Extremal Graphs with Respect to Degree Distance Index

Since 1864

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DECLARATION

I, **Miss Salma Kanwal** Registration No. **29-GCU-PHD-SMS-07** student at **Abdus Salam School of Mathematical Sciences GC University, Lahore** in the subject of **Mathematics**, **Year of Admission (2007)**, hereby declare that the matter printed in this thesis titled

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RESEARCH COMPLETION CERTIFICATE

It is certified that the research work contained in this thesis titled

“Extremal Graphs with Respect to Degree Distance Index”

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To My Family…

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SYMBOL INDEX

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$BS(p,q); p+q = n-2$, Bistar, 14

$\beta_1(G)$, edge independence number, 12

$c(G)$, circumference of G, 11

$C_{n,d}$, 15

C_k, cycle with k vertices, 15

$d(x)$, degree of vertex x, 4

$d(x,y)$, distance between vertices x and y, 10

$diam(G)$, diameter of graph G, 10

$D(x)$, sum of distances of all other vertices from x, 18

$D(G)$, sum of all distances of graph G, 18

$D'(x)$, degree distance of vertex x, 18

$D'(G)$, degree distance of graph G, 18

${}^rD'(G)$, reverse degree distance of graph G, 18

$E(G)$, edge set of graph G, 4

$|E(G)|$, number of edges in G, or size of G, 4

$e = xy$, edge e joining x and y, 4

$ecc(x)$, eccentricity of vertex x, 10

$G - v$, deletion of vertex v from G, 7

$G - e$, deletion of edge e from G, 7

$g(G)$, girth of G, 11

$H_{n,k}$, 15

$H(G)$, harmonic index of G, 19

$H(n,k;n_1,n_2,\ldots,n_k)$, 15

$K_{1,n-1}$, star graph, 14

K_n, complete graph on n vertices, 15

$K_{a,b}$, complete bipartite graph, 15

$K_{1,n-1}+e$, addition of an edge to star graph, 21

$MTI(G)$, molecular topological index, 18

$MS(n_1, n_2, \ldots, n_{d-1})$, multistar, 55

$m_G(uv)$, multiplicity of edge uv in multigraph G, 61

$M_{k,m}(K_{1,n-1})$, set of multigraphs, 63

$N(x)$ or $V(x)$, neighborhood of vertex x, 4

$N_G(x)$, open neighborhood of x in G, 5

$N_G[x]$, closed neighborhood of x in G, 5

$P(G)$, periphery of G, 10

P_d, path of length $d-1$, 10

$R(G)$, Randić index, 19

$R_\alpha(G)$, general product-connectivity index of G, 19

$R_{-1/2}(G)$, classical Randić connectivity index of G, 19

$rad(G)$, radius of G, 10

$S_{n,p}$, 56

$V(G)$, vertex set of G, 4

$|V(G)|$, order of G, 4

$W(G)$, Wiener index of G, 18

$\delta(G)$, minimum degree in graph G, 6

$\Delta(G)$, maximum degree in G, 6

$\chi_\alpha(G)$, general sum-connectivity index of graph G, 19

$\chi_{-1/2}(G)$, sum-connectivity index of G, 19

$Z(G)$ or $C(G)$, center of G, 10

$Zg(G)$, first Zagreb index of graph G, 18

$\mu(G)$, cyclomatic number of G, 15

Abstract

In Chapter 1, some necessary definitions and results from graph theory are given along with a description on the progress towards the relationship of graph theory with other sciences like chemistry. Involvement of graph theory in Chemistry has emerged as a separate science known as chemical graph theory.

In Chapter 2, we study the ordering of connected graphs having small degree distances. Families of graphs that are mainly considered there are trees, unicyclic graphs, bicyclic graphs and general simple connected graphs. While giving an ordering to these graphs having small degree distances results were proved dealing with the diameter in ascending order.

In Chapter 3, using the ideas presented in last chapter trees and unicyclic connected graphs were separately ordered with respect to the degree distance index (in increasing order). Same technique (as in Chapter 2) was used in proving the main results of this chapter *i.e.* dealing with the diameter of trees (resp. unicyclic graphs). A list of four trees and four extremal unicyclic graphs is given there.

In Chapter 4, lower and upper bounds on degree distance index are determined in terms of various graphical parameters like Zagreb index, order, size, diameter, radius, minimum degree, and graphs for which these bounds are attained are characterized. Chapter 5 deals with an ordering of trees having small general sum-connectivity index. In last Chapter some comments are given, in the same chapter some open problems are also proposed.

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Lahore, Pakistan Salma Kanwal

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Preface

Graph theory is an exciting branch of pure mathematics, full of elegant and innovative ideas. The deepening and broadening of the subject is evidence that graph theory has reached a point where it is treated as a basis for all the well-established disciplines of pure mathematics. Problems arising in computer science and other areas of sciences greatly influence the direction taken by graph theory. In the past few years graph theory has established itself as an important mathematical tool in a wide variety of subjects. This subject has been highly successful in certain academic fields such as the natural sciences, engineering and operational research. Many decades have passed since the appearance of those graph theory concepts that still set the basis for most of academic fields seen today. It is proved to be a rapidly maturing subject. Its involvement in chemistry has developed a separate field known as *chemical graph theory*. Topological indices based on distances between vertices of a graph are widely used in mathematical chemistry [10, 12] because of their correlations with physical, chemical and thermodynamic parameters of chemical compounds.

The parameter $D'(G)$ of a connected graph G is called the degree distance of G. $W(G)$ denotes the Wiener index (for graph G), a well−known topological index in mathematical chemistry.

The new parameter $D'(G)$, was introduced by Dobrynin and Kochetova [13] and Gutman [20] as a weighted version of the Wiener index. This parameter was intensively studied in the literature. In [43] it was shown that for $n \geq 2$ in the class of connected graphs of order n, the minimum of $D'(G)$ equals $3n^2 - 7n + 4$ and the unique extremal graph is $K_{1,n-1}$ and a conjecture raised in [13] was disproved. In [41] two more graphs having smallest degree distances were found. Author proved that the next graphs of order $n \geq 4$ having smallest degree distances are $BS(n-3, 1)$ and $K_{1,n-1}+e$, having $D'(BS(n-3, 1)) = 3n^2-3n-8$ and $D'(K_{1,n-1}+e) = 3n^2-3n-6$, where $BS(n-3, 1)$ denotes the bistar consisting of vertex disjoint stars $K_{1,n-3}$ and $K_{1,1}$ with central vertices joined by an edge. In [5] and [42] the authors reported several properties of connected graphs of fixed order and size. In [40, 44] the minimum degree distance of unicyclic and bicyclic graphs was obtained. In the case of unicyclic graphs the unique extremal graph is $K_{1,n-1}+e$. In [9] an asymptotically sharp upper bound of degree distance of graphs with given order and diameter was presented and in [26] the degree distance of partial Hamming graphs was obtained. In [24] the maximum degree distance among unicyclic graphs on n vertices was deduced and in [27] the unicyclic graphs of order n and girth k, having minimal and maximal degree distances respectively, were characterized. In chapter 2 of this thesis, the list of three graphs having smallest degree distances deduced in [41] is completed up with six new members with the condition that the number of vertices are greater than or equal to 15. Note that, degree distance index and Wiener index of trees are connected by relation $D'(G) = 4W(G) - n(n-1)$ [20], which implies that the ordering of trees on n vertices with respect to the Wiener index is the same for the degree distance parameter. There are various transformations on trees and general graphs (see [27]) that decrease degree distance and/or Wiener index. Extremal trees and unicyclic graphs with respect to degree distance index could be also determined using this method. In [8, 11] the authors proved that the caterpillar $C_{n,d}$ is the unique tree with n vertices and diameter d that minimizes Wiener index. Also the maximum degree distance among unicyclic graphs on n vertices was deduced in [7] and the extremal unicyclic connected graphs of order n and girth k, having minimal and maximal degree distances respectively, were characterized in [10]. In [27] n-vertex unicyclic graphs with girth k, having minimum and maximum degree distance were characterized and was proved that the graph B_n, obtained from two triangles linked by a path, is the unique graph having the maximum degree distance among bicyclic graphs of order n.

