G has no such path, then $d(u,v) = \infty$. The *diameter* (diam G) is $\max_{u,v\in V(G)} d(u,v)$. The *eccentricity* of a vertex u, written $\epsilon(u)$. The *radius* of a graph G, written rad G, is $\min_{u\in V(G)} \epsilon(u)$. The diameter equals the maximum of the vertex eccentricities. A *caterpillar* is a tree in which a single path (the spine) is incident to (or contains) every edges.

1.2 Motivation

To determine whether two graphs are isomorphic or not is one of the most important and difficult problems in graph theory. It is known that solving the problem by using an algorithm is an NP-hard problem. Similarly, given a graph G, to determine the set of automorphisms of G is not easy at all. Practically, we may have to check all permutations of $V(G)$ in order to find Aut(G). Therefore, some permutations are indeed automorphisms, but there are permutations which are not automorphisms. Among all the permutations of $V(G)$, we are interested in knowing a way to measure how close (or how far) a permutation is from being an automorphism.

From the definition of an automorphism f of G, it is not difficult to see that $d_G(u,v) = d_G(f(u), f(v))$, i.e., the permutation f is an isometric mapping (keeping distance fixed). So, if a permutation g of $V(G)$ fails to do the job, it is not an automorphism. This phenomenon motivates us to observe how much can a permutation φ affect the distance of u and v to the distance of $\varphi(u)$ and $\varphi(v)$ for each pair of vertices u and v in $V(G)$. So, we define the *total relative displacement* of G, $\delta_f(G) = \sum_{u,v\in V(G)} |d_G(u,v) - d_G(f(u), f(v))|$. Clearly, $\delta_f(G) = 0$ if and only if f is an automorphism of G. Furthermore, if a permutation f which gives the smallest positive value in $\{\delta_\varphi(G) : \varphi$ is a permutation of $V(G)\}$, f is very close to being an automorphism. Such a permutation is now known as a *near automorphism* of G. On the other (opposite) direction, we may also try to find a permutation f such that $\delta_f(G)$ attains the largest value of $\{\delta_\varphi(G) : \varphi$ is a permutation of $V(G)\}$, f is then called a chaotic mapping of G. The later part of this research is also motivated by the sorting problem in computer science.

Due to practical reasons, in order to study the disorderedness of input data, they only consider the situation in which data are arranged on a path or a cycle. For convenience, we use a path to explain the notion. Now, let $P_n = 1, 2, \cdots, n$ be a path with n vertices $1, 2, \cdots, n$ arranged as $< 1, 2, \cdots, n >$. Clearly, for $i = 1, 2, \cdots, n-1$, $(i, i+1)$ is an edge of P_n and thus $d_{P_n}(i, i+1) = 1$. Moreover, $d_{p_n}(i, j) = |i - j|$. So, if the sorting data are distributed randomly to another path with the same set of vertices of $Z = < z_1, z_2, \cdots, z_n >$, then $d_{P_n}(i, i+1)$ may not be the same as $d_{P_n}(z_i, z_{i+1})$. It is natural to define the oscillation Z of P_n by

$$O_{sc}(Z) = \sum_{i=1}^{n-1}(|z_i - z_{i+1}| - 1).$$

Then, finding $\max_{Z \in S_n} O_{sc}(Z)$ reveals the maximum disorderedness of the input data arranged on a path. See [4,10] for references.

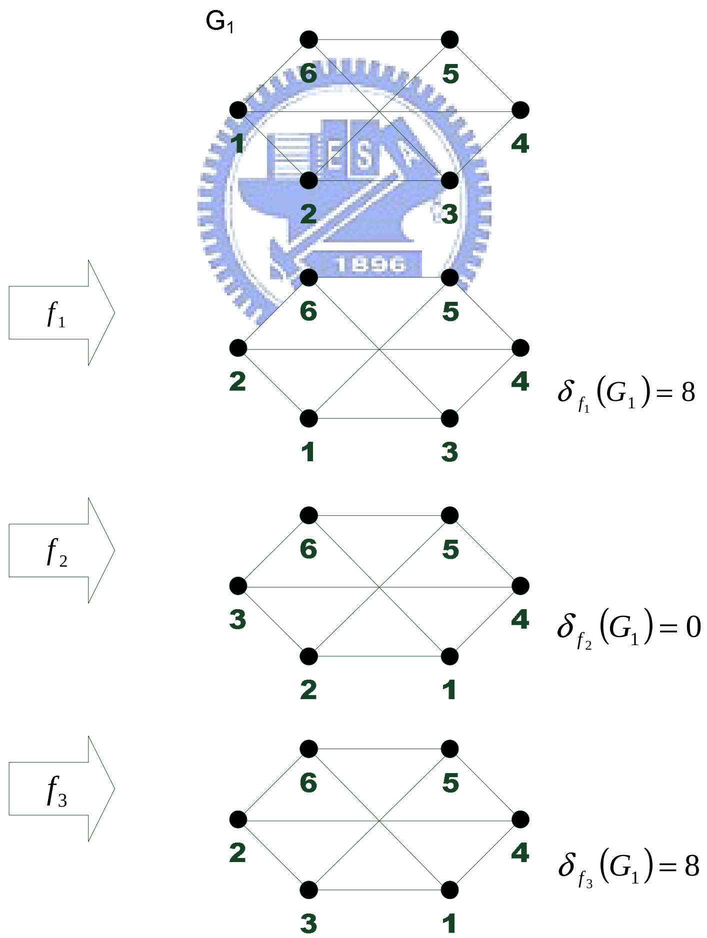
1.3 Total Relative Displacement

Let $G = (V, E)$ be a connected graph of order n and f be a permutation of V. The relative displacement of two distinct vertices u and v in G is then denoted by $\delta_f(u, v) = |d(u, v) - d(f(u), f(v))|$. In addition, let $\delta_f(u) = \sum_v \delta_f(u, v)$, and then the *total relative displacements of permutation f in G* is the sum of $\delta_f(u, v)$ over all the $\binom{n}{2}$ unordered pairs $\{u, v\}$ of distinct vertices of G denoted by $\delta_f(G)$, i.e., $\delta_f(G) = \sum_{u \neq v} \delta_f(u, v) = \frac{1}{2} \sum_{u} \delta_f(u)$.

It is clear that a permutation f is an automorphism of G if and only if $\delta_f(G) = 0$. Let $\pi(G)$ and $\pi^*(G)$ denote the smallest nonzero total relative displacement and the largest total relative displacement in G, respectively. The permutations which realize $\pi(G)$ and $\pi^*(G)$ are called the near automorphism and the chaotic mapping of G, respectively.

For clearness, we give an example here.

Example 1.3.1. Let $f_1 = (1, 2)$, $f_2 = (1, 3)$ and $f_3 = (1, 2, 3)$, then



By checking all permutations of the six vertices, we are able to see that $\pi(G) = 8$ and $\pi^*(G) = 8$. From this example, it is not difficult to realize that finding $\pi(G)$ and $\pi^*(G)$ for a general graph is going to be very challenging.

In what follows, we explore some properties of total relative displacements.

Lemma 1.3.2. *Let G be a graph and let f be a permutation of $V(G)$. Then $\delta_f(G)$ is even. Moreover, $\pi(G)$ and $\pi^*(G)$ are even.*

Proof. Let f be a permutation of $V(G)$ and k be a positive integer. Then

$$|\{\{x,y\} : d(x,y) = k\}| = |\{\{x,y\} : d(f(x), f(y)) = k\}|$$

which implies that

$$\sum_{x \neq y \in V(G)} d(x,y) = \sum_{x \neq y \in V(G)} d(f(x), f(y)).$$

Let $\delta(x,y) = \begin{cases} 0 & if\ d(x,y) \geq d(f(x), f(y)) \\ 1 & if\ d(x,y) < d(f(x), f(y)). \end{cases}$ Then,

$$\begin{aligned}
\delta_f(G) &= \sum_{x,y \in V(G)} |d(x,y) - d(f(x), f(y))| \\
&= \sum_{x,y \in V(G)} (-1)^{\delta(x,y)} d(x,y) - \sum_{x,y \in V(G)} (-1)^{\delta(x,y)} d(f(x), f(y)).
\end{aligned}$$

Since $\sum_{x,y \in V(G)} d(x,y) \equiv \sum_{x,y \in V(G)} (-1)^{\delta(x,y)} d(x,y) \pmod 2$ and

$$\sum_{x,y \in V(G)} d(f(x), f(y)) \equiv \sum_{x,y \in V(G)} (-1)^{\delta(x,y)} d(f(x), f(y)) \pmod 2,$$

$$\sum_{x,y \in V(G)} (-1)^{\delta(x,y)} d(x,y) \equiv \sum_{x,y \in V(G)} (-1)^{\delta(x,y)} d(f(x), f(y)) \pmod 2.$$

So, $\delta_f(G) \equiv 0 \pmod 2$ and $\pi(G)$ and $\pi^*(G)$ are even. ∎

Lemma 1.3.3. *If f is a permutation of $V(G)$ and h is an automorphism of a graph G, then $\delta_{h \circ f}(G) = \delta_f(G) = \delta_{f \circ h}(G)$.*

Proof. Since h is an automorphism, each vertex pair of $V(G)$ preserves their distance by h. Thus $d(h(f(x)), h(f(y))) = d(f(x), f(y))$ for each vertex pair $\{x, y\}$. Then the equality follows.

$$\begin{aligned}
\delta_{h\circ f}(G) &= \sum_{x,y\in V(G)} |d(x,y) - d(h(f(x)), h(f(y)))| \\
&= \sum_{x,y\in V(G)} |d(x,y) - d(f(x), f(y))| = \delta_f(G) \\
&= \sum_{j=1}\sum_{i=1} |\{\{x,y\} : x,y \in V(G), d(x,y) = i, d(f(x), f(y)) = j\}| \cdot |i-j| \\
&= \sum_{j=1}\sum_{i=1} |\{\{h(x),h(y)\} : h(x),h(y) \in V(G), d(h(x),h(y)) = i, \\
&\qquad d(f(h(x)), f(h(y))) = j\}| \cdot |i-j| \\
&= \delta_{f\circ h}(G)
\end{aligned}$$

∎

Lemma 1.3.4. *Let f be a permutation of $V(G)$ and $f(v) = v$ for some $v \in V(G)$. Then $\delta_f(v)$ is even.*

Proof. Since $\delta_f(v) = \sum_{u\neq v} \delta_f(u,v) = \sum_{u\neq v} |d(u,v) - d(f(u),v)|$, $\delta_f(v) \equiv \sum_{u\neq v}(d(u,v) - d(f(u),v)) \equiv \sum_{u\neq v} d(u,v) - \sum_{u\neq v} d(f(u),v) \pmod 2$. By the fact that f is a permutation, $\sum_{u\neq v} d(u,v) = \sum_{u\neq v} d(f(u),v))$. Hence, $\delta_f(v) \equiv 0 \pmod 2$. ∎

If the graph we consider is vertex-transitive, for example C_n, then we have better properties.

Lemma 1.3.5. *If G is a vertex-transitive graph and f is a near automorphism of G, then $\delta_f(v)$ is even for each $v \in V(G)$.*

Proof. Let h be an automorphism of G. Then, for each $v \in V(G)$, $\delta_{h\circ f}(v) = \sum_{u\in V(G)\setminus\{v\}} |d(v,u) - d((h\circ f)(v), (h\circ f)(u))| = \sum_{u\in V(G)\setminus\{v\}} |d(v,u) - d(f(v), f(u))| = \delta_f(v)$. Now, consider f. If there exists an $v \in V(G)$ such that $f(v) = v$, then by Lemma 1.3.4, we have the proof. Otherwise, since G is vertex-transitive, there exists an automorphism h of G such that $h(u) = v$ where $u = f(v)$. Therefore, $(h \circ f)(v) = h(f(v)) = h(u) = v$. This implies that $\delta_{h \circ f}(v)$ is even. By Lemma 1.3.3, $\delta_{h \circ f}(v) = \delta_f(v)$. Hence $\delta_f(v)$ is even. ∎

Lemma 1.3.6. *Let $v \in V(G)$, $f(v) = v$ and $\delta_f(v) \neq 0$. Then there exist at least two distinct vertices u and w such that $\delta_f(u, v)$ and $\delta_f(w, v)$ are positive.*

Proof. Suppose there exists a unique $u \in V(G)$ such that $\delta_f(v) = \delta_f(v, u) \neq 0$. Then $\sum_{w \in V(G) \setminus \{v,u\}} |d(v, w) - d(f(v), f(w))| = 0$. This implies that for each $w \in V(G) \setminus \{v, u\}, d(v, w) = d(f(v), f(w)) = d(v, f(w))$. Now, since $f(u) \neq v$ and $f(u) \neq u, d(v, f(u)) = d(v, f^2(u)) = d(v, f^3(u)) = \cdots$. By the fact that f is a permutation of finite order, there exists a $t \leq |V(G)|$ such that f^t is an identity and thus $d(v, f(u)) = d(v, u)$. This contradicts $\delta_f(v, u) \neq 0$, and we have the proof. ∎

For convenience, we need a notion called the *displacement graph* of graph G.

Definition 1.3.7. Suppose G is a graph and f is a permutation of $V(G)$. The displacement graph of G with respect to f is the directed multigraph $G[f]$ whose vertex set $V(G[f]) = \{a_1, a_2, \cdots, a_t\}$, where $t = \mathrm{diam}(G)$, and the arc set $A(G[f]) = \{\langle a_i, a_j\rangle : i \neq j$, there is a pair of vertices u and v such that $d(u, v) = i$ and $d(f(u), f(v)) = j\}$.

It is not difficult to see that for each displacement graph of G with respect to a non-automorphism, $deg^+(a_1) = deg^-(a_1) \neq 0$.