In [9], Dankelmann, Gutman, Mukwembi and Swart gave an asymptotically sharp upper bound $D'(G) \leq \frac{1}{4}nd(n-d)^2 + O(n^{\frac{7}{2}})$ for graphs of order n and as a corollary they obtained the bound $D'(G) \leq \frac{1}{27}n^4 + O(n^{\frac{7}{2}})$ for graphs of order n; this essentially proves a conjecture proposed by Tomescu [43]. In [27] it was proved that $H_{n,k}$

is the unique unicyclic graph G of girth $g(G) = k$ having minimum degree distance for $n \geq k$.

The list of connected graphs having smallest degree distances deduced in [37] includes nine members, three of them being trees and three of them are unicyclic.

In the third chapter of this work the list of three unicyclic connected graphs in [37] having smallest degree distances is completed up with a new member.

This thesis is divided into five chapters. Chapter 1 covers the basic concepts, notations and terminologies of graphs which are needed to have a better understanding of this work. In chapter 2 an ordering of connected graphs having small degree distances is provided as a continuation of work done in [41], we have added six new members to the list of three connected graphs having small degree distances presented in [41]. Chapter 3 provides us a list of four trees having smallest degree distance and a list of four unicyclic connected graphs having smallest degree distances. Chapter 4 deals with lower and upper bounds for degree distance index in terms of various graphical parameters. Chapter 5 gives us an ordering of trees having small general sum-connectivity index. The general sum-connectivity index, proposed by Zhou and Trinajstić [49] in 2010, is defined as

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha.$$

Several extremal properties of the sum-connectivity ($\alpha = -1/2$) and general sum-connectivity index for trees, unicyclic graphs and general graphs were given in [14, 15, 48, 49]. Thus for a tree T with $n \geq 4$ vertices, it was shown in Proposition 3 of [49] that if $\alpha > 0$, then $\chi_\alpha(T) \leq (n-1)n^\alpha$ and if $\alpha < 0$ then $\chi_\alpha(T) \geq (n-1)n^\alpha$. The unique extremal graph is the n-vertex star S_n (also denoted by $K_{1,n-1}$) in both cases. In [48] the tree minimizing $\chi_{-1/2}$ in the set of trees with $n \geq 5$ vertices and p pendant vertices was characterized, where $3 \leq p \leq n-2$. This result will be extended in section 3 of chapter 5 for index χ_α with $-1 \leq \alpha < 0$.

Chapter 1

Preliminaries

In this chapter we recall some basic notions and some preliminary results in combinatorics and graph theory that will be used in our later discussions in next chapters. Throughout this work all graphs are considered to be simple and connected.

1.1 Elements of Graph Theory

A *graph* $G = (V(G), E(G))$ consists of two sets $V(G)$ and $E(G)$. Denote $|V(G)| = n$ and $|E(G)| = m$, the elements of $V(G)$ are called *nodes* (or *vertices*), and the elements of $E(G)$ are called *edges* of graph G. Each edge has a set of one or two vertices associated to it, which are called its *endpoints*. An edge $e = xy$ is said to be *join* of its endpoints x and y, also we say e is *incident* to x and y. A vertex x joined by an edge to a vertex y is called *neighbor* of x, in this case both vertices x and y are called *adjacent vertices*. The *(open) neighborhood* of a vertex x in a graph G, denoted by $N(x)$ or sometimes by $V(x)$ is given as the set of vertices adjacent to x other than x. For a vertex $x \in V(G)$ *degree of* x, denoted by $d(x)$, is given as $d(x) = |N(x)|$, *i.e.* number of neighbors of x is the degree of x. If $d(x)$ is even (odd) for some $x \in V(G)$ then x is called an *even vertex* (*odd vertex*). x is called a *pendant or leaf vertex* if $d(x) = 1$, and is called isolated vertex if $d(x) = 0$. For a connected graph G and $x \in V(G)$, $d(x) \geq 1$. A graph G all of whose vertices have equal degrees is called *regular graph* and if $d(x) = k\,; k \geq 0$ for all $x \in V(G)$ is known as *k-regular graph*. The closed neighborhood of x is given by $N[x] = N(x) \cup \{x\}$. When G is not the only graph under consideration, these neighborhoods are denoted as $N_G(x)$ and $N_G[x]$ respectively. If $V(G)$ and $E(G)$ are finite sets then G is called *finite graph*, otherwise *infinite graph*. A graph G, for which $V(G) = \emptyset$ and $E(G) = \emptyset$ is called *null graph* and a graph consisting of one vertex and no edge is called *trivial graph*. An edge e is said to be a *proper edge* if it joins two distinct vertices otherwise it is called a *loop* or *self loop*. A *multi - edge* is a collection of two or more edges with same end points. Number of edges in that multi - edge is called *edge multiplicity*. Graph G is called *simple graph* if it does not contain self loops and multi - edges. A *general graph* may have self loops and/ or multi - edges. In Figure 1.1, a finite simple graph G is shown, where $n = 8$, $m = 8$ $e = xy$ is a proper edge and is a join of its end points x and y, so x and y are neighbors of each other. A much closer observation gives us $N(x) = \{z, y, u, w\}$ and $N[x] = \{x, z, y, u, w\}$ also $d(x) = |N(x)| = 4$. In G as $d(x) = 4$ so x is an even vertex and $d(u) = 3$ giving that u is an odd vertex whereas z, v, w, r are leaf vertices. In the same Figure 1.1 a multi - graph (*general graph*) M is also shown in which l is self loop and we have multi - edge e' between y' and u' and multiplicity of this multi - edge is 3. For a graph G, suppose we have arranged all $x_i \in V(G)$; $1 \leq i \leq n$ so that $d(x_1) \geq d(x_2) \geq \ldots \geq d(x_n)$. Then the ordered (in non - increasing order) $n-$ *tuple* $(d(x_1), d(x_2), \ldots, d(x_n))$ gives us *degree sequence* for graph G. Given an $n-$ *tuple* of non - negative integers, ordered in non - increasing order, is called *graphic* if there exists some graph having that $n-$ *tuple* as its degree sequence. Following theorem provides us a necessary and sufficient condition for a degree sequence to be graphic.

Theorem 1.1.1. *[23] Consider the following two degree sequences, assume (i) is in decreasing order.*

(i) $l,\ u_1,\ u_2, \ldots,\ u_l,\ d_1, \ldots,\ d_n$

(ii) $u_1 - 1,\ u_2 - 1, \ldots, u_{l-1},\ d_1, \ldots,\ d_n$

Then (i) is graphic if and only if (ii) is graphic.

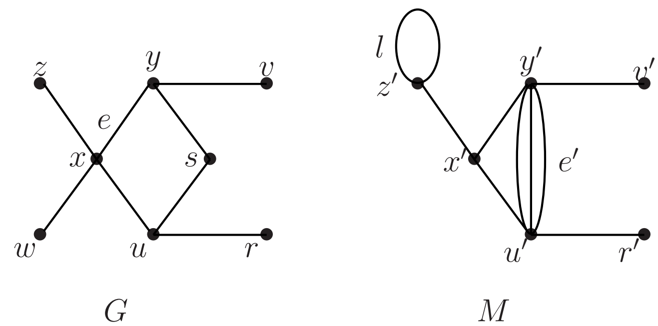


Figure 1.1: Simple graph G and multiple graph (multigraph) M

Denote by $\delta(G)$ the minimum degree in G; it is given by $\delta(G) = min_{x \in V(G)} d(x)$. We also have analogous concept of maximum degree in graph G, denoted by $\triangle(G)$, given by $\triangle(G) = max_{x \in V(G)} d(x)$. In Figure 1.1, for graph G, its degree sequence is $(4, 3, 3, 2, 1, 1, 1, 1)$ with $\delta(G) = 1$ and $\triangle(G) = 4$. Coming back to the degree $d(x)$ of vertex $x \in V(G)$, we have a significant result that is also known as *First Theorem of Graph Theory* and will be used in almost all main results of this work.

Theorem 1.1.2. *[4] For every graph G,*

$$\sum_{x \in V(G)} d(x) = 2m.$$

Corollary 1.1.3. *[4] In any graph G, the number of odd vertices is even.*

1.2 Connected and Disconnected Graphs

For two vertices x and y in G, a finite alternating sequence $x = x_0, e_1, x_1, e_2, x_2, e_3, \ldots, e_n, x_n = y$ of vertices and edges such that every edge e_i in the sequence joins vertex x_{i-1} with vertex x_i, is called a *walk* from x to y. The vertices and the edges in the walk need not be distinct. The number of edges in a walk is the length of the walk. *Trial* is a walk with no edge repeated and a $x - y$

walk with distinct vertices is called a *path* between x and y. x and y are called *extremities* of this path and the remaining vertices are called *intermediate vertices* of the path. For the sake of simplicity, in some books short expression for walks and paths is used due to the fact that an edge in simple graph is incident to two distinct vertices so we can write $x = x_0, x_1, x_2, \ldots, x_n = y$ for a $x - y$ walk by ignoring edges as it is assumed obvious that edge e_i is incident to two consecutive vertices x_{i-1} and x_i for $1 \leq i \leq n$. If $x_0 = x_n$, then this $x-y$ walk is a *closed walk*. A closed walk with no edges repeated is a *circuit*. A *cycle* is a circuit with no vertex repeated. In a simple graph G, any cycle consisting of $p\,; p \geq 3$ vertices ia called $p-$ *cycle* in G, it is an odd cycle if p is odd and an even cycle if p is even. For graph G shown in Figure 1.2 $x,\ f,\ y,\ h,\ z,\ g,\ x,\ f,\ y,\ e,\ v$ is a $x-v$ walk having length 5 but this is not $x-v$ path. $x,\ g,\ z,\ h,\ y,\ e,\ v$ is a $x-v$ path with $z,\ y$ as intermediate vertices, also in the same figure $y,\ h,\ z,\ g,\ x,\ f,\ y,\ e,\ v$ is a $y-v$ trial, also $x,\ g,\ z,\ h,\ y,\ f,\ x$ is a $3-$ cycle hence is an odd cycle. The graph G in which it is possible to move from one vertex to other will be of special interest to us. $x, y \in V(G)$ are *connected*, if G contains a $x-y$ path, in this case we say that x is connected to y. A graph in which every two vertices are connected is known as *connected graph* and *disconnected graph* otherwise. For $x, y \in V(G)$, $x-y$ geodesic is a shortest path between x and y. For $x, y \in V(G)$, denote by $d(x, y)$ the distance between x and y and this is given by the length of a $x-y$ geodesic (if exists), otherwise $d(x, y) = \infty$. It is easy to see that for $y \in N(x)$, $d(x, y) = 1$.

1.3 Subgraphs

Given a graph G, there are two natural ways of deriving smaller graphs from G [4]. If $e \in E(G)$, then we can obtain $G - e$ (a graph on $m-1$ edges) from G by deleting edge e and leaving remaining vertices and edges intact. Similarly if $v \in V(G)$ then the graph $G-v$ is derived form G by deleting vertex v together with all edges incident with v. These operations of *edge deletion* and *vertex deletion* are illustrated in Figure 1.2. A graph H for which $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$, is called *subgraph* of graph G or G is a *super graph* of H. Thus the graphs $G - e$ and $G - v$ derived from G are subgraphs of G. If H is a subgraph of G with the property that $V(H) = V(G)$, then H is called *spanning subgraph* of G and if K is a subgraph of G such that for $u, v \in V(K)$, $uv \in E(K)$ whenever u and v form an edge in G, K is known as *induced subgraph* of G. In Figure 1.2 graph G is shown along with its two subgraphs $G - e$ (denoted by H) and $G - v$ (denoted by K), so G is super graph of both graphs H and K. H is also spanning subgraph of G whereas K is not, but another subgraph S of G, also shown in the same figure, is induced subgraph of G.

If G is a disconnected graph then a *component* of G is a maximal connected subgraph of G, *i.e.* a subgraph C of G is a component of G if C itself is connected and is not contained in any other connected subgraph of G. Graph G is connected if and only if G has exactly one component (G itself). A vertex $x \in V(G)$ with the property that its deletion increases the number of components of G is called *cut vertex or cut node*, analogously when the same role is played by some edge $e \in E(G)$ then that specific edge is given the name of *cut edge or bridge* of graph G. In Figure 1.2 graph G is connected whereas graph H is not. $x - u$ geodesic is given as x, y, v, u so its length gives us that $d(x, u) = 3$ but in H, $d(x, u) = \infty$ and vertex v is cut node of G and edge e is a bridge for graph G. A nontrivial graph G that has no cut vertices and bridges is called *non separable* graph. We have a very nice characterization for non separable graphs.