Note that if there are exactly s pairs of vertices u and v such that $d(u, v) = i$ and $d(f(u), f(v)) = j$, then $\langle a_i, a_j\rangle$ occurs in $G[f]$ exactly s times, i.e., $\langle a_i, a_j\rangle$ is of multiplicity s. For each unordered pair $\{u, v\}$ of distinct vertices of G, let $\alpha(u, v)$ denote $\langle a_i, a_j\rangle$, where $d(u, v) = i$ and $d(f(u), f(v)) = j$.

We now have a couple of conclusions about the structure of $G[f]$.

Lemma 1.3.8. *For each vertex* $a_i \in V(G[f])$, $1 \le i \le \mathrm{diam}(G)$, $\deg^+(a_i) = \deg^-(a_i)$.

Proof. This is a direct consequence of the fact that $|\{\{u,v\} : u, v \in V(G), d(u,v) = i\}| = |\{\{z,w\} : z, w \in V(G), d(f(z), f(w)) = i\}|$ where $1 \le i \le \mathrm{diam}(G)$. ∎

Lemma 1.3.9. $\delta_f(G) = \sum_{\langle a_i, a_j\rangle \in A(G[f])} |i - j|$.

Proof. The lemma follows from Definition 1.3.7 easily. ∎

Lemma 1.3.10. *Let G be a graph and f be a permutation of G but not an automorphism, then there is an edge uv of G such that $\delta_f(u,v) \ge 1$.*

Proof. If $\delta_f(u,v) = 0$ for each edge $uv \in E(G)$, then $f(u)f(v)$ is still an edge in G, i.e., f is an automorphism.

Lemma 1.3.11. *If f is a permutation of $V(G)$, then $\delta_f(G) = \delta_{f^{-1}}(G)$.*

Proof. Obviously, $G[f]$ and $G[f^{-1}]$ have the same vertex set, but their arc sets have the inverse direction. Thus, by Lemma 1.3.9, we have $\delta_f(G) = \delta_{f^{-1}}(G)$. ∎

Lemma 1.3.12. *Let G be a connected graph which is not complete. Then $2 \le \pi(G) \le 2|V(G)| - 4$.*

Proof. Note that there exist no near automorphisms for a complete graph. Therefore, we only consider those graphs which are not complete. Since G is not a complete graph, there exist three vertices x, y and z such that $xy, xz \in E(G)$ and $yz \notin E(G)$. Then, let f be the transposition (xy). Clearly, f is not an automorphism, since x is adjacent to z but y is not adjacent to z. As for $\pi(G)$, since $\delta_f(G) = \sum\{\delta_f(u,v) \mid |\{u,v\} \cap \{x,y\}| = 1\} \le 2|V(G)| - 4$, we conclude that $\pi(G) \le 2|V(G)| - 4$. By the fact that $\pi(G)$ is even and $\pi(G) \ne 0$, $2 \le \pi(G)$ follows. ∎

1.4 Known Results

The notion of near automorphism was first introduced by Chartrand et al. in [5] and they conjectured that $\pi(G) = 2n - 4$ where G is a path with n vertices. Later, Aitken [1] proved this conjecture and among other things, characterized those permutations f for which $\pi(G) = \delta_f(G) = 2n - 4$ when G is a path with n vertices. He also proved that, if $n \geq 25$, then the only values of $\delta_f(G)$ less than $4n$ are $2n-4$, $4n-12$, and $4n-10$, and he classified the permutation f that give these values.

Theorem 1.4.1. [1] $\pi(P_n) = 2n - 4$.

Theorem 1.4.2. [1] *Let G be a path with n vertices where $n \geq 25$, and let f be a permutation of $V(G)$. If $0 < \delta_f(G) < 4n$ then $\delta_f(G)$ is one of the following: $2n-4$, $4n-12$, or $4n-10$. Let $h : V(G) \to V(G)$ be the function which sends i to $n-i+1$. Then either f or $h \circ f$ is of the following form :* (i) *a transposition switching i and $i+1$ for some $1 \leq i \leq n-1$, here $\delta_f(G) = 2n-4$,* (ii) *a transposition switching i and $i+2$ for some $1 \leq i \leq n-2$, here $\delta_f(G) = 4n-12$,* (iii) *a three cycle permuting i, $i+1$, and $i+2$ for some $1 \leq i \leq n-2$, here $\delta_f(G) = 4n-10$, or* (iv) *a product of a transposition switching i and $i+1$ with a transposition switching j and $j+1$ where $1 \leq i < i+1 < j \leq n-1$, here $\delta_f(G) = 4n-12$.*

In 1999, Chartrand, Gavlas and Vander Jagt [5] claimed that $\pi(K_{m,n}) = 2(m+n-2)$, for all integers $2 \leq m \leq n$, but, as a special case of a more general treatment, Reid [12] proved Theorem 1.4.3. He also determined $\pi(K_{n_1,n_2,\cdots,n_t})$ and described the permutations f of $K_{n_1,n_2,\cdots,n_t}$ for which $\delta_f(K_{n_1,n_2,\cdots,n_t}) = \pi(K_{n_1,n_2,\cdots,n_t})$.

Let $K_{n_1,n_2,\cdots,n_t}$ be a complete t-partite graph with partite sets $X_1, X_2, \cdots, X_t$ and $|X_i| = n_i$. Let f be a permutation of $V(K_{n_1,n_2,\cdots,n_t})$. For each $1 \leq i,j \leq t$, define

$$a_{ij} = |A_{ij}(f)| = |\{x : x \in X_i \text{ and} f(x) \in X_j\}|.$$

Then,

$$\delta_f(K_{n_1,n_2,\cdots,n_t}) = \sum_{i=1}^{t} n_i^2 - \sum_{1\le i,j\le t} a_{ij}^2. \tag{1.1}$$

Reid then transformed the problem into the combinatorial optimization problem of maximizing the sums of the squares of the entries in certain t by t matrices with non-negative integer entries in which the sum of the entries in the ith row and the sum of the entries in the ith column were each equal to n_i, $1 \le i \le t$. Following this effort, he obtained the following two results.

Theorem 1.4.3. [12] *For all positive integers m and n, where* $\max(m,n) \ge 2$. *Then*

$$\pi(K_{m,n}) = \begin{cases} 2m & \textit{if } n = m+1, \\ 2(m+n-2) & \textit{otherwise.} \end{cases}$$

.

Theorem 1.4.4. [12]

$$\pi(K_{n_1,n_2,\ldots,n_t}) = \begin{cases} 2n_{h+1}-2 & \textit{if } 1 = n_1 = \cdots = n_h < n_{h+1} \le \cdots \le n_t, \\ & \textit{and } t \ge (h+1),\ \textit{for some } h \ge 2; \\ 2n_{k_0} & \textit{if } 1 = n_1 < n_2 \textit{ or } n_h \ge 2 \textit{ and} \\ & n_{k+1} = n_k + 1 \textit{ for some } k, 1 \le k \le t-1, \\ & \textit{and } 2 + n_{k_0} \le n_1 + n_2,\ \textit{where } k_0 \\ & \textit{is the smallest index for which} \\ & n_{k_0+1} = n_{k_0} + 1; \\ 2(n_1+n_2-2) & \textit{otherwise.} \end{cases}$$

where $K_{n_1,n_2,\cdots,n_t}$ denotes the complete t-partite graph with t-partite sets of cardinality $n_1 \le n_2 \le \cdots \le n_t$.

In the other direction, Fu et al. [9] studied the maximum value of the total relative displacements of permutations in a graph G. They transformed the problem of finding $\pi^*(K_{n_1,n_2,\cdots,n_t})$ into a quadratic integer programming problem, equation (1.1), and developed a characterization of the optimal solution. A polynomial time algorithm running in $O(n^5 logn)$ time was then developed to solve the problem, where

n was the number of vertices in the multipartite graph. Moreover, in [7], they studied the total relative displacement of the permutations in complete bipartite graphs and complete tripartite graphs with an approach different from that in [9]. They also developed an algorithm running in $O(n_3^4)$ time for finding the chaotic numbers of complete tripartite graphs, where n_3 is the number of vertices of the largest partite set.

In this thesis, we shall mainly study the near automorphisms of certain graphs such as cycles and trees. For cycles C_n, we prove that $\pi(C_n) = 4\lfloor \frac{n}{2} \rfloor - 4$ for $n \geq 4$, and for the trees, we characterize the trees T where $\pi(T) = 2$ or 4 or $2n-4$ respectively. As to $\pi^*(G)$, we obtain a better lower bound for $G \cong P_n$ than that achieved earlier by Chiang et al. in [6].

Chapter 2

Graphs G with $\pi(G) = 2$ and $\pi(G) = 4$

We start this chapter with a review. It was shown in Lemma 1.3.12 that if G is a connected graph which is not complete, then $2 \leq \pi(G) \leq 2n - 4$. Aitken showed that $\pi(P_n) = 2n - 4$ in [1], therefore, it is interesting to know the oppositive case for which graphs G, $\pi(G) = 2$.

In this chapter, we shall first consider the graphs G such that $\pi(G) = 2$. Then, for the rest of this chapter, the trees T with $\pi(T) = 2$ or 4 are characterized.

2.1 $\pi(G) = 2$

The following lemma plays an important role in determining the graphs G with $\pi(G) = 2$.

Lemma 2.1.1. *If there are two vertices u and v of graph G such that $|N[u]| = |N[v]| + 1$, $N(u) \setminus N[v] = \{w\}$, $d(v, w) = 2$ and $d(x, w) \geq d(x, v) - 1$ for all $x \neq w$, then $\pi(G) = 2$.*

Proof. Let f be a transposition (uv). Then $\delta_f(G) = |d(u, w) - d(f(u), f(w))| + |d(v, w) - d(f(v), f(w))| = 2$. ∎

The lemma is not the sufficient condition, for example, see Figure 2.1

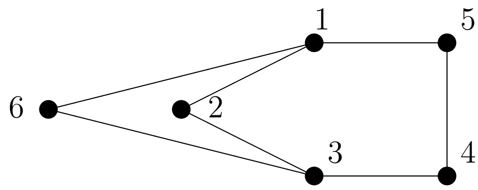


Figure 2.1: $f = (34)(56)$ and $\delta_f(G) = 2$.

Proposition 2.1.2. If $\pi(G) = 2$ and the near automorphism is a transposition (uv), then $|N[u]| = |N[v]| + 1$, $N(u) \setminus N[v] = \{w\}$, $d(v, w) = 2$ and $d(x, w) \geq d(x, v) - 1$ for all $x \neq w$. (see Figure 2.2.)

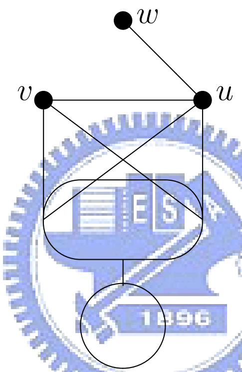


Figure 2.2: $f = (uv)$ and $\delta_f(G) = 2$.

Unfortunately, we are not able to characterize all graphs G with $\pi(G) = 2$ at this moment. But, if G is a bipartite graph, then we are able to do so. In fact, we prove a more general case.

Theorem 2.1.3. *Suppose G is a connected graph without 3-cycles and 5-cycles, and $|V(G)| \geq 3$. Then, $\pi(G) = 2$ if and only if $G \simeq P_3$.*

Proof. It is clear that $\pi(P_3) = 2$. On the other hand, suppose $\pi(G) = 2$ but $G \not\simeq P_3$. In this case, $|V(G)| \geq 4$. Choose a near automorphism f of G such that $\delta_f(G) = 2$. By Lemma 1.3.10, there exists an edge $uv \in E(G)$ such that $\delta_f(u, v) \geq 1$.

Also, by Lemma 1.3.8 and Lemma 1.3.10 $\deg^+(a_1) = \deg^-(a_1) \geq 1$ and so in fact $A(G[f]) = \{\langle a_1, a_2\rangle, \langle a_2, a_1\rangle\}$ as $\pi(G) = 2$.

Let $\alpha(u, v) = \langle a_1, a_2\rangle$. Therefore, $d(f(u), f(v)) = 2$. Let w be the vertex in G such that $(f(u), f(w), f(v))$ is a path in G. Clearly, $d(f(u), f(w)) = d(f(w), f(v)) = 1$. Thus, $d(u, w) \leq 2$ and $d(w, v) \leq 2$, and at most one of them is equal to 2. Furthermore, w is not adjacent to both u and v, for otherwise there is a C_3, which is not possible. By symmetry we may assume that $d(w, v) = 1$ and $d(u, w) = 2$, and so (u, v, w) is a path in G.

Since $|V(G)| \geq 4$ and G is connected, there exists a vertex z adjacent to some vertex of $\{u, v, w\}$. If z is adjacent to u, then z is not adjacent to v and so $d(z, v) = d(f(z), f(w)) = 2$ implying that $d(z, w) = 2$ and so there is a C_5, a contradiction. The case z is adjacent to w can be treated similarly. If z is adjacent to v, then $d(z, u) = d(z, w) = 2$ implies that $d(f(z), f(u)) = d(f(z), f(w)) = 2$, and so there is a C_5, again a contradiction. Hence the theorem is true. ∎

2.2 Trees T with $\pi(T) = 4$

By Theorem 2.1.3, if T is a tree with $\pi(T) = 2$, then T is a path with three vertices. Therefore, the smallest total relative displacement left to consider is $\pi(T) = 4$. In what follows, we obtain a characterization of such trees T. First, we need a lemma.