Theorem 1.3.1. *[7] Let G be a graph with $n \geq 3$. Then G is non separable if and only if every two vertices of G lie on a common cycle.*

Graph S shown in Figure 1.2 is non separable graph but graph G is not. The graph G of Figure 1.2 provides us a better understanding for disconnected graph and its components. Components can be looked by means of an equivalence relation.

Theorem 1.3.2. *[7] Let R be the relation defined on the vertex set of a graph G by*

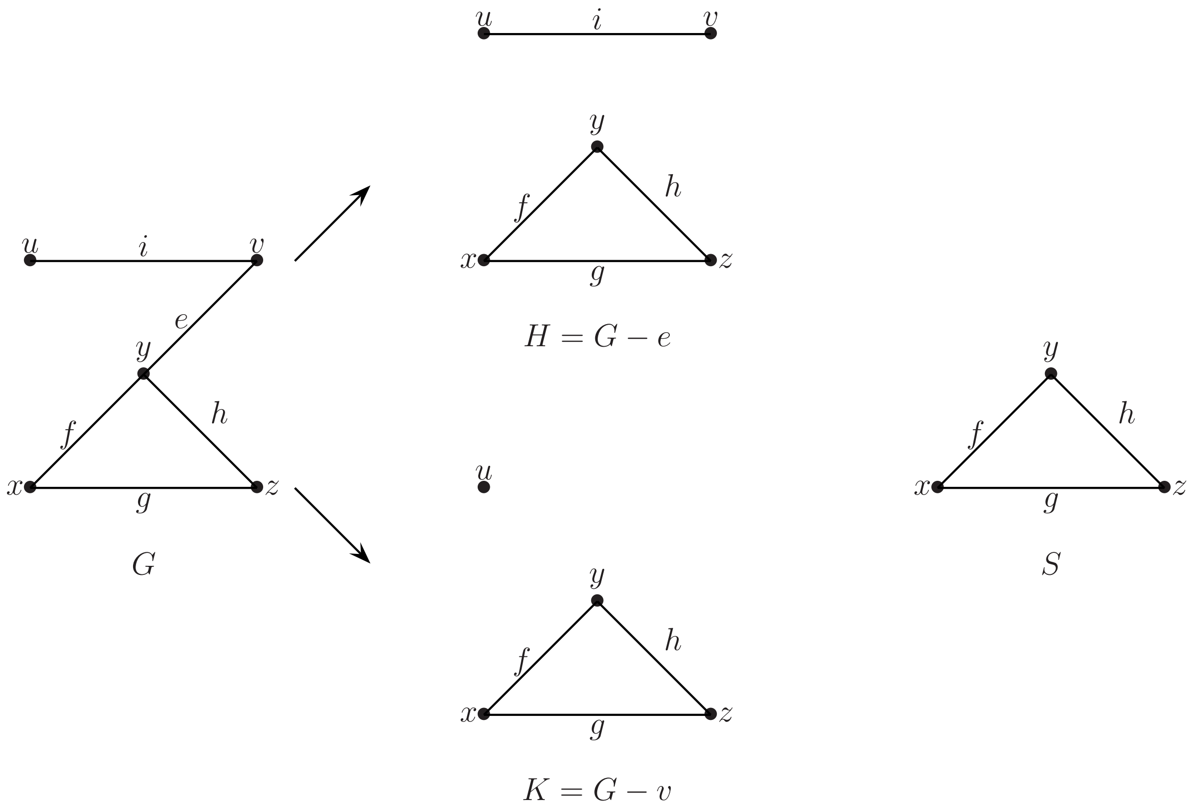


Figure 1.2: Subgraphs and super graphs

$x\,R\,y$, where $x, y \in V(G)$, if x is connected to y. Then R is an equivalence relation.

A non separable subgraph that is not properly contained in any other proper subgraph of G, is referred as *block* of G. Blocks can also be looked upon by considering the following equivalence relation on $E(G)$.

Theorem 1.3.3. *[7] Let G be a nontrivial connected graph with the relation R defined on $E(G)$ by $e\,R\,f$, where $e, f \in E(G)$, if $e = f$ or e and f lie on a common cycle of G. Then R is an equivalence relation.*

As a result of this equivalence relation, equivalence classes obtained are in fact blocks of G and as a corollary of this result we obtain nice properties of blocks.

Corollary 1.3.4. *[7] Every two distinct blocks B_1 and B_2 in a nontrivial connected graph G have the following properties:*
(i) B_1 and B_2 are edge disjoint.
(ii) B_1 and B_2 have at most one vertex in common.
(iii) If B_1 and B_2 have a vertex x in common, then x is a cut node.

In Figure 1.2 subgraph S is a block in graph G. Graph H shown in the same figure has two connected components.

1.4 Distances in Graphs

From now on, we assume that the graph G under our consideration is simple connected graph. As we have already seen that for $x, y \in V(G)$, $d(x, x) = 0$; if $x \neq y$ then $d(x, y)$, the distance between x and y, is the length of a $x - y$ geodesic in G. This distance function possesses the same properties as ordinary distance function.

Theorem 1.4.1. *[22] Let G be a connected graph. The distance function d is a* metric *on V(G).*

For any $x \in V(G)$, *eccentricity* of x denoted by $ecc(x)$, is defined as the distance of x from the vertex farthest from x, *i.e.* $ecc(x) = max_{y \in V(G)} d(x, y)$. The diameter of a graph G, denoted by $diam(G)$, is the maximum of the vertex eccentricities in G equivalently,

$$diam(G) = max_{x \in V(G)} ecc(x) = max_{x,y \in V(G)} d(x, y).$$

For graph G *radius* of G, denoted by $rad(G)$ is given by the minimum of the vertex eccentricities, *i.e.* $rad(G) = min_{x \in V(G)} ecc(x)$. A vertex x in G with the minimum eccentricity is called *central vertex* of G, and the subgraph induced by set of central vertices of G is called *center* of G and is denoted as $Z(G)\, or\, C(G)$. A graph G for which $Z(G) = G$ is called *self centered graph. Periphery* $P(G)$ of a graph is the opposite of the center. *Peripheral vertex* of graph G is a vertex with the maximum eccentricity, *i.e.* a vertex x for which $ecc(x) = diam(G)$ and just like the notion of center of graph, the set all peripheral vertices gives rise to *periphery* of G. Two vertices $x, y \in V(G)$, for which $d(x, y) = diam(G)$ are called *diametral vertices* of G and the shortest path between them is called *diametral path.* For the vertex $x \in V(G)$, y is called *eccentric vertex* for x if $d(x, y) = ecc(x)$. Now as a consequence of definitions of radius and diameter of G and triangular inequality for distance function d, we have the following result.

Theorem 1.4.2. *[22] For a connected graph G,*

$$rad(G) \leq diam(G) \leq 2rad(G)$$

Blocks in a graph G play a vital role in locating the center of the graph, as shows the following result.