Lemma 2.2.1. *If u, v and w are three vertices in a tree T, then $d(u, v) \equiv d(w, u) + d(w, v) \pmod 2$.*

Theorem 2.2.2. *If T is a tree of order at least 4. Then $\pi(T) = 4$ if and only if there exists a vertex x such that $T - x$ contains an isolated vertex and a component K_2, with the only exception that $\pi(S_3) = 4$.*

Proof. By Theorem 2.1.3, we have $\pi(T) \geq 4$ if $|V(T)| \geq 4$. Hence the trees with order 4 are P_4 and S_3, and $\pi(P_4) = 4$ and $\pi(S_3) = 4$. Assume that u is an isolated vertex in $T - x$, and v belongs to the component K_2 of $T - x$ and is adjacent to x. Let the transposition $f = (uv)$. Then $\delta_f(T) = \delta_f(w, u) + \delta_f(w, v) = 2 + 2 = 4$, see Figure 2.3. Thus, $\pi(T) = 4$.

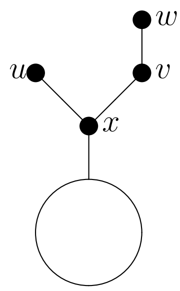


Figure 2.3: $f = (uv)$ and $\delta_f(G) = 4$.

Conversely, suppose that $\pi(T) = 4$. Then $A(T[f])$ is equal to $\{\langle a_1, a_2\rangle, \langle a_2, a_1\rangle, \langle a_i, a_{i+1}\rangle, \langle a_{i+1}, a_i\rangle$: for some $i, 1 \leq i \leq t\}$, $\{\langle a_1, a_2\rangle,\langle a_2, a_3\rangle,\langle a_3, a_1\rangle\}$, $\{\langle a_1, a_3\rangle, \langle a_2, a_1\rangle, \langle a_3, a_2\rangle\}$ or $\{\langle a_1, a_3\rangle, \langle a_3, a_1\rangle\}$.

Case 1. $A(T[f]) = \{\langle a_1, a_2\rangle, \langle a_2, a_1\rangle, \langle a_i, a_{i+1}\rangle, \langle a_{i+1}, a_i\rangle :$ for some $i, 1 \leq i \leq t\}$. When $i = 1$, we claim that $T \simeq S_3$. By the same argument as in Theorem 2.1.3, there are three vertices u, v, w of $V(T)$ such that (u, v, w) and $(f(u), f(w), f(v))$ are two paths in T, and $|V(T)| \geq 4$. Since $d(u, w) = 2$, $d(f(u), f(w)) = d(f(v), f(w)) = 1$ and $\langle a_i, a_j\rangle \notin A(T[f])$ for $i \geq 3$ or $j \geq 3$. Hence, none of the vertices of $V(T) \setminus \{u, v, w\}$ is adjacent to u or w in T. With the same argument, since $d(f(u), f(v)) = 2$, $d(u, v) = d(v, w) = 1$ and $\langle a_i, a_j\rangle \notin A(T[f])$ for $i \geq 3$ or $j \geq 3$, we get that for each vertex y of $V(T) \setminus \{u, v, w\}$, $f(y)$ must be adjacent to $f(w)$. Then each vertex of $V(T) \setminus \{u, v, w\}$ contributes 2 to $\pi(T)$. Hence $\delta_f(G) = 2(|V(T)| - 2) = 4$ implies that $|V(T)| = 4$, and $T \simeq S_3$.

Otherwise, for $i \geq 2$, we have $|V(T)| \geq 5$. Let $\alpha(x_0, x_i) = \langle a_i, a_{i+1}\rangle$ and the path from x_0 to x_i in T be $(x_0, x_1, \ldots, x_i)$ and y be a vertex of $V(T)$ such that $f(y)$ lies on the path from $f(x_0)$ to $f(x_i)$. Without loss of generality, we let $d(x_0, y) \geq d(x_i, y)$. Since $d(x_0, x_i) \neq d(f(x_0), f(x_i))$, we have $d(x_0, x_1) \neq d(f(x_0), f(x_1))$ or $d(x_1, x_i) \neq d(f(x_1), f(x_i))$, i.e. $\alpha(x_0, x_1)$ or $\alpha(x_1, x_i) \in A(T[f])$.

If $\alpha(x_0, x_1) \in A(T[f])$, then $\alpha(x_0, x_1) = \langle a_1, a_2\rangle$. Furthermore, if $i \geq 3$, then $\alpha(x_0, x_2) = \langle a_2, a_1\rangle$ or $\alpha(x_2, x_i) = \langle a_2, a_1\rangle$. But, when $\alpha(x_0, x_2) = \langle a_2, a_1\rangle$, $d(f(x_0), f(x_i)) \leq d(f(x_0), f(x_2)) + d(f(x_2), f(x_i)) = 1 + (i - 2) = i - 1$, a contradiction. On the other hand, if $\alpha(x_2, x_i) = \langle a_2, a_1\rangle$, $i = 4$, $d(f(x_0), f(x_4)) \leq d(f(x_0), f(x_2)) + d(f(x_2), f(x_4)) = 2 + 1 = 3$, also a contradiction. Thus the only possible case left is $i = 2$. Then, $\alpha(x_0, x_1) = \langle a_1, a_2\rangle$ and $\delta_f(x_1, x_2) = 0$ imply that $d(f(x_0), f(x_2)) = d(f(x_0), f(x_1)) + d(f(x_1), f(x_2))$, $f(x_1)$ is on the path from $f(x_0)$ to $f(x_2)$ and the path is $(f(x_0), f(y), f(x_1), f(x_2))$. Since $d(x_0, y) \geq d(x_2, y)$, $\alpha(x_0, y) \in A(T[f])$, in fact $\alpha(x_0, y) = \langle a_2, a_1\rangle$. The induced subgraph of $\{x_0, x_1, x_2, y\}$ in T is a star with center x_1. Since $|V(T)| \geq 5$, there exists another vertex z which is adjacent to one of $\{x_0, x_1, x_2, y\}$, and no matter which one is adjacent to z, $\delta_f(z) \geq 2$, a contradiction.

Now, suppose that $\alpha(x_1, x_i) \in A(T[f])$ and $\delta_f(x_0, x_1) = 0$. Then $\alpha(x_1, x_i)$ is equal to $\langle a_1, a_2\rangle$ or $\langle a_2, a_1\rangle$, $i = 2$ or $i = 3$. First, for $i = 3$, we have $d(f(x_0), f(x_3)) \leq d(f(x_0), f(x_1)) + d(f(x_1), f(x_3)) = 1 + 1 = 2$, a contradiction. Hence, $i = 2$ and the path from $f(x_0)$ to $f(x_2)$ is $(f(x_0), f(x_1), f(y), f(x_2))$. Since $d(f(y), f(x_1)) = d(f(y), f(x_2)) = 1$ and $d(x_1, x_2) = 1$, by Lemma 2.2.1, we have $\alpha(y, x_1) = \langle a_2, a_1\rangle$ or $\alpha(y, x_2) = \langle a_2, a_1\rangle$ in the tree T. If $\alpha(y, x_1) = \langle a_2, a_1\rangle$, then we have $\delta_f(y, x_2) = 0$ and the induced subgraph of $\{x_0, x_1, x_2, y\}$ is a path (x_0, x_1, x_2, y); if $\alpha(y, x_2) = \langle a_2, a_1\rangle$, then we have $\delta_f(y, x_1) = 0$ and the induced subgraph of $\{x_0, x_1, x_2, y\}$ is a star with the center x_1. Since $|V(T)| \geq 5$, there exists a vertex z' which is adjacent to one of the vertices in $\{x_0, x_1, x_2, y\}$. Clearly, no matter which one is adjacent to z', we also have $\delta_f(z') \geq 2$. Thus, this case is not possible.

Case 2. $A(T[f]) = \{\langle a_1, a_2\rangle, \langle a_2, a_3\rangle, \langle a_3, a_1\rangle\}$. Let $\alpha(u, v) = \langle a_1, a_2\rangle$ and $(f(u), f(w), f(v))$ be the path in T for some vertex w. Then $d(f(w), f(u)) = d(f(w), f(v)) = 1$ implies that one of the elements in $\{d(w, u), d(w, v)\}$ is 1 and the other one is 3. By Lemma 2.2.1, this case is impossible.

Case 3. $A(T[f]) = \{\langle a_1, a_3\rangle, \langle a_2, a_1\rangle, \langle a_3, a_2\rangle\}$. By Lemma 1.3.11, if f is a near automorphism, then f^{-1} is also a near automorphism. Moreover, $A(T[f^{-1}]) = \{\langle a_1, a_2\rangle, \langle a_2, a_3\rangle, \langle a_3, a_1\rangle\}$. Thus, by **Case 2**, **Case 3** is also not possible.

Case 4. $A(T[f]) = \{\langle a_1, a_3\rangle, \langle a_3, a_1\rangle\}$. Let $\alpha(u, v) = \langle a_1, a_3\rangle$ and $\{x, y\}$ be a pair of vertices of T such that $(f(u), f(x), f(y), f(v))$ is a path in T. Then, $d(f(u), f(y)) = d(f(x), f(v)) = 2$ implies that $d(u, y) = d(x, v) = 2$, and $d(f(u), f(x)) = d(f(x), f(y)) = d(f(y), f(v)) = 1$ implies that one of the elements in $\{d(u, x), d(x, y), d(y, v)\}$ is 3 and the other two are 1 in tree T.

If $\alpha(x, y) = \langle a_3, a_1\rangle$, then in T the graph induced by the vertex set $\{u, v, x, y\}$ is the path (x, u, v, y). If $|V(T)| = 4$, then $T \simeq P_4$. If $|V(T)| \geq 5$, then there is a vertex w which is adjacent to one vertex in $\{u, v, x, y\}$ and keeps the condition that $\delta_f(w) = 0$. This is impossible, since $\delta_f(w) \geq \delta_f(w, x) + \delta_f(w, y) > 0$.

In addition, since $\alpha(u, x) = \langle a_3, a_1\rangle$ and $\alpha(y, v) = \langle a_3, a_1\rangle$ are similar cases, we consider the case $\alpha(u, x) = \langle a_3, a_1\rangle$. Then the graph induced by $\{u, v, x, y\}$ is (u, v, y, x), and it's obviously an exchange of x and v. If $|V(T)| \geq 5$, then for each vertex w in $V(T) \setminus \{u, v, x, y\}$, $\delta_f(w) = 0$. Moreover, in order to maintain $\delta_f(w) = 0$, all the paths which combine each vertex in $\{u, v, x, y\}$ to each vertex in $V(T) \setminus \{u, v, x, y\}$ must pass through y. This implies that $T - y$ contains an isolated vertex x and K_2 induced by $\{u, v\}$. Furthermore, the near automorphism is the transposition (vx).

This concludes the proof. ∎

So, we have obtained the trees T of order n such that $\pi(T) = 4$. But, for larger values t, $4 < t \leq 2n - 4$, to determine the trees T with $\pi(T) = t$ seems quite difficult. We shall make an effort in Chapter 4 to find those trees T with $\pi(T) = 2n - 4$.

Chapter 3

Near Automorphisms of Cycles

As mentioned earlier in Theorem 1.4.1, the near automorphisms have been characterized by Aitken and he also proved that $\pi(P_n) = 2n - 4$. Therefore, it is natural to ask what are the set of near automorphisms of C_n, the cycle of order n, and we shall answer this question in this chapter. Furthermore, by using the idea we obtained in showing $\pi(C_n) = 4\lfloor \frac{n}{2} \rfloor - 4$, we obtain an alternative proof of $\pi(P_n) = 2n - 4$.

3.1 $\pi(C_n) = 4\lfloor \frac{n}{2} \rfloor - 4$

For convenience, the n-cycle C_n we consider throughout this chapter is denoted by $(v_{-\lfloor \frac{n}{2} \rfloor}, \cdots, v_{-1}, v_0, v_1, \cdots, v_{\lfloor \frac{n}{2} \rfloor})$ (for n even we let $v_{-\lfloor \frac{n}{2} \rfloor} = v_{\lfloor \frac{n}{2} \rfloor}$) and the vertices are distributed on the cycle evenly. Now, clearly the permutations $g(v_i) = v_{-i}$ and $h(v_i) = v_{i+j}$ for some j, $1 \leq j \leq t$, and for all i, $1 \leq i \leq t$, are automorphisms of C_n. The permutations g and h are the mirror reflection and the rotation respectively (geometrically speaking).

Theorem 3.1.1. $\pi(C_n) = 4\lfloor \frac{n}{2} \rfloor - 4$.

Proof. Let the permutation be the transposition $(v_0 v_1)$. Then, by direct counting, we have $\pi(C_n) \leq \delta_f(C_n) = 4\lfloor \frac{n}{2} \rfloor - 4$. For $n \leq 3$, all permutations of C_n are automorphisms. Therefore, we start our proof by showing that for each positive integer

$n \geq 4$, $\delta_f(C_n) \geq 4\lfloor \frac{n}{2} \rfloor - 4$ for any non-automorphism f.

Since C_n is a vertex-transitive graph, by Lemma 1.3.5, we may assume that f is a non-automorphism of C_n such that $f(v_0) = v_0$ and $\delta_f(v_0) = \min\{\delta_f(v) : v \in V(C_n)\}$.

Clearly, if $\delta_f(v_0) \geq 4$, then $\delta_f(C_n) \geq 2n$ and the proof follows. Hence we assume that $\min\{\delta_f(v) : v \in V(C_n)\}$ is equal to 0 or 2. Note that, by Lemma 1.3.4, $\delta_f(v_0)$ is even.

Case 1. $\delta_f(v_0) = 0$.