Theorem 1.4.3. *[22] The center of every connected graph G lies within a single block.*

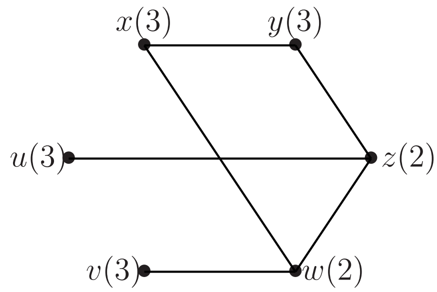
Other graph related terminologies are as follows:
A *unicyclic graph* is a connected graph G of order n and size n. It contains exactly one cycle; by contracting this cycle to a unique vertex the resulting graph is a tree. *Girth* of a graph G, denoted by $g(G)$, is the length of the shortest cycle in G (if any) also moving in the same direction *circumference* of G, denoted by $c(G)$, is the length of the longest cycle in G (if any). For a graph G containing cycles, girth and diameter are related as shown by the following theorem.

Theorem 1.4.4. *[11]A unicyclic graph G satisfies $g(G) \leq 2diam(G) + 1$.*

For connected G shown in Figure 1.3, eccentricities of all vertices are shown in parentheses along with labels of vertices, also it is easy to see that $diam(G) = 3$, $rad(G) = 2$ and w, z are central vertices of G so center of G, $Z(G)$ is subgraph induced by $\{z, w\}$. x, y, u, v are peripheral vertices of G hence forming the periphery of G induced by $\{x, y, u, v\}$. Moreover u, v are diametral vertices of G and u, z, w, v is a diametral path in G, $g(G) = 4$ and for this graph girth and circumference are the same.

1.5 Matchings

For a connected graph G, a set of edges (say) $M \subseteq E(G)$ is said to be *independent* if no two edges in this set have a vertex in common. Thus a *matching* in graph



G

Figure 1.3: Distances in graphs

G is given by this independent set of edges and a matching M in graph G with maximum cardinality is called *maximum matching* and cardinality of this maximum matching is a well known graphic parameter known as *edge independence number* of graph G, and is denoted by $\beta_1(G) = |M|$. This parameter $\beta_1(G)$ provides an association between matchings (maximum matchings) and independence of edges. Another notion relating these two ideas is that of *perfect matching.* Matching M, that covers all nodes of a graph G is referred as perfect matching, *i.e.* a perfect matching of a graph G is a subset M of the edge set of G such that

(a) every two edges of M have no common end;

(b) every vertex of G is incident to an edge of M.

Note that if G has a perfect matching then its order is even. We have several results giving us information about matchings for several well - known graph families like trees, complete graphs *etc.* Following result provides us information about perfect matchings in trees.

Theorem 1.5.1. *[6] A tree has at most one perfect matching.*

For a graph G of order n,

$$|\beta_1(G)| \leq \lfloor \frac{n}{2} \rfloor$$

$i.e$, if G is a graph of odd order (say) $2m + 1$; $m \geq 1$, then no matching contains more than m edges; whereas if G has even order (say) $2t$; $t \geq 1$, then no matching

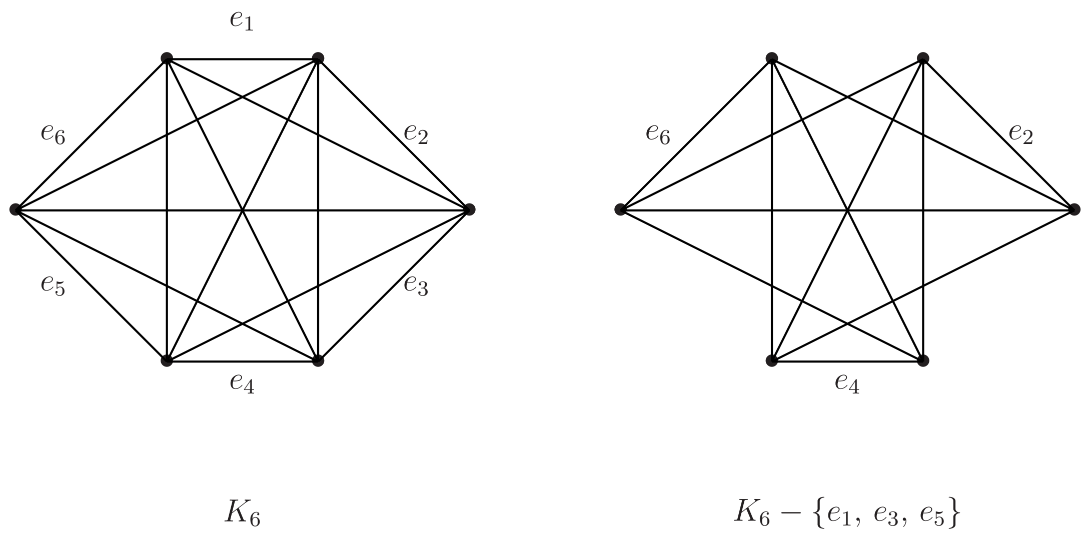


Figure 1.4: Matchings

contains more than t edges and if a graph G of order $2t$ has a matching M of cardinality t, then this (necessarily) maximum matching M is a perfect matching. In Figure 1.4, complete graph K_6 is shown, it can be seen that $M = \{e_1, e_3, e_5\}$ is a perfect matching for K_6 and in the same figure 1.4 another graph $K_6 - \{e_1, e_3, e_5\}$ is shown, that is in fact obtained from K_6 after deleting the edges of perfect matching M.

1.6 Graph Invariants or Graph Parameters

Two simple graphs G and H are *isomorphic graphs* if there exists a bijection $\Theta : V(G) \to V(H)$ which preserves adjacency (that is, the vertices u and v are adjacent in G if and only if their images $\theta(u)$ and $\theta(v)$ are adjacent in H). An *invariant* of a graph G is a number associated with G which has the same value for any graph isomorphic to G [6]. Major role played by these invariants is that they helps us in distinguishing non isomorphic graphs: some of these graph parameters are very common like n (the number of vertices), m (the number of edges), *degree sequence* of the graph G. Having defined the notions of distance related concepts, we can now add some other invariants to this list:

1. the number of components
2. the diameter
3. the radius
4. the girth
5. the circumference
6. the distance between pairs of vertices of given degree.

1.7 Some Well Known Graph Families

A graph with no cycles is known as *acyclic* graph. A *forest* is an acyclic graph and an acyclic connected graph is a *tree*. *Star graph* $K_{1,n-1}$ and *bistar* (also known as double star) $BS(1, n-3)$ are trees. Star graph $K_{1,n-1}$ consists of a center and $n-1$ pendant vertices, it is a tree of diameter 2. On the other hand $BS(p, q)$ where $p + q = n - 2$ denotes the bistar, which is obtained by joining the central vertices of $K_{1,p}$ and $K_{1,q}$ by an edge. Bistar is a tree of diameter 3. In Figure 1.5 star graph $K_{1,4}$ and bistar $BS(2, 3)$ are shown. We have many equivalent characterizations for trees:

Theorem 1.7.1. *[45] For an $n-$vertex graph G (with $n \geq 1$), the following properties are equivalent:*
(a) G is tree.
(b) G is connected and acyclic.
(c) G is connected and $|E(G)| = n - 1$.
(d) G is acyclic and $|E(G)| = n - 1$.
(e) G has no loops and for each $x, y \in V(G)$, $x \neq y$, G has exactly one $x - y$ path.

Further properties of trees T are as follows:

Theorem 1.7.2. *[46] For a tree T, the following properties are equivalent.*

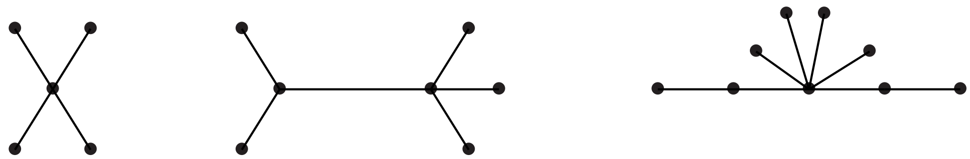
(a) T is connected and each edge is a bridge.

(b) T is acyclic and addition of any new edge produces a cycle in G.

As a consequence we have the following corollary.

Corollary 1.7.3. *[46] Any forest on n vertices and k components has $n-k$ edges.*

Another example of tree is a *caterpillar*. A caterpillar is a tree having the property that deleting all pendant vertices the resulting graph is a path. A caterpillar denoted by $C_{n,d}$ (where d represents the diameter of the caterpillar and n, its number of vertices) is obtained from a path P_{d+1} and $n-d-1$ pendant vertices attached to a central vertex. In order to be more clear, in Figure 1.5, $C_{9,4}$ is shown. Similar to the concept of spanning subgraph of a graph, we have the notion of spanning tree T in a graph G which is an acyclic connected subgraph of G such that $V(T) = V(G)$; in this case G is not necessarily a tree. A graph which contains exactly one cycle is called unicyclic graph and a graph G containing exactly two cycles is called *bicyclic graph*. Denote by $H_{n,k}$, the unicyclic graph of order n obtained from a cycle C_k by adding $n-k$ pendant vertices to a vertex of C_k, here k is the girth of this unicyclic graph. Considering somehow more general form of $H_{n,k}$ denoted by $H(n, k; n_1, n_2, \ldots, n_k)$ gives us another unicyclic graph of order n and girth k, which is again obtained from the cycle $C_k = v_1, v_2, \ldots, v_k, v_1$ with $n_i \geq 0$ pendant vertices attached at v_i for $1 \leq i \leq k$. In Figure 1.6, two unicyclic graphs $H_{8,5}$ and $H(14, 5; 2, 2, 1, 1, 3)$ are shown. The *cyclomatic number* $\mu(G)$ represents the number of linearly independent cycles in G and is given by $\mu(G) = m - n + 1$ if G is connected. A graph G on n vertices is *complete graph* if any two vertices of G are adjacent, thus a complete graph on n vertices is $(n-1)$ - regular and is denoted by K_n with $|E(K_n)| = \frac{n(n-1)}{2}$. Another important class of graphs is that of *bipartite graphs*. A graph G is called bipartite graph if the set $V(G)$ is the disjoint union of two nonempty sets (say) A and B (called partite classes of G) such that no two vertices in the same partite set are adjacent. A bipartite graph is called *complete bipartite graph* if any two ver-



$K_{1,4}$ $BS(2,3)$ $C_{9,4}$

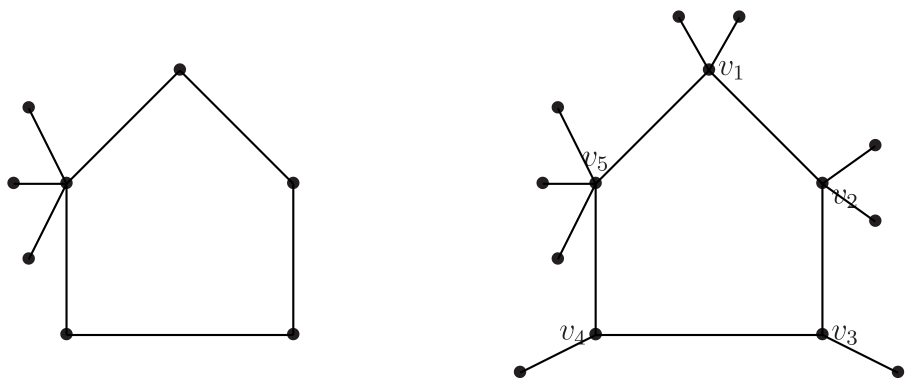
Figure 1.5: Some well known trees

tices in G belonging to different partite sets are adjacent and the complete bipartite graph on n vertices is denoted by $K_{a,b}$, where $|A| = a$ and $|B| = b$, with $a + b = n$ and $|E(K_{a,b})| = ab$. For the sake of completeness, in Figure 1.7 complete graph K_4 and complete bipartite graph $K_{2,3}$ are shown. Let $k \geq 2$ be an integer, in general a graph G is called $k-$ partite if $V(G)$ can be partitioned into k disjoint nonempty subsets such that each edge has its end points in different subsets and a $k-$ partite graph in which every two vertices from different partite classes are adjacent is called *complete* $k-$ *partite graph*. Here is given a characterization for a bipartite graph.

Theorem 1.7.4. *[23] A graph G is bipartite if and only if every cycle in G has even length.*

1.8 Chemical Graph Theory

Graph theoretical (GT) applications in chemistry underwent a dramatic revival lately. Constitutional (molecular) graphs have points (vertices) representing atoms and lines (edges) symbolizing covalent bonds. Graph theory provides the basis for definition, enumeration, systematization, codification, nomenclature, correlation, and computer programming. Chemical graph theory has attracted increasing research interest in recent years. Among the large variety of topics treated we



$H_{8,5}$ $\quad$ $H_{(14,5;2,2,1,1,3)}$

Figure 1.6: Unicyclic graphs

mention here the most important one: chemical indices in graph theory, that have origin in chemistry and graph theory lead to results that are used in a wide range by chemists. Well known chemical indices are Wiener index, First Zagreb index, Second Zagreb index, Multiplicative Zagreb indices, Reverse degree distance, Schultz molecular topological index, Balaban's index, Harary index, Degree distance index, Estrada index, Randić index, Harmonic index *etc.* In the last few years, a large number of mathematical investigations were reported on graph invariants originating from chemistry, and which have chemical applications (see [10, 12, 18, 36]). Quite a few of these graph invariants are based on vertex degrees and the distances between vertices. In this paper an invariant of connected graphs called the degree distance is considered. Chemical indices that will be in our discussion in later chapters of this work are *Wiener Index*, *First Zagreb Index*, *Reverse Degree Distance*, *Degree Distance Index*, *Harmonic Index*, *Sum-Connectivity Index*, *General Sum-Connectivity Index*, *Randić Index*, *Product-Connectivity Index* and *General Product-Connectivity Index*.