This implies that for each $v_i \in V(C_n)$, $i \neq 0$, $f(v_i) \in \{v_i, v_{-i}\}$. Let $A = \{k : f(v_k) = v_k, k = 1, 2, \cdots, \lceil \frac{n}{2} \rceil - 1\}$ and $B = \{h : f(v_h) = v_{-h}, h = 1, 2, \cdots, \lceil \frac{n}{2} \rceil - 1\}$. Since f is not an automorphism, then $|A| \neq 0$ and $|B| \neq 0$. Thus in this case, $n \geq 5$. Then, for each $k \in A$ and $h \in B$, $|d_{C_n}(v_k, v_h) - d_{C_n}(f(v_k), f(v_h))| \geq 1$ whenever n is odd and $|d_{C_n}(v_k, v_h) - d_{C_n}(f(v_k), f(v_h))| \geq 2$ whenever n is even. Now, let $A^- = \{-k : k \in A\}$ and $B^- = \{-h : h \in B\}$. The above inequalities also hold for $k \in A^-$ and $h \in B$ or $k \in A$ and $h \in B^-$ or $k \in A^-$ and $h \in B^-$ depending on whether n is odd and even, respectively. Thus, we conclude that $\delta_f(C_n) \geq 4|A||B|$ or $8|A||B|$ depending on whether n is odd or even, respectively. Nevertheless, by the fact that $|A| + |B| = \lceil \frac{n}{2} \rceil - 1$, we have $\delta_f(C_n) \geq 4 \cdot 1 \cdot (\lceil \frac{n}{2} \rceil - 2)$ or $8 \cdot 1 \cdot (\lceil \frac{n}{2} \rceil - 2)$ with respect to whether n is odd or even, respectively and the equality holds only if $|h| = \lceil \frac{n}{2} \rceil - 1$ for all odd n and special for $n = 6$ since $8 \cdot (\lceil \frac{n}{2} \rceil - 2) = 4\lfloor \frac{n}{2} \rfloor - 4$.

Case 2. $\delta_f(v_0) = 2$.

By Lemma 1.3.6, there exist two distinct vertices v_h and v_k such that $\delta_f(v_0) = \delta_f(v_0, v_h) + \delta_f(v_0, v_k)$, where $h, k \in \{-\lfloor \frac{n}{2} \rfloor, \cdots, 0, \cdots, \lfloor \frac{n}{2} \rfloor\}$ (again, for n even we let $v_{-\lfloor \frac{n}{2} \rfloor} = v_{\lfloor \frac{n}{2} \rfloor}$) and $|h| = |k| + 1$. Hence, the near automorphism f satisfies one of the following four conditions: (a) $f(v_h) = v_k$ and $f(v_k) = v_h$, (b) $f(v_h) = v_k$ and $f(v_k) = v_{-h}$, (c) $f(v_h) = v_{-k}$ and $f(v_k) = v_h$, (d) $f(v_h) = v_{-k}$ and $f(v_k) = v_{-h}$. Since

$\delta_f(v_0) = 2$, for each $v_i, i \neq h, k, f(v_i) = v_i$ or $f(v_i) = v_{-i}$. Obviously, if we compose an automorphism g to all the possible permutations in (a), then we can get all the possible permutations in (d), where g is a mirror reflection such that $g(v_0) = v_0$ and $g(v_i) = v_{-i}$ for all i, and so do (b) and (c). Thus, it suffices to find $\delta_f(C_n)$ for the f's satisfying (a) and (b) respectively. By considering the displacement of v_h and v_k, we have

$$\begin{aligned}\delta_f(C_n) &\geq \sum_{i\neq h,k}\{\delta_f(v_h, v_i) + \delta_f(v_k, v_i)\}\\ &= \sum_{i\neq h,k}\{|d(v_h, v_i) - d(f(v_h), f(v_i))| + |d(v_k, v_i) - d(f(v_k), f(v_i))|\}\end{aligned}$$

Let $C = \{i : f(v_i) = v_i, i \neq h, k\}$ and $D = \{j : f(v_j) = v_{-j}, j \neq h, k\}$. Since $v_0 \in C$, $|C| \neq 0$, and $|C| + |D| = n - 2$. Then, for the f satisfying (a), we have

$$\begin{aligned}\delta_f(C_n) \geq &\sum_{\substack{i\neq h,k\\ i\in C}}\{|d(v_h, v_i) - d(v_k, v_i)| + |d(v_k, v_i) - d(v_h, v_i)|\}+\\ &\sum_{\substack{i\neq h,k\\ i\in D}}\{|d(v_h, v_i) - d(v_k, v_{-i})| + |d(v_k, v_i) - d(v_h, v_{-i})|\}.\end{aligned}\tag{3.1}$$

By the fact that $|d(v_h, v_i) - d(v_k, v_i)| \geq 1$ and $|d(v_h, v_i) - d(v_k, v_{-i})| \geq 1$ for each $i \neq h, k$ in the case n is even, we have $\delta_f(C_n) \geq 2(|C| + |D|) = 2(n - 2)$, as desired. On the other hand, if n is odd, there is exactly one vertex $v_j, j \neq h, k$ in $V(C_n)$ that satisfies $d(v_h, v_j) = d(v_k, v_j)$. Thus, $\delta_f(C_n) \geq 2(n-3) = 4\lfloor\frac{n}{2}\rfloor-4$ in the case when n is odd, since $|C| \neq 0$, $\delta_f(C_n) = 4\lfloor\frac{n}{2}\rfloor-4$ if $|d(v_h, v_i)-d(v_k, v_i)| = 1$. In fact, $d(v_h, v_k) = 1$ for all i and for all n but $i = \lfloor\frac{n}{2}\rfloor$ or $-\lfloor\frac{n}{2}\rfloor$, and we have $|d(v_h, v_i) - d(v_k, v_i)| = 1$; if $d(v_h, v_k) \neq 1$, then there are four and two vertices such that $|d(v_h, v_i) - d(v_k, v_i)| = 1$ and the other vertices $|d(v_h, v_i) - d(v_k, v_i)| \geq 3$ and 2 in all n even and odd case, respectively.

Next, for the f satisfying (b), we have

$$\begin{aligned}\delta_f(C_n) \geq &\sum_{\substack{i\neq h,k\\ i\in C}}\{|d(v_h, v_i) - d(v_k, v_i)| + |d(v_k, v_i) - d(v_{-h}, v_i)|\}+\\ &\sum_{\substack{i\neq h,k\\ i\in D}}\{|d(v_h, v_i) - d(v_k, v_{-i})| + |d(v_k, v_i) - d(v_{-h}, v_{-i})|\}.\end{aligned}\tag{3.2}$$

By observation, we are able to see that at least one of the summands is larger than 2. Therefore, we conclude that $\delta_f(C_n) > 4\lfloor \frac{n}{2} \rfloor - 4$ in this case. In conclusion that we have the lower bound $\delta_f(C_n) \geq 4\lfloor \frac{n}{2} \rfloor - 4$. ∎

By the way, in the above argument, we also have the near automorphisms of C_n are $f \circ g$ and $g \circ f$ where $f = (v_0 v_1)$ and g is an automorphism of C_n, (since C_n is a vertex-transitive graph, we prefer $(v_0 v_1)$ to any transposition of two adjacent vertices), and special for $n = 5$, $f = (v_0 v_1)$ or $(v_0 v_2)$ and for $n = 6$, $f = (v_0 v_1)$, $(v_0 v_2)$ or $(v_0 v_3)$. This concludes the following theorem.

Theorem 3.1.2. *The near automorphisms of C_n are $f \circ g$ and $g \circ f$ where $f = (v_0 v_1)$ and g is an automorphism of C_n, and special for $n = 5$, $f = (v_0 v_1)$ or $(v_0 v_2)$ and for $n = 6$, $f = (v_0 v_1)$, $(v_0 v_2)$ or $(v_0 v_3)$.*

3.2 An Alternative Proof of $\pi(P_n) = 2n - 4$

In this section, we would like to point out that the study of near automorphisms of paths and cycles does have some similarity. With the following proposition, we provide a short proof of $\pi(P_n) = 2n - 4$ which was obtained by Aitken [1].

Proposition 3.2.1. $\pi(P_n) \geq \pi(C_n)$, the equality holds only when n is even.

Proof. Let $P_n = \langle v_1, v_2, \cdots, v_n \rangle$ and $C_n = (v_1, v_2, \cdots, v_n)$. Now, it is easy to see that $d_{P_n}(v_i, v_j) = |j - i|$ and $d_{C_n}(v_i, v_j) = \min\{|j - i|, n - |j - i|\}$. In order to prove the proposition, we will first show that for each permutation f of $V(P_n) = V(C_n)$ and for each pair of distinct vertices $\{x, y\}$, $|d_{P_n}(x, y) - d_{P_n}(f(x), f(y))| \geq |d_{C_n}(x, y) - d_{C_n}(f(x), f(y))|$. Clearly, if both $d_{P_n}(x, y)$ and $d_{P_n}(f(x), f(y))$ are not larger than $\lfloor \frac{n}{2} \rfloor$, neither are $d_{C_n}(x, y)$ and $d_{C_n}(f(x), f(y))$, and thus the proof follows. On the other hand if both $d_{P_n}(x, y)$ and $d_{P_n}(f(x), f(y))$ are larger than $\lfloor \frac{n}{2} \rfloor$, then $|d_{C_n}(x, y) -$

$d_{C_n}(f(x), f(y))| = |n - d_{P_n}(x,y) - n + d_{P_n}(f(x), f(y))| = |d_{P_n}(x,y) - d_{P_n}(f(x), f(y))|$. Therefore, it is left to consider the case that one of them is larger and the other is smaller than $\lfloor \frac{n}{2} \rfloor$ or equivalently $d_{P_n}(x,y) > \lfloor \frac{n}{2} \rfloor$ and $d_{P_n}(f(x), f(y)) \leq \lfloor \frac{n}{2} \rfloor$ (by symmetry). Now, we have two subcases to consider.

(i) $d_{P_n}(x,y) + d_{P_n}(f(x), f(y)) \geq n$.
$|d_{C_n}(x,y) - d_{C_n}(f(x), f(y))| = |n - d_{P_n}(x,y) - d_{P_n}(f(x), f(y))| = d_{P_n}(x,y) + d_{P_n}(f(x), f(y)) - n \leq d_{P_n}(x,y) - d_{P_n}(f(x), f(y)) = |d_{P_n}(x,y) - d_{P_n}(f(x), f(y))|$.

(ii) $d_{P_n}(x,y) + d_{P_n}(f(x), f(y)) < n$.
$|d_{C_n}(x,y) - d_{C_n}(f(x), f(y))| = |n - d_{P_n}(x,y) - d_{P_n}(f(x), f(y))| = n - d_{P_n}(x,y) - d_{P_n}(f(x), f(y)) \leq d_{P_n}(x,y) - d_{P_n}(f(x), f(y)) = |d_{P_n}(x,y) - d_{P_n}(f(x), f(y))|$.

Note that the equalities in (i) and (ii) hold when $n = 2d_{P_n}(x,y)$ and $n = 2d_{P_n}(f(x), f(y))$ respectively. Therefore, n must be even. Thus, for each non-automorphism f, we have $\delta_f(P_n) \geq \delta_f(C_n)$. Hence, we left with the case that when f is an automorphism of C_n but not an automorphism of P_n, $\delta_f(P_n) \geq 2n - 4$.

Clearly, $g(v_i) = v_{n-i+1}$ and $h(v_i) = v_{i+j}$ (mod n) are a mirror reflection and rotation of C_n here, respectively, and they can create all the automorphisms of C_n. Obviously, if $\{f(v_1), f(v_n)\} = \{v_1, v_n\}$ for some automorphism f of C_n, then f is also an automorphism of P_n. Otherwise, if $\{f(v_1), f(v_n)\} = \{v_j, v_{j+1}\}$ for $1 \leq j < n$, then $\{f(v_j), f(v_{j+1})\} = \{v_1, v_n\}$ or $\{f(v_{n-j}), f(v_{n-j+1})\} = \{v_1, v_n\}$, and $\delta_f(P_n) \geq \delta_f(v_1, v_n) + \delta_f(v_j, v_{j+1}) + \delta_f(v_{n-j}, v_{n-j+1}) = (n-2) + (n-2) = 2n - 4$. Thus this concludes the proof. ∎

Hence, by Theorem 3.1.1 and Proposition 3.2.1, we can get $\pi(P_n) \geq 2n - 4$. Then, $\pi(P_n) = 2n - 4$ [1] follows by the fact that $\pi(P_n) \leq 2n - 4$ (Lemma 1.3.12).

Chapter 4

Trees T with $\pi(T) = 2n - 4$

4.1 Necessary Conditions

It should be recalled that if G is a graph of order n, then $\pi(G) \leq 2n-4$. Therefore, it is interesting to know for which graphs G, $\pi(G) = 2n-4$. By Theorem 1.4.1 [1], it is known that if P_n is a path with n vertices, then $\pi(P_n) = 2n-4$ for each $n \geq 3$. Since P_n is a special tree, we intend to find more trees T of order n such that $\pi(T) = 2n-4$ and finally find all trees T of order n with $\pi(T) = 2n-4$.

First, we obtain the necessary conditions for the trees T having $\pi(T) = 2n-4$.

Lemma 4.1.1. *Let T be a tree of order n such that $\pi(T) = 2n-4$. Then, the following conditions hold:*

(a) *If there exists a vertex x with $deg_T(x) \geq 3$ and $T-x$ has an isolated vertex, then $T-x$ has at most one non-trivial component.*

(b) *For each $y \in V(T)$, if $T-y$ contains only non-trivial components, then $deg_T(y) \leq 3$.*

Proof. We verify (a) first. Assume that x is a vertex in T with $deg_T(x) \geq 3$, $T-x$ has an isolated vertex x_0 and $T-x$ contains at least two non-trivial components. Let H be one of the non-trivial components which has the minimum number of vertices, and let $|V(H)| = s$. Clearly, $s \geq 2$ and $s < \frac{n}{2}$. Let $z \in V(H)$ and $zx \in E(T)$. Now, by letting $f = (x_0 z)$, the transposition of x_0 and z, we have $\delta_f(T) = 4(s-1)$. Since $\pi(T) = 2n-4$, $4(s-1) \geq 2n-4$ which implies $s \geq \frac{n}{2}$, a contradiction. Hence, (a) is verified.