1.9 Well Known Indices in Chemical Graph Theory

Wiener index is a well−known topological index in mathematical chemistry. For a simple connected graph G, Wiener index is given as:

$$W(G) = \frac{1}{2}D(G)$$

where $D(G) = \sum_{x \in V(G)} D(x)$ with $D(x) = \sum_{y \in V(G)} d(x, y)$.

The new parameter $D'(G)$, called the degree distance of G, was introduced by Dobrynin and Kochetova [13] and Gutman [20] as a weighted version of the Wiener index, who used a different name for it. The degree distance $D'(x)$ of a vertex x is defined as $D'(x) = d(x)D(x)$, where $d(x)$ is the degree of x and the degree distance of G, denoted by $D'(G)$ is

$D'(G) = \sum\limits_{x \in V(G)} D'(x) = \sum\limits_{x \in V(G)} d(x)D(x) = \frac{1}{2} \sum\limits_{x,y \in V(G)} d(x, y)(d(x) + d(y))$.

This parameter was intensively studied in the literature. If G is a tree on n vertices, in [6] it was shown that $D'(G) = 2D(G) - n(n-1)$, which implies that for a tree of order n we have $D'(G) = 4W(G) - n(n-1)$, a relation which relies the Wiener index on the degree distance for trees. The expression $\sum_{x \in V(G)} d^2(x)$ is known as first Zagreb index of G, denoted by $Zg(G)$ [21]. Another molecular descriptor is the molecular topological index of G, denoted by $MTI(G)$ [34] and defined by $MTI(G) = Zg(G) + D'(G)$. In [50] Zhou and Trinajstić reported some properties of the reverse degree distance, including its bounds for connected (molecular) graphs, expressed in terms of other indices like first Zagreb index and Wiener index. For a connected graph of order n, size m and diameter d, since reverse degree distance ${}^{r}D'(G)$ and degree distance are related by

$${}^{r}D'(G) = 2(n-1)md - D'(G),$$

properties given in [50] give us some further information about relationship of degree distance with other indices.

The Randić index $R(G)$, is defined as

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2}.$$

The general Randić connectivity index (or general product-connectivity index), denoted by R_α, of G is defined as [2]:

$$R_\alpha = R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^{\alpha},$$

where α is a real number. Then $R_{-1/2}$ is the classical Randić connectivity index. The sum-connectivity of G, denoted by $\chi_{-1/2}(G)$ is defined by:

$$\chi_{-1/2}(G) = \sum_{uv \in E(G)} (d(u) + d(v))^{-1/2}.$$

The sum-connectivity index was proposed in [48] and both sum-connectivity index and Randić index correlate well with the π - electronic energy of benzenoid hydrocarbons [31]. This concept was extended to the general sum-connectivity index $\chi_\alpha(G)$ in [49], which is defined as

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^{\alpha},$$

where α is a real number. Then $\chi_{-1/2}(G)$ is the sum-connectivity index [48]. Another variant of the Randić index of a graph G is the harmonic index, denoted by $H(G)$ and defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)} = 2\chi_{-1}(G).$$

We have $H(G) \leq R(G)$ by the inequality between arithmetic and geometric means, with equality if and only if G is a regular graph. This index first appeared in [16] and was studied for simple connected graphs and trees in [47].

1.10 Preliminary Results

The technical results which follow will be useful for main results in next chapters. As in [41] , for parameters $m, n, p, t \in \mathbb{N}$, $t, m, n \geq 2$ and $n + t - 1 \leq p \leq nt$,

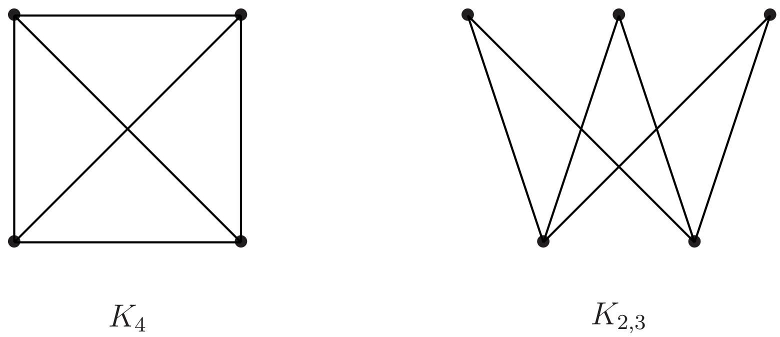


Figure 1.7: Complete graph and complete bipartite graph

denote by $S_{p,m,t}(x_1,...,x_n)$, the symmetric function

$$S_{p,m,t}(x_1,...,x_n) = \sum_{i=1}^{n} x_i(m-x_i)\,.$$

This function is defined for $(x_1,...,x_n) \in D_1$, where D_1 is the set of all vectors $(x_1,...,x_n)$ with positive integer coordinates such that $1 \le x_i \le t$ for $1 \le i \le n$, $x_1 \ge x_2 \ge ... \ge x_n$ and $\sum_{i=1}^{n} x_i = p$. Note that $S_{p,m,t}$ is strictly increasing in each variable on D_1 if $m \ge 2n-2$ and $t \le n-2$. Consider the following transformation denoted by T_1 of vectors in D_1: If $1 \le i < j \le n$ and $x_i \le t-1$ and $x_j \ge 2$ then $(x_1,...,x_n)$ is replaced by $(x_1,...,x_i+1,...,x_j-1,...,x_n)$. By reordering the components of this vector we get the vector $(x_1^*,...,x_n^*) \in D_1$, which will be denoted by $\mathbf{z}$. Since $i < j$ implies $x_i \ge x_j$ we deduce as in [41] that $S_{p,m,t}(x_1,...,x_n) - S_{p,m,t}(\mathbf{z}) = 2 + 2(x_i - x_j) > 0$. Eventually applying several times T_1 we deduce:

Lemma 1.10.1. *[41] $S_{p,m,t}(x_1,...,x_n)$ is minimum over D_1 if and only if there is an index k, $1 \le k \le n$ such that $x_1 = ... = x_k = t$, $1 \le x_{k+1} \le t-1$ and $x_i = 1$ for every $k+2 \le i \le n$.*

Note that the index k may be precisely determined; since $kt+n-k \le p \le kt+n-k+t-2$ it follows that $k(t-1) \le p-n \le k(t-1)+t-2$, which implies

$k = \lfloor \frac{p-n}{t-1} \rfloor$. We shall also use the function $F(x_1, ..., x_r, y_1, ..., y_{n-r})$ (defined in [41]) for $n, r \in \mathbb{N}$, $n \geq 4$, $5 \leq r \leq n-2$, $\alpha, \beta \in \mathbb{R}$ such that $\beta \geq \alpha + 1 \geq 2n - 1$ by

$$F(x_1, ..., x_r, y_1, ..., y_{n-r}) = \sum_{i=1}^{r} x_i(\alpha - x_i) + \sum_{j=1}^{n-r} y_j(\beta - y_j).$$

It is symmetric in the first r variables and in the last $n-r$ variables. F is defined for $(x_1, \ldots, x_r, y_1, \ldots, y_{n-r}) \in D$, where the domain D is the set of all vectors $(x_1, \ldots, x_r, y_1, \ldots, y_{n-r})$ with integer coordinates such that $x_1 \geq x_2 \geq ... \geq x_r$; $y_1 \geq y_2 \geq ... \geq y_{n-r}$; $2 \leq x_i \leq n-2$ for $1 \leq i \leq r$; $1 \leq y_j \leq n-2$ for $1 \leq j \leq n-r$ and $\sum_{i=1}^{r} x_i + \sum_{j=1}^{n-r} y_j = 2n-2$. F is strictly increasing in each variable on D.