Now, we verify (b). Observe that if y is a pendent vertex of T, then the assertion follows. So, let y be a cut vertex of T. Let H_1 and H_2 be two non-trivial components in $T - y$ which have minimum number of vertices t and r, respectively ($t \leq r$). Let $y_i \in V(H_i)$, $i = 1, 2$, such that $yy_i \in E(T)$. By a similar argument, let $f = (y_1 y_2)$, then $\delta_f(T) = 4(t+r-2) \geq 2n-4$. Hence $t + r \geq \frac{n}{2} + 1$. This implies that $T - y$ has at most three non-trivial components, and thus $deg_G(x) \leq 3$. ∎

By Lemma 4.1.1, it is not difficult to see that if $\pi(T) = 2n-4$ where T is a tree of order n, then T must be a graph in the following two classes of graphs, see Figure 4.1 and Figure 4.2. For convenience, the class of graphs in Figure 4.1 is denoted by $T^{(2)}$ (double broom) and the other class of graphs in Figure 4.2 is denoted by $T^{(3)}$ (triple broom). Since $T \in T^{(2)}$ is a star (path) whenever $t = 1$ ($s = 2$) and $\pi(T) = 2n-4$, we consider this case a special one and assume that $t \geq 2$ ($s \geq 2$) throughout of the rest of this chapter.

$T^{(2)}$:

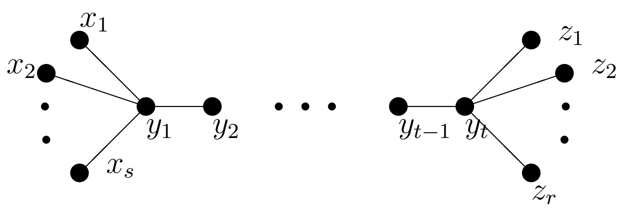


Figure 4.1: Double Broom ($s \geq r$).

$T^{(3)}$:

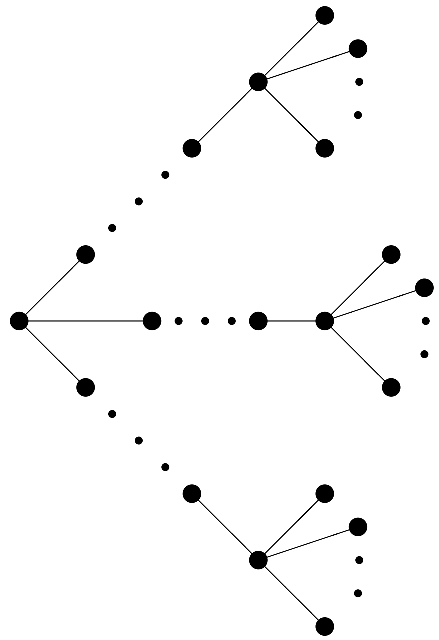


Figure 4.2: Triple Broom.

4.2 Double Broom T with $\pi(T) = 2n - 4$

In this section, we shall focus on the trees T in $T^{(2)}$ with constraints on the number of pendent vertices. By observation, both transpositions $\alpha = (y_2 x_s)$ and $\beta = (y_{t-1} z_r)$ are not automorphisms. It is not difficult to see that $\delta_\alpha(T) = 4(r + t - 2)$ and $\delta_\beta(T) = 4(s + t - 2)$. This implies that $\pi(T) \leq \min\{4(r + t - 2), 4(s + t - 2)\}$. Therefore, if $\pi(T) = 2n - 4$, then $r + t \geq \frac{n}{2} + 1$ and $s + t \geq \frac{n}{2} + 1$. That is to say, without these two extra constraints, $\pi(T) < 2n - 4$ for the trees in $T^{(2)}$. Therefore, we have

Lemma 4.2.1. *If $T \in T^{(2)}$ is a tree of order n and $\pi(T) = 2n-4$, then $r+t \geq \frac{n}{2}+1$ where $s \geq r$.*

In what follows, we shall prove that all the trees $T \in T^{(2)}$ with $s \geq r$ and $r + t \geq \frac{n}{2} + 1$ attain $\pi(T) = 2n - 4$.

It is worth of noting again that if T is a path of order $n \geq 3$, then $T \in T^{(2)}$ and also T satisfies the constraints mentioned above. Therefore, the result obtained in what follows implies that $\pi(P_n) = 2n - 4$.

In order to evaluate $\pi(T)$, we introduce a notion which is interesting in itself. Let $A = (a_1, a_2, \cdots, a_m)$ and $B = (b_1, b_2, \cdots, b_m)$ be two ordered m-tuples of real numbers where $a_1 \leq a_2 \leq \cdots \leq a_m$. Define $\|A - B\|$ to be $\sum_{i=1}^{m} |a_i - b_i|$. So, $\|A - B\|$ is a non-negative value. Also, let $\phi(B) = (b_{\phi(1)}, b_{\phi(2)}, \cdots, b_{\phi(m)})$ where ϕ is a permutation of $\{1, 2, \cdots, m\}$, i.e., $\phi \in S_m$ (the symmetric group of order m). Now, it is interesting to find $\min_{\phi \in S_m} \|A - \phi(B)\|$.

Lemma 4.2.2. *Let* $\phi \in S_m$ *such that* $b_{\phi(1)} \leq b_{\phi(2)} \leq \cdots \leq b_{\phi(m)}$. *Then* $\|A - \phi(B)\|$ *attains* $\min_{\phi \in S_m} \|A - \phi(B)\|$.

Proof. It suffices to prove that if $b_i > b_j$ for some $i < j$, then $\|A - B'\| \leq \|A - B\|$ where $B' = (b_1, b_2, \cdots, b_{i-1}, b_j, b_{i+1}, \cdots, b_{j-1}, b_i, b_{j+1}, \cdots, b_m)$. The proof is then obtained by sorting the sequence B step by step.

We now claim that $|a_i - b_j| + |a_j - b_i| \leq |a_i - b_i| + |a_j - b_j|$. Since for all the orders the other differences are the same , the proof follows.

By checking all six cases of the distributions of b_i and b_j compared with a_i and a_j, we have (1) $b_j \leq b_i \leq a_i \leq a_j$, (2) $b_j \leq a_i \leq b_i \leq a_j$, (3) $b_j \leq a_i \leq a_j \leq b_i$, (4) $a_i \leq b_j \leq b_i \leq a_j$, (5) $a_i \leq b_j \leq a_j \leq b_i$, (6) $a_i \leq a_j \leq b_j \leq b_i$. Then, the proof follows by calculating the values $|a_i - b_j|$, $|a_j - b_i|$, $|a_i - b_i|$ and $|a_j - b_j|$ in each respective case. ∎

We are now ready to evaluate the total relative displacements. First, we consider two distinct vertices u and v in G. Since $A_u = \{d_G(u, w) : u \neq w\}$ and $A_v =$

$\{d_G(v,w) : v \neq w\}$ are two sets of positive integers, we let $\hat{A}_u = (a_1, a_2, \cdots, a_{n-1})$ and $\hat{A}_v = (b_1, b_2, \cdots, b_{n-1})$ where n is the order of G, $\hat{A}_u$ and $\hat{A}_v$ are two non-decreasing sequences obtained from A_u and A_v, respectively, by sorting their orders. For convenience, we define $P(u,v) = \|\hat{A}_u - \hat{A}_v\| = \sum_{i=1}^{n-1} |a_i - b_i|$. Obviously, $P(u,v) = P(v,u)$. Moreover, we have the following property, which holds for all graphs, not only trees.

Lemma 4.2.3. *For each vertex $x \in V(G)$ and each permutation f of $V(G) = \{v_1, v_2, \cdots, v_n\}$, $\delta_f(x) \geq P(x, f(x))$.*

Proof. $\delta_f(x) = \sum_{w \neq x} \delta_(x,w) = \sum_{w \neq x} |d(x,w) - d(f(x), f(w))| \geq \|\hat{A}_x - \hat{A}_{f(x)}\| = P(x, f(x))$. ∎

Observe that Lemma 4.2.3 provides a way to estimate the lower bound of $\delta_f(G)$. In order to find $\delta_f(T)$ where $T \in T^{(2)}$, we also need the following results. Without mentioning otherwise, all trees T we consider in what follows are of order n and $T \in T^{(2)}$, furthermore, $s \geq r$ and $r + t \geq \frac{n}{2} + 1$.

Lemma 4.2.4. *Let T be the tree in Figure 4.1. Then,*

(1) $\sum_{w \in V(T)} d(x_i, w) = [t^2 + (2r+1)t + (2r + 4s - 4)]/2,$

(2) $\sum_{w \in V(T)} d(z_i, w) = [t^2 + (2s+1)t + (2s + 4r - 4)]/2,$ *and*

(3) $\sum_{w \in V(T)} d(y_i, w) = i^2 - (1 - s + r + t)i + (t+1)(r + \dfrac{t}{2}).$

Proof. Since (1) and (2) are easy to see, we check (3) here.

$$\begin{aligned}
\sum_{w \in V(T)} d(y_i, w) &= si + (i-1) + (i-2) + \cdots + 1 + 1 + \cdots + (t-i) + r(t-i+1) \\
&= si + \tfrac{i(i-1)}{2} + \tfrac{(t-i)(t-i+1)}{2} + r(t-i+1) \\
&= si + \tfrac{i^2}{2} - \tfrac{i}{2} + \tfrac{t^2}{2} - ti + \tfrac{i^2}{2} + \tfrac{t}{2} - \tfrac{i}{2} + rt - ri + r \\
&= i^2 - (1 - s + r + t)i + (t+1)(r + \tfrac{t}{2}).
\end{aligned}$$

$\blacksquare$

Lemma 4.2.5. *Let $T \in \mathcal{T}^{(2)}$ with $s \geq r$ and $r+t \geq \frac{n}{2}+1$. Then, we have the following sorting values.*

(1) $P(x_i, z_j) = (s-r)t$.

(2) $P(x_i, y_j) \geq n-2$, *for* $1 \leq j \leq t-(s-r)$; *and*

$P(x_i, y_j) = 2$, *for* $j = t$ *and* $s = r+1 = 2$.

(3) $P(z_i, y_j) \geq n-2$, *for all* j.

(4)
$$P(y_i, y_j) = \begin{cases} 0, & i=j, \text{ or } i+j=t+1 \text{ for } s=r; \\ 1, & i=\frac{t}{2}, j=\frac{t}{2}+1 \text{ for } s-r=1; \\ 2, & i=\frac{t-1}{2}, j=\frac{t+1}{2} \text{ for } s=r+1=2; \\ & i=\frac{t+1}{2}, j=\frac{t+3}{2} \text{ for } s=r+1=2; \\ & i=\frac{t}{2}, j=\frac{t}{2}+1 \text{ for } s=r+2; \\ 3, & i=\frac{t}{2}-1, j=\frac{t}{2} \text{ for } s=r+1=2; \\ & i=\frac{t-1}{2}, j=\frac{t+1}{2} \text{ for } s=r+2=3; \\ & i=\frac{t-1}{2}, j=\frac{t+1}{2} \text{ for } s=r=2; \\ & i=\frac{t+1}{2}, j=\frac{t+3}{2} \text{ for } s=r=2; \\ & i=\frac{t}{2}+1, j=\frac{t}{2}+2 \text{ for } s=r+1=2; \\ & i=\frac{t}{2}-1, j=\frac{t}{2}+2 \text{ for } s=r+1; \\ & i=\frac{t}{2}-1, j=\frac{t}{2}+1 \text{ for } s=r+1=2; \\ & i=\frac{t}{2}, j=\frac{t}{2}+1 \text{ for } s=r+3; \text{ and} \end{cases}$$

$P(y_i, y_j) \geq 4$, *otherwise.*

Proof.

(1) Clearly, $\hat{A}_{x_i} = (1, \underbrace{2, \cdots, 2}_{s}, 3, 4, \cdots, t, \underbrace{t+1, \cdots, t+1}_{r})$ and

$$\hat{A}_{z_j} = (1, \underbrace{2, \cdots, 2}_{r}, 3, 4, \cdots, t, \underbrace{t+1, \cdots, t+1}_{s}).$$

Therefore, $P(x_i, z_j) = \|\hat{A}_{x_i} - \hat{A}_{z_j}\| = (1+2+\cdots+(s-r))\cdot 2 + (s-r)\cdot(n-2s-1) = (s-r)(s-r+1) + (s-r)(n-2s-1) = (s-r)(n-s-r) = (s-r)t.$

(2) Since $P(x_i, y_j) = \sum |a_i - b_i| \geq \sum (a_i - b_i) = \sum a_i - \sum b_i = \sum_{w \in V(T)} d(x_i, w) - \sum_{w \in V(T)} d(y_j, w)$, thus we have $P(x_i, y_j) \geq n-2$ for $1 \leq j \leq t-(s-r)$.
Also, we have

$$\hat{A}_{x_i} = (1, \underbrace{2, \cdots, 2}_{s}, 3, 4, \cdots, t, \underbrace{t+1, \cdots, t+1}_{r}), \text{ and}$$

$$\hat{A}_{y_t} = (\underbrace{1, \cdots, 1}_{s+1}, 2, \cdots, t-1, \underbrace{t, \cdots, t}_{r}). \text{ This implies that}$$

$$P(x_i, y_t) = \begin{cases} n-2, & \text{if } s = r; \\ 2r + (s-r-1)(t-2), & \text{if } s - r \geq 1. \end{cases}$$ Hence, the claim follows.

(3) $P(z_i, y_j) \geq \sum_{w \in V(T)} d(z_i, w) - \sum_{w \in V(T)} d(y_j, w) \geq n-2$, for all j.

(4) The proof follows by considering the following cases: $1 \leq i < j < \frac{t+1}{2}$, $1 \leq i < j = \frac{t+1}{2}$, $1 \leq i < \frac{t+1}{2} < j \leq t$, $\frac{t+1}{2} = i < j \leq t$, and $\frac{t+1}{2} < i < j \leq t$.

Since they can be obtained by a routine calculation, we omit the details here.

∎

We now are ready to find $\pi(T)$. Recall that if f is a permutation of $V(G)$ such that $f(u) = u$ for some vertex $u \in V(G)$, then $\delta_f(u)$ is even.

Lemma 4.2.6. *Let f be a permutation which is not an automorphism of T with $f(u) = u$ and $\delta_f(u) = 0$ or 2 for some $u \in V(T)$. Then, $\delta_f(T) \geq 2n-4$.*

Proof. First, let $\delta_f(u) = 0$. If $u = x_i$ for some i, then f maps a vertex of $\{x_1, x_2, \cdots, x_{i-1}, x_{i+1}, \cdots, x_s, y_2\}$ into a vertex of the same set (maintaining adjacency). Since f is not an automorphism, $f(y_2) = x_j$ for some $j \in \{1, 2, \cdots, i-1, i+1, \cdots, s\}$. Moreover, $f(y_k) = y_k$ for $k = 1, 3, 4, \cdots, t$ and $f(z_{i'}) = z_{i''}$ where i', i'' are elements in $\{1, 2, \cdots, r\}$. So, $\delta_f(y_2) = 2(t-2) + 2r$ and $\delta_f(T) = 4(r + t - 2)$. By assuming that $r + t \geq \frac{n}{2} + 1$, we conclude that $\delta_f(T) \geq 2n - 4$. Similarly, if $u = z_j$ for some j, then $\delta_f(T) \geq 2n - 4$. So, we are left to consider $u = y_k$ for some $k \in \{1, 2, \cdots, t\}$. Again, since $\delta_f(y_k) = 0$, the set $S_l = \{x \in V(T) : d(y_k, x) = l\}$ maps onto S_l, $l = 1, 2, \cdots$. For convenience, we depict T by Figure 4.3, in which the vertices to the left (right) of the dot line are called left vertices (right vertices). Now, let the set of vertices $w \in V(T) \setminus \{y_k\}$ such that $f(w)$ stays on the same side be A, and the set of vertices which move to the other side be $B = V(T) \setminus (A \cup \{y_k\})$. This implies that $\delta_f(T) \geq 2|A||B| = 2|A|(n - 1 - |A|)$.

Since $|A| \neq n - 1, |A| \neq 0$ and $|A| \geq 2$ (f is not an automorphism), we have $\delta_f(T) \geq 4(n-3) \geq 2n - 4$ for $n \geq 4$. This concludes the proof of the case $\delta_f(u) = 0$.

Next, if $\delta_f(u) = 2$, then by Lemma 1.3.6, there exist two vertices v and w such that $\delta_f(u, v) = \delta_f(u, w) = 1$. Therefore, for each $x \in V(T) \setminus \{u, v, w\}$, we have $\delta_f(u, x) = 0$. This implies that $\delta_f(v, x) \geq 1$ and $\delta_f(w, x) \geq 1$. Hence, $\delta_f(T) \geq \delta_f(v) + \delta_f(w) \geq 2(n-2) = 2n - 4$. ∎

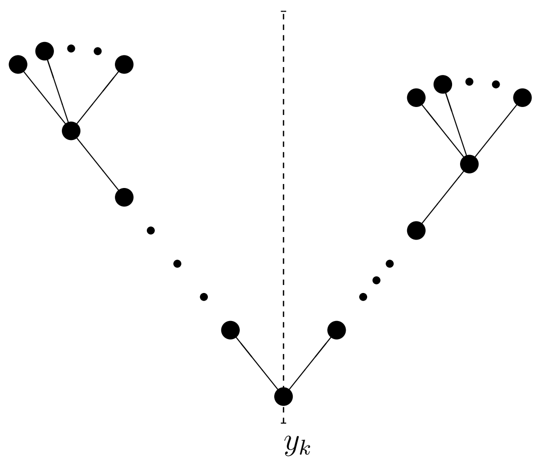


Figure 4.3: The graph with respect to y_k.

Lemma 4.2.7. *If $f(x_i) = x_i$ and $\pi(T - x_i) = 2|V(T - x_i)| - 4$ for some $i \in \{1, 2, \cdots, s\}$, then $\delta_f(T) \geq 2n - 4$.*

Proof. Since $\delta_f(T) = \delta_f(x_i) + \delta_f(T - x_i)$, $\delta_f(T) = \delta_f(x_i) + (2n - 6)$ by assumption. Now, if $\delta_f(x_i) \geq 2$, then $\delta_f(T) \geq 2n - 4$. On the other hand, if $\delta_f(x_i) = 0$, then the possible near automorphisms are the composition of an automorphism and a transposition $(y_2 x_j)$ for some $j \neq i$. This implies that $\delta_f(T) \geq 2n - 4$. ∎

Now, we prove the main result.

Theorem 4.2.8. *Let $T \in T^{(2)}$, $s \geq r$ and $r + t \geq \frac{n}{2} + 1$. Then $\pi(T) = 2n - 4$.*

Proof. When $s = 1$ (or $t = 1$), then T is a path (star) and thus $\pi(T) = 2n - 4$. So, in what follows, we assume that $s \geq 2$ and $t \geq 2$, i.e., $n \geq 6$.

For convenience, the proof is split into three cases.

Case 1. $s = r$. By definition, we have $\delta_f(T) = \frac{1}{2} \sum_{v \in V(T)} \delta_f(v)$. Therefore, if $\delta_f(v) \geq 4$ for each vertex v in T, then the assertion is true. In what follows, we find those vertices u in T such that $\delta_f(u) \leq 3$. Since $\delta_f(u) \geq P(u, f(u))$, we evaluate $P(u, f(u))$ first. Recall that $P(u, f(u)) = \|\hat{A}_u - \hat{A}_{f(u)}\|$. Therefore, by direct counting in Lemma 4.2.5, $P(u, f(u)) \leq 3$ if $(u, f(u)) \in A \cup B$, where $A = \{(x_i, x_j), (x_i, z_j), (z_i, z_j), (z_i, x_j), (y_k, y_k), (y_k, y_{t+1-k})\}$ and $B = \{(y_{\frac{t-1}{2}}, y_{\frac{t+1}{2}}), (y_{\frac{t+1}{2}}, y_{\frac{t-1}{2}}), (y_{\frac{t+1}{2}}, y_{\frac{t+3}{2}}), (y_{\frac{t+3}{2}}, y_{\frac{t+1}{2}})\}$. Note that for $(u, f(u)) \in B$, $P(u, f(u)) = 3$. If the permutation f gives a pair $(u, f(u)) \in A$, then there exists an automorphism g of T, such that $(g \circ f)(u) = u$. Since f is not an automorphism, $g \circ f$ is not an automorphism either. Furthermore, by Lemma 4.2.6, $\delta_f(T) = \delta_{g \circ f}(T) \geq 2n - 4$. Otherwise, the permutation f does not provide any pairs $(u, f(u)) \in A$ satisfying $\delta_f(u) \leq 3$ but in B we have a pair $(u, f(u))$ such that $\delta_f(u) \leq 3$. This implies that for each pair $(u, f(u)) \in A$, $\delta_f(u) \geq 4$. Since B has four pairs and $P(u, f(u)) = 3$ for each pair,

$\delta_f(T) \geq 2n-2 \geq 2n-4$. This concludes the proof of **Case 1**.

Case 2. $s = r+1$.

Assume that $f(x_i) \neq x_j$ for all j, and there is no fixed vertex u ($f(u) = u$) with $\delta_f(u) \leq 3$. For convenience, we let $\xi_f(u) = 4 - \delta_f(u)$. It suffices to show that if f is a near automorphism of T, $\sum_{u \in V(T)} \xi_f(u) \leq 8$. By the fact that $\delta_f(u) \geq P(u, f(u))$, $\xi_f(u) \leq 4 - P(u, f(u))$. Therefore, the pairs $(u, f(u))$ such that $P(u, f(u)) < 4$ are what we are concerned with. First, assume that $t \geq 4$ and $r \geq 2$. Then, the permutation (near automorphism) f gives $\delta_f(u) < 4$ for vertex pairs $(u, f(u)) \in \{ (y_{\frac{t}{2}}, y_{\frac{t}{2}+1}), (y_{\frac{t}{2}+1}, y_{\frac{t}{2}}), (y_{\frac{t-1}{2}}, y_{\frac{t+3}{2}}), (y_{\frac{t+3}{2}}, y_{\frac{t-1}{2}}), (y_{\frac{t}{2}-1}, y_{\frac{t}{2}+2}), (y_{\frac{t}{2}+2}, y_{\frac{t}{2}-1})\}$. Since a permutation f can be represented by disjoint union of cycles (Algebra), for each vertex y_i, y_i is in exactly one cycle $(y_i, f(y_i), f^2(y_i), \cdots, y_i)$. Then, by direct counting, we have $\sum \xi_f(u) \leq 8$. Hence, $\delta_f(T) \geq 2n-4$.

Consider $t \geq 4$ and $r = 1$. Then the near automorphism f gives $\delta_f(u) < 4$ for vertices $(u, f(u)) \in \{(y_{\frac{t}{2}-1}, y_{\frac{t}{2}}), (y_{\frac{t}{2}}, y_{\frac{t}{2}-1}), (y_{\frac{t-1}{2}}, y_{\frac{t+1}{2}}), (y_{\frac{t+1}{2}}, y_{\frac{t-1}{2}}), (y_{\frac{t+1}{2}}, y_{\frac{t+3}{2}}), (y_{\frac{t+3}{2}}, y_{\frac{t+1}{2}}), (y_{\frac{t}{2}+1}, y_{\frac{t}{2}+2}), (y_{\frac{t}{2}+2}, y_{\frac{t}{2}+1}), (y_{\frac{t}{2}}, y_{\frac{t}{2}+1}), (y_{\frac{t}{2}+1}, y_{\frac{t}{2}}), (y_{\frac{t-1}{2}}, y_{\frac{t+3}{2}}), (y_{\frac{t+3}{2}}, y_{\frac{t-1}{2}}), (y_{\frac{t}{2}-1}, y_{\frac{t}{2}+2}), (y_{\frac{t}{2}+2}, y_{\frac{t}{2}-1}), (y_{\frac{t}{2}-1}, y_{\frac{t}{2}+1}), (y_{\frac{t}{2}+1}, y_{\frac{t}{2}-1})\} \cup \{(x_i, y_t), (y_t, x_i)\}$. Again, since f has a cycle $(y_i, f(y_i), f^2(y_i), \cdots, y_i)$ or (x_i, y_t), but not both, we conclude that $\sum \xi_f(u) \leq 8$ by direct counting.

Finally, we have special cases left to check, namely $t = 3$ and $r \geq 2$; and $t = 3$, $s = 2$ and $r = 1$. Since they are easy to obtain, we omit the details. This concludes the proof of **Case 2**.

Case 3. $s \geq r+2$.

The proof follows by a similar argument as in **Case 1** and **Case 2.** Since the permutation (near automorphism) f gives $\delta_f(u) < 4$ for vertices $u \in V(T)$ satisfying $(u, f(u)) \in \{(y_{\frac{t-1}{2}}, y_{\frac{t+1}{2}}) : r = 1 \text{ and } s = 3\} \cup \{(y_{\frac{t}{2}}, y_{\frac{t}{2}+1}) : s = r+2\} \cup \{(y_{\frac{t}{2}-1}, y_{\frac{t}{2}+1}) :$

$s = r + 3\}$, the conclusion can be obtained easily by direct counting. Hence, $\delta_f(T) \geq 2n - 4$ and we have the proof of the theorem. ∎

To conclude this chapter, we would like to mention one more result which can be obtained from the main theorem.

Corollary 4.2.9. *Let T be a caterpillar of order n. Then $\pi(T) = 2n - 4$ if and only if $T \in T^{(2)}$, $s \geq r$ and $r + t \geq \frac{n}{2} + 1$.*

Chapter 5

Chaotic Mappings

As mentioned earlier in the introduction, motivated by the study of total disorderedness via permutations, we investigate the maximum value of the total relative displacements of graphs. This chapter is devoted to introducing several known results and presenting recent progress in finding $\pi^*(P_n)$.

5.1 Basic Notions

Recall that the maximum value of the total relative displacements of permutations in a graph G is denoted by $\pi^*(G)$ and called the chaotic number of G. In [9], the problem of finding $\pi^*(K_{n_1,n_2,\cdots,n_t})$ was transformed into a quadratic integer programming problem (QIP), and a characterization of the optimal solution was given. Furthermore, they gave a polynomial time algorithm to solve the problem. For completeness, we describe their work here. Mainly, we should minimize $\sum a_{ij}^2$ of $A = (a_{ij})$.

Let $A = (a_{ij})$ be a $t \times t$ non-negative matrix. We call

$$C = (a_{i_1j_1}, a_{i_1j_2}, a_{i_2j_2}, a_{i_2j_3}, a_{i_3j_3}, \cdots, a_{i_sj_s}, a_{i_sj_1})$$

a cycle of length $2s$, $s \geq 2$, in A. A cycle C of length $2s$ is said to be overweight if either $a_{i_kj_k} \geq 1$ for $1 \leq k \leq s$ and

$$a_{i_1j_1} - a_{i_1j_2} + a_{i_2j_2} - a_{i_2j_3} + a_{i_3j_3} - \cdots + a_{i_sj_s} - a_{i_sj_1} > s,$$

or $a_{i_k j_{k+1}} \geq 1$ for $1 \leq k \leq s$, where $j_{s+1} = j_1$ and

$$-a_{i_1j_1} + a_{i_1j_2} - a_{i_2j_2} + a_{i_2j_3} - a_{i_3j_3} + \cdots - a_{i_sj_s} + a_{i_sj_1} > s.$$

Below, we show a matrix with an overweight cycle of length 4:

$$A = \begin{bmatrix} 3 & \rightarrow & 1 & 1 \\ \uparrow & & \downarrow & \\ 1 & \leftarrow & 2 & 1 \\ & & & \\ 1 & & 1 & 0 \end{bmatrix}.$$

It is not difficult to see that, since $A = (a_{ij})$ has an overweight cycle, $\sum a_{ij}^2 = 19$ is not of minimum value under the constraints that the row sums and column sums are fixed. The next matrix $A' = (a'_{ij})$ reaches a smaller value $\sum a_{ij}'^2 = 17$,

$$A' = \begin{bmatrix} 2 & 2 & 1 \\ 2 & 1 & 1 \\ 1 & 1 & 0 \end{bmatrix}.$$

Theorem 5.1.1. *$A = (a_{ij})$ is an optimal solution of the problem* (QIP) *,i.e. $\sum a_{ij}^2$ is minimum, if and only if no overweight cycle exists in A.*

Proof. Necessity. Suppose that A has an overweight cycle $C = (a_{i_1j_1}, a_{i_1j_2}, \cdots, a_{i_sj_s}, a_{i_sj_1})$. Without loss of generality, assume that $a_{i_kj_k} \geq 1$ for $1 \leq k \leq s$ and

$$a_{i_1j_1} - a_{i_1j_2} + a_{i_2j_2} - a_{i_2j_3} + a_{i_3j_3} - \cdots + a_{i_sj_s} - a_{i_sj_1} > s.$$

Define $A' = (a'_{ij})$, where

$$a'_{ij} = \begin{cases} a_{ij} - 1, & \text{if } (i,j) = (i_k, j_k) \text{ for some } 1 \leq k \leq s, \\ a_{ij} + 1, & \text{if } (i,j) = (i_k, j_{k+1}) \text{ for some } 1 \leq k \leq s, \\ a_{ij}, & \textit{otherwise}. \end{cases}$$

Now,

$$\begin{aligned}\sum a_{ij}^2 - \sum a_{ij}'^2 &= a_{i_1j_1}^2 + a_{i_1j_2}^2 + \cdots + a_{i_sj_1}^2 - a_{i_1j_1}'^2 - a_{i_1j_2}'^2 - \cdots - a_{i_sj_1}'^2 \\ &= 2(a_{i_1j_1} + a_{i_2j_2} + \cdots + a_{i_sj_s}) \\ &\quad -2(a_{i_1j_2} + a_{i_2j_3} + \cdots + a_{i_sj_1}) - 2s \\ &> 0.\end{aligned}$$

Therefore, $\sum a_{ij}^2$ is not the minimum. Note that the row sums and column sums of A and A' are equal, respectively. Hence, we have the proof for necessity.

Sufficiency. For contradiction, assume that all cycles of A are not overweight and $\sum a_{ij}^2$ is not the minimum. Let $A^* = (a_{ij}^*)$ denote an optimal solution.

Let

$$\triangle_{ij} = a_{ij} - a_{ij}^*, \quad 1 \leq i, j \leq t.$$

Define a directed bipartite multigraph G with bipartition (X, Y), where

$$X = \{x_1, x_2, \cdots, x_t\}, \quad Y = \{y_1, y_2, \cdots, y_t\},$$

x_i joins to y_i with $\triangle_{ij}$ edges if $\triangle_{ij} > 0$, and x_i joins from y_j with $\triangle_{ij}$ edges if $\triangle_{ij} < 0$. Since

$$\sum_{j=1}^{t} \triangle_{ij} = 0, \quad \text{for } 1 \leq i \leq t,$$

and

$$\sum_{i=1}^{t} \triangle_{ij} = 0, \quad \text{for } 1 \leq j \leq t,$$

the outdegree and indegree of each vertex in G are equal. Thus, each component of G has a directed Eulerian circuit, and hence G can be decomposed into directed cycles $C_1, C_2, \cdots, C_m$. For each cycle C_l, define

$$w(C_l) = \sum_{(x_i,y_j)\in C_l} a_{ij} - \sum_{(y_j,x_i)\in C_l} a_{ij}.$$

Note that,

$$\triangle_{ij} > 0, \text{ for } (x_i, y_j) \in C_l,$$

and that $\triangle_{ij} > 0$ implies $a_{ij} \geq 1$, since $a^*_{ij} \geq 0$. Thus,

$$a_{ij} \geq 1, \text{ for } (x_i, y_j) \in C_l.$$

This means that, if $w(C_l) > |E(C_l)|/2$, where $|E(C_l)|$ is the number of edges in cycle C_l, then C_l introduces an overweight cycle in A. Since A has no overweight cycle, we have

$$w(C_l) \leq |E(C_l)|/2, \text{ for } 1 \leq l \leq m.$$

Therefore,

$$\begin{aligned}
\sum_{1\leq i,j\leq t} a_{ij}^2 - \sum_{1\leq i,j\leq t} a_{ij}^{*2} &= \sum_{1\leq i,j\leq t} a_{ij}^2 - \sum_{1\leq i,j\leq t} (a_{ij} - \triangle_{ij})^2 \\
&= 2\sum_{1\leq i,j\leq t} a_{ij}\triangle_{ij} - \sum_{1\leq i,j\leq t} \triangle_{ij}^2 \\
&= 2\sum_{l=1}^{m} w(C_l) - \sum_{1\leq i,j\leq t} \triangle_{ij}^2 \\
&\leq 2\sum_{l=1}^{m} |E(C_l)|/2 - \sum_{1\leq i,j\leq t} \triangle_{ij}^2 \\
&= |E(G)| - \sum_{1\leq i,j\leq t} \triangle_{ij}^2 \\
&= \sum_{i,j} |\triangle_{ij}| - \sum_{1\leq i,j\leq t} \triangle_{ij}^2 \\
&\leq 0,
\end{aligned}$$

where $|E(G)|$ denotes the number of edges in G. This contradicts the fact that $A^* = (a^*_{ij})$ is an optimal solution, while $A = (a_{ij})$ is not. ∎

The following algorithm is the algorithm to compute $\pi^*(K_{n_1,n_2,\cdots,n_t})$.

Algorithm Start from an initial matrix (a_{ij}),

$$a_{ij} = \begin{cases} n_i, & \text{if } i = j, \\ 0, & \text{if } i \neq j \end{cases}$$

Carry out the following steps in each iteration.

Step 1. Check whether the matrix (a_{ij}) has an overweight cycle. If not, then stop; we obtain

$$\pi^*(K_{n_1,n_2,\cdots,n_t}) = \sum_{i=1}^{t} n_i^2 - \sum_{1\leq i,j\leq t} a_{ij}^2.$$

Step 2. Suppose that $(a_{i_1j_1}, a_{i_1j_2}, a_{i_2j_2}, \cdots, a_{i_sj_s}, a_{i_sj_1})$ is an overweight cycle, with $a_{i_kj_k} \geq 1$ for $1 \leq k \leq s$ and $a_{i_1j_1} - a_{i_1j_2} + a_{i_2j_2} - a_{i_2j_3} + a_{i_3j_3} - \cdots + a_{i_sj_s} - a_{i_sj_1} > s$. Then, set

$$\begin{aligned} a_{i_1j_1} &\leftarrow a_{i_1j_1} - 1, \\ a_{i_1j_2} &\leftarrow a_{i_1j_2} + 1, \\ a_{i_2j_2} &\leftarrow a_{i_2j_2} - 1, \\ &\vdots \\ a_{i_sj_s} &\leftarrow a_{i_sj_s} - 1, \\ a_{i_sj_1} &\leftarrow a_{i_sj_1} + 1. \end{aligned}$$

Go to the next iteration.

Later, in order to find a better upper bound of $\pi^*(G)$, Chiang and Tzeng [8] studied total self-variations of sequences as follows.

Let $X = (x_1, x_2, \cdots, x_k)$ be a sequence, and $Y = (y_1, y_2, \cdots, y_k)$ be a sequence obtained by permuting all the terms of X. The total self-variation of sequence X with respect to Y is

$$\zeta_Y(X) = \sum_{i=1}^{k} |x_i - y_i|.$$

Define $\eta^*(X) = \max\{\zeta_Y(X) : Y$ is a sequence that permutes all the terms of $X\}$. Chiang and Tzeng proved the following property.

Theorem 5.1.2. [8] *Let $X = (x_1, x_2, \cdots, x_k)$ be a non-decreasing sequence. If $Y = (x_k, x_{k-1}, \cdots, x_1)$, then $\eta^*(X) = \zeta_Y(X)$.*

The following lemma is an easy consequence of the definitions of $\pi^*(G)$ and $\eta^*(X)$. The result is very useful in finding the upper bound of $\pi^*(G)$.

Lemma 5.1.3. [8] *Let $G = (V, E)$ be a graph of order n and X be a sequence consisting of all the distances of the $\binom{n}{2}$ unordered pairs of distinct vertices of G. Then $\delta_f(G) \leq \pi^*(G) \leq \eta^*(X)$ for any permutation f of V.*

In [6], they studied the total relative displacement of permutations in a path and a cycle, they got the upper and lower bound for $\pi^*(P_n)$ and $\pi^*(C_n)$. We list their results in what follows.

Theorem 5.1.4. [6] *Let $t = \lfloor \frac{\sqrt{2n(n-1)+1}-1}{2} \rfloor$. Then*

$$\pi^*(P_n) \leq \tfrac{2}{3}t(t+1)(t+2) = \tfrac{1}{3}n(n-1)(2n-4-3t).$$

Corollary 5.1.5. [6] $\pi^*(P_n) \leq \frac{4}{3}(n+1)^3$.

Let f be the permutation of $V(P_n)$ defined by

$$f(i) = \begin{cases} \frac{n}{2} - i + 1 & \text{, if } 1 \leq i \leq \frac{n}{2}; \\ \\ \frac{3n}{2} - i + 1 & \text{, if } \frac{n}{2} + 1 \leq i \leq n; \text{ or} \end{cases}$$

$$f(i) = \begin{cases} \frac{n-2i+1}{2} & \text{, if } 1 \leq i \leq \frac{n-1}{2}; \\ \\ \frac{n+1}{2} & \text{, if } i = \frac{n+1}{2}; \\ \\ \frac{3(n+1)}{2} - i & \text{, if } \frac{n+1}{2} + 1 \leq i \leq n, \end{cases}$$

for whether n is even or odd, respectively. Then the lower bound follows.

Theorem 5.1.6. [6] *Suppose that n is even. Then $\pi^*(P_n) \geq \frac{n^3}{12} - \frac{n}{3}$.*

Theorem 5.1.7. [6] *Suppose that n is odd. Then*

$$\pi^*(P_n) \geq \begin{cases} \frac{(n-1)^3}{12} + \frac{(n-1)^2}{4} - \frac{n-1}{3}, & \text{if } \frac{n-1}{2} \text{ is even;} \\ \\ \frac{(n-1)^3}{12} + \frac{(n+1)(n-3)}{4} - \frac{n-1}{3}, & \text{if } \frac{n-1}{2} \text{ is odd.} \end{cases}$$

Theorem 5.1.8. [6]

$$\pi^*(C_n) \leq \begin{cases} \frac{1}{8}n^3 - \frac{1}{4}n^2 + \frac{1}{8}n & , \text{if } n \equiv 1 \pmod 4; \\ \\ \frac{1}{8}n^3 - \frac{1}{4}n^2 - \frac{3}{8}n & , \text{if } n \equiv 3 \pmod 4; \\ \\ \frac{1}{8}n^3 - \frac{1}{4}n^2 & , \text{if } n \text{ is even.} \end{cases}$$

Let f be the permutation of $V(C_n)$ defined by

$$f(i) = \begin{cases} 2i-1 & , \text{if } 1 \leq i \leq \frac{n}{2}; \\ \\ 2i-n & , \text{if } \frac{n}{2}+1 \leq i \leq n; \end{cases} \text{ or}$$

$$f(i) = \begin{cases} \frac{i+1}{2} & , \text{if } i \text{ is odd ;} \\ \\ \frac{i+n+1}{2} & , \text{if } i \text{ is even,} \end{cases}$$

where n is even or odd, respectively. Then the lower bound follows.

Theorem 5.1.9. [6] *Let C_n be an even cycle. Then $\pi^*(C_n) \geq \frac{n^3}{12} - \frac{n}{3}$.*

Theorem 5.1.10. [6] *Let C_n be an odd cycle. Then $\pi^*(C_n) \geq \frac{n^3}{12} - \frac{n}{3}$ for $n \equiv 1$ or $5 \pmod 6$; and $\pi^*(C_n) \geq \frac{n^3}{12} - \frac{3n}{4}$ for $n \equiv 3 \pmod 6$.*

In order to see how close these bounds are, we present a couple of tables (Table 5.1 and 5.2) for P_n and C_n, respectively where n is not too large.

n	2	3	4	5	6	7	8
Thm. 5.1.4	0	2	8	16	30	52	80
$\pi^*(P_n)$	0	2	8	16	28	44	68
Thm. 5.1.6 and Thm. 5.1.7	0	0	4	8	16	24	40

n	9	10	11	12	13	14
Thm. 5.1.4	116	164	224	292	376	478
$\pi^*(P_n)$	96	134	180	234	298	374
Thm. 5.1.6 and Thm. 5.1.7	56	80	104	140	176	224

Table 5.1: $\pi^*(P_n)$ and its upper and lower bounds

n	4	5	6	7	8	9	10
Thm. 5.1.8	4	10	18	28	48	72	100
$\pi^*(C_n)$	4	10	16	28	40	58	80
Thm. 5.1.9 and Thm. 5.1.10	4	10	16	28	40	54	80

n	11	12	13	14	15	16	17
Thm. 5.1.8	132	180	234	294	360	448	544
$\pi^*(C_n)$	110	140	182	224	278	336	408
Thm. 5.1.9 and Thm. 5.1.10	110	140	182	224	270	336	408

Table 5.2: $\pi^*(C_n)$ and its upper and lower bounds

Note that $\pi^*(P_n)$ and $\pi^*(C_n)$ in the tables are obtained by computer , and they are the correct values.

5.2 Improved Bounds

In this section, we mainly improve the upper bound for $\pi^*(P_n)$. First, we consider two examples:

n = 9										
	v	1	2	3	4	5	6	7	8	9
	$f(v)$	9	7	5	3	1	8	6	4	2

n = 10											
	v	1	2	3	4	5	6	7	8	9	10
	$f(v)$	9	7	5	3	1	10	8	6	4	2

In the following we list all the displacements of $\binom{n}{2}$ order pairs of P_9 and P_{10}, respectively.

By direct counting, we have that $\pi^*(P_9) \geq 84$ and $\pi^*(P_{10}) \geq 128$, respectively, from Tables 5.3 and 5.4.

$\delta_f(1,2)=1$	$\delta_f(2,3)=1$	$\delta_f(3,4)=1$	$\delta_f(4,5)=1$	$\delta_f(5,6)=6$
$\delta_f(1,3)=2$	$\delta_f(2,4)=2$	$\delta_f(3,5)=2$	$\delta_f(4,6)=3$	$\delta_f(5,7)=3$
$\delta_f(1,4)=3$	$\delta_f(2,5)=3$	$\delta_f(3,6)=0$	$\delta_f(4,7)=0$	$\delta_f(5,8)=0$
$\delta_f(1,5)=4$	$\delta_f(2,6)=3$	$\delta_f(3,7)=3$	$\delta_f(4,8)=3$	$\delta_f(5,9)=3$
$\delta_f(1,6)=4$	$\delta_f(2,7)=4$	$\delta_f(3,8)=4$	$\delta_f(4,9)=4$	
$\delta_f(1,7)=3$	$\delta_f(2,8)=3$	$\delta_f(3,9)=3$		
$\delta_f(1,8)=2$	$\delta_f(2,9)=2$			
$\delta_f(1,9)=1$				
$\delta_f(6,7)=1$	$\delta_f(7,8)=1$	$\delta_f(8,9)=1$		
$\delta_f(6,8)=2$	$\delta_f(7,9)=2$			
$\delta_f(6,9)=3$				

Table 5.3: $\delta_f(i,j)$ in P_9

$\delta_f(1,2)=1$	$\delta_f(2,3)=1$	$\delta_f(3,4)=1$	$\delta_f(4,5)=1$	$\delta_f(5,6)=8$
$\delta_f(1,3)=2$	$\delta_f(2,4)=2$	$\delta_f(3,5)=2$	$\delta_f(4,6)=5$	$\delta_f(5,7)=5$
$\delta_f(1,4)=3$	$\delta_f(2,5)=3$	$\delta_f(3,6)=2$	$\delta_f(4,7)=2$	$\delta_f(5,8)=2$
$\delta_f(1,5)=4$	$\delta_f(2,6)=1$	$\delta_f(3,7)=1$	$\delta_f(4,8)=1$	$\delta_f(5,9)=3$
$\delta_f(1,6)=4$	$\delta_f(2,7)=4$	$\delta_f(3,8)=4$	$\delta_f(4,9)=4$	$\delta_f(5,10)=4$
$\delta_f(1,7)=5$	$\delta_f(2,8)=5$	$\delta_f(3,9)=5$	$\delta_f(4,10)=5$	
$\delta_f(1,8)=4$	$\delta_f(2,9)=4$	$\delta_f(3,10)=4$		
$\delta_f(1,9)=3$	$\delta_f(2,10)=3$			
$\delta_f(1,10)=2$				
$\delta_f(6,7)=1$	$\delta_f(7,8)=1$	$\delta_f(8,9)=1$	$\delta_f(9,10)=1$	
$\delta_f(6,8)=2$	$\delta_f(7,9)=2$	$\delta_f(8,10)=2$		
$\delta_f(6,9)=3$	$\delta_f(7,10)=3$			
$\delta_f(6,10)=4$				

Table 5.4: $\delta_f(i,j)$ in P_{10}

Now, compare these two values to the values obtained earlier by [6] $\pi^*(P_9) \geq 56$ and $\pi^*(P_{10}) \geq 80$, respectively, and the ones we found are indeed larger. In what follows, we obtain larger lower bounds for $\pi^*(P_n)$.

Theorem 5.2.1. $\pi^*(P_n) \geq \begin{cases} \frac{13}{108}n^3 + \frac{1}{9}n^2 - \frac{1}{3}n, & n \equiv 0 \pmod 6; \\ \frac{13}{108}n^3 - \frac{7}{36}n + \frac{2}{27}, & n \equiv 1 \pmod 6; \\ \frac{13}{108}n^3 + \frac{1}{9}n^2 - \frac{5}{9}n - \frac{8}{27}, & n \equiv 2 \pmod 6; \\ \frac{13}{108}n^3 - \frac{5}{12}n, & n \equiv 3 \pmod 6; \\ \frac{13}{108}n^3 + \frac{1}{9}n^2 - \frac{1}{3}n - \frac{4}{27}, & n \equiv 4 \pmod 6; \ \textit{and} \\ \frac{13}{108}n^3 - \frac{7}{36}n - \frac{2}{27}, & n \equiv 5 \pmod 6. \end{cases}$

Proof. The results are obtained by six congruent classes and the following permutations defined for odd n and even n, respectively. For odd n, let

$$f(i) = \begin{cases} n+2-2i & , \text{if } 1 \leq i \leq \frac{n+1}{2}; \\ 2(n+1-i) & , \text{if } \frac{n+3}{2} \leq i \leq n. \end{cases}$$

We partition the set of all relative displacements into 4 parts, see Table 5.3 for reference. The first part (left-upper corner) is equal to

$$\sum_{i=1}^{\frac{n-1}{2}} \{1+2+3+\cdots+i\} = \frac{1}{48}(n-1)(n+1)(n+3).$$

The other part can be obtained by direct calculation and they are equal to

$$\begin{cases} \frac{1}{16}n^3 - \frac{11}{432}n^2 - \frac{11}{432}n - \frac{5}{432}, & n \equiv 1 \pmod 6; \\ \frac{43}{432}n^3 - \frac{1}{16}n^2 - \frac{19}{48}n + \frac{1}{16}, & n \equiv 3 \pmod 6; \\ \frac{43}{432}n^3 - \frac{1}{16}n^2 - \frac{25}{144}n - \frac{5}{432}, & n \equiv 5 \pmod 6, \text{ respectively.} \end{cases}$$

Similarly, we define $f(i) = \begin{cases} n+1-2i & , \text{if } 1 \leq i \leq \frac{n}{2}; \\ 2(n+1-i) & , \text{if } \frac{n}{2}+1 \leq i \leq n, \end{cases}$ when n is even, then the proof follows by the same technique as in the case "n is odd". ∎

In the following, we compare the results of Theorem 5.2.1 and the results of Theorem 5.1.6 and Theorem 5.1.7. Clearly, this result is a better lower bound. The differences of these bounds are listed in the following, but we still can't accomplish the goal of finding $\pi^*(P_n)$.

$$\begin{cases} \frac{1}{27}n^3+\frac{1}{9}n^2, & n\equiv 0 \pmod 6; \\ \frac{1}{27}n^3-\frac{11}{18}n-\frac{23}{54}, & n\equiv 1 \pmod{12}; \\ \frac{1}{27}n^3-\frac{1}{9}n^2-\frac{2}{9}n-\frac{8}{27}, & n\equiv 2 \pmod 6; \\ \frac{1}{27}n^3+\frac{1}{6}n+\frac{1}{2}, & n\equiv 3 \pmod{12}; \\ \frac{1}{27}n^3+\frac{1}{9}n^2-\frac{4}{27}, & n\equiv 4 \pmod 6; \\ \frac{1}{27}n^3-\frac{11}{18}n-\frac{31}{54}, & n\equiv 5 \pmod{12}; \\ \frac{1}{27}n^3+\frac{7}{18}n+\frac{31}{54}, & n\equiv 7 \pmod{12}; \\ \frac{1}{27}n^3-\frac{5}{6}n-\frac{1}{2}, & n\equiv 9 \pmod{12}; \\ \frac{1}{27}n^3+\frac{7}{18}n-\frac{23}{54}, & n\equiv 11 \pmod{12}; \end{cases}$$

From the partial results obtained in this chapter, it is not difficult to see that finding the chaotic number of a graph seems to be a much harder task. We believe that no polynomial time algorithms can be found for finding $\pi^*(G)$ where G is an arbitrarily given graph. However, we are not able to prove this at the moment.

Chapter 6

Conclusion

From the results we obtained in Chapter 4, we have seen a chance of finding the trees T of order n where $\pi(T) = 2n-4$. To prove that for each $T \in T^{(3)}$, $\pi(T) = 2n-4$ deserves to be considered in our further research, even it can be foreseen that more details are involved in estimating $\delta_f(v)$ for each $v \in V(T)$. Fortunately, we do now have a tool to find its lower bound by using the sorting values. This idea should work for other graphs too.

On the other hand, the study of chaotic mappings has a long way to go. As can be seen in Chapter 5, to determine $\pi^*(P_n)$ or $\pi^*(C_n)$ is still very far from being settled. Between the results obtained so far and expected values, there are gaps. A smarter idea is in need, and hopefully we can also find these two values in the near future.

To conclude this thesis, we would like to mention one more result which we have worked on. Let Q_k denote the k-dimensional hypercube. It is well-known that $Q_2 \cong K_{2,2}$ and $Q_k = Q_{k-1} \times K_2$ for $k \geq 3$. Since Q_k is vertex-transitive, there exists a permutation f such that $\pi(Q_k)$ can be achieved by f in which $\delta_f(v)$ is even for each $v \in V(Q_k)$. In fact, $\delta_f(v) \equiv 0 \pmod 4$ by Lemma 1.3.4. Thus, $\pi(Q_k) \equiv 0 \pmod 4$. This is what we can do so far, by the fact that $\pi(Q_3) = 8$, we believe that $\pi(Q_k) = 2 \cdot 2^k - 8 = 2^{k+1} - 8$ is true.

Bibliography

[1] W. Aitken, Total relative displacement of permutations, *J. Combin. Theory, Series A* 87 (1999), 1-21.

[2] C. F. Chang and H. L. Fu, Near automorphisms of trees with small total relative displacements, J. Combin. Optimization, 14 (2007), No. 2-3, 191-195.

[3] C. F. Chang, B. L. Chen and H. L. Fu, Near automorphisms of cycles, *Discrete Math.*, to appear.

[4] C. C. Chao, and W. Q. Liang, Arranging n Distinct Numbers on a Line or a Circle to Reach Extreme Total Variations, *European Journal of Combinatorics* 13 (1992), 325-334.

[5] G. Chartrand, H. Gavlas and D. W. VanderJagt, Near-automorphisms of graphs, Graph Theory, Combinatorics and Applications, Vol I, (Proceedings of the 1996 Eighth Quadrennial International Conference on Graph Theory, Combinatorics, Algorithms and Applications), Y. Alavi, D. Lick and A. J. Schwenk (Editors), New Issues Press, Kalamazoo, 1999, 181-192.

[6] K. C. Cheng, N. P. Chiang, H. L. Fu and C. K. Tzeng, A study of total relative displacement of permutations in paths and cycles, Utilitas Mathematica, to appear.

[7] N. P. Chiang, Chaotic numbers of complete bipartite graphs and tripartite graphs, *J. of Optimization Theory Appl.*, 131 (2006), No. 3, 485-491.

[8] N. P. Chiang and C. K. Tzeng, An upper bound for the total relative displacement, submitted.

[9] H. L. Fu, C. L. Shiue, X. Cheng, D. Z. Du, and J. M. Kim, Quadratic integer programming with application in chaotic mappings of complete multipartite graphs, *J. of Optimization Theory Appl.*, 110 (2001), No. 3, 545-556.

[10] F. K. Hwang, Extremal Permutations with Respect to Weak Majorizations, *European Journal of Combinatorics*, 17 (1996), 637-645.

[11] C. Leveopoulos, and O. Petersson, Heapsort-Adapted for Presorted Files, Proceedings of a 1989 Workshop on Algorithms and Data Structures, Lecture Notes in Computer Science, Springer Verlag, Berlin, Germany, 382 (1989), 499-509.

[12] K. B. Reid, Total relative displacement of vertex permutations of $K_{n_1,n_2,\ldots,n_t}$, *J. Graph Theory*, 41 (2002), 85-100.

[13] D. B. West, Introduction to Graph Theory, 2nd Edition, Prentice-Hall, Inc., 2001.