Lemma 1.10.2. *[41](a) $F(x_1, \ldots, x_r, y_1, \ldots, y_{n-r})$ is minimum over D if and only if $(x_1, \ldots, x_r) = (n-r, 2, \ldots, 2)$ and $(y_1, \ldots, y_{n-r}) = (1, \ldots, 1)$.*
(b) Let $D_1 = D \setminus \{(\underbrace{n-r, 2, \ldots, 2}_{r}, 1, \ldots, 1)\}$. If $n \geq r+4$ then $F(x_1, ..., x_r, y_1, ..., y_{n-r})$ is minimum over D_1 if and only if $(x_1, \ldots, x_r) = (n-r-1, 3, 2, \ldots, 2)$ and $(y_1, \ldots, y_{n-r}) = (1, \ldots, 1)$.

Following Lemma gives us a lower bound for $D'(x)$ depending upon the eccentricity of the vertex x.

Lemma 1.10.3. *[41] Let G be a connected graph of order n and x be a vertex of G having eccentricity equal to p. Then $D'(x) = (n-1)^2$ for $p = 1$, $D'(x) = d(x)(2n-2-d(x))$ for $p = 2$ and $D'(x) \geq d(x)(2n - d(x) + \frac{p^2-3p}{2} - 1)$ for $p \geq 3$.*

In order to complete the result given above, an upper bound for $D'(x)$ is also provided in chapter 4 and also we will observe when these inequalities become equalities.

Chapter 2

Ordering Connected Graphs Having Small Degree Distances

In [41] the author found three graphs having smallest degree distances. They are $K_{1,n-1}$, $BS(n-3,1)$ and $K_{1,n-1}+e$. Here the next six graphs of order n in this sequence are determined provided $n \geq 15$: two have diameter 2, three diameter 3 and one diameter 4.

2.1 Main Result

Main result if this chapter can be concluded as follows:

Theorem 2.1.1. *The connected graphs of order $n \geq 15$ having the smallest degree distances are (in this order): $K_{1,n-1}$, $BS(n-3,1)$, $K_{1,n-1}+e$, G_1, G_2, G_3, G_4, G_5, G_6, the last two graphs having equal degree distances.*

Graphs G_1 - G_6 are illustrated in Figure 2.1. The technical results which follow will be useful in the main results of this chapter. As we have already given detail of symmetric function $S_{p,m,t}(x_1,...,x_n)$ and also explained transformation T_1. Now in order to find next minimum point we apply this transformation several times and get the following result providing us more information about minimum points of function mentioned above.

Lemma 2.1.2. *Let $D_1^* = D_1 \setminus (t, ..., t, x_{k+1}, 1, ..., 1)$, where $(t, ..., t, x_{k+1}, 1, ..., 1)$ is the unique point of minimum of $S_{p,m,t}(x_1, ..., x_n)$ over D_1. Then $S_{p,m,t}(x_1, ..., x_n)$ is minimum over D_1^* if and only if*
$(x_1, ..., x_n) = (t, ..., t, t-2, 2, 1, ..., 1)$ *if* $x_{k+1} = t-1$;
$(x_1, ..., x_n) = (t, ..., t, t-1, x_{k+1}+1, 1, ..., 1)$ *if* $x_{k+1} \in \{1, 2\}$;
$(x_1, ..., x_n) \in \{(t, ..., t, t-1, x_{k+1}+1, 1, ..., 1), (t, ..., t, x_{k+1}-1, 2, 1, ..., 1)\}$ *if* $3 \leq x_{k+1} \leq t-2$.

As before, the index k may be precisely determined; since $kt+n-k \leq p \leq kt+n-k+t-2$ it follows that $k(t-1) \leq p-n \leq k(t-1)+t-2$, which implies $k = \lfloor \frac{p-n}{t-1} \rfloor$. We shall use the function $F(x_1, ..., x_r, y_1, ..., y_{n-r})$ (defined in [41]), to find the minimum of degree distance function of graphs with different diameters. This time F is defined on an extended domain D_2, consisting of all vectors $(x_1, ..., x_r, y_1, ..., y_{n-r})$ having positive integer coordinates such that $x_1 \geq x_2 \geq ... \geq x_r$; $y_1 \geq y_2 \geq ... \geq y_{n-r}$; $2 \leq x_i \leq \gamma$ for $1 \leq i \leq r$; $1 \leq y_j \leq \gamma$ for $1 \leq j \leq n-r$ and $\sum_{i=1}^{r} x_i + \sum_{j=1}^{n-r} y_j = \delta$, where $\gamma \in \{n-2, n-3\}$, $\delta \in \{2n-2, 2n\}$. For $\alpha = 2n-2$ and $\beta = 2n-1$, F is strictly increasing in each variable on D_2. Consider now the transformation T_2 of vectors in D_2 defined by :
If $y_1 \geq 2$ then $(x_1, ..., x_r, y_1, ..., y_{n-r})$ is replaced by $(x_1, ..., x_r + y_1 - 1, 1, y_2, ..., y_{n-r})$; reorder separately the first r components and the last $n-r$ components and we get $\mathbf{z} = (x_1^*, ..., x_r^*, y_1^*, ..., y_{n-r}^*) \in D_2$. From given conditions it follows that $x_r + y_1 - 1 \leq 2n - 1 - \sum_{i=1}^{r-1} x_i - \sum_{j=2}^{n-r} y_j \leq n - r + 2 \leq n - 3 \leq \gamma$ for any $r \geq 5$. As in [41] we get $F(x_1, ..., x_r, y_1, ..., y_{n-r}) - F(\mathbf{z}) = (y_1 - 1)(\beta - \alpha - 2 + 2x_r) > 0$.

Lemma 2.1.3. *If $F(x_1, ..., x_r, y_1, ..., y_{n-r})$ is minimum over D_2 then*
$(x_1, ..., x_r) = (\delta - n - r + 2, 2, ..., 2)$ *and* $(y_1, ..., y_{n-r}) = (1, ..., 1)$.

Proof. Suppose that $\mathbf{z}^0 = (x_1^0, x_2^0, ..., x_r^0, y_1^0, ..., y_{n-r}^0)$ is a point of minimum for F in D_2. Applying T_1 on the first r components and the last $n-r$ components and T_2 we deduce that $x_3^0 = ... = x_r^0 = 2$ and $y_1^0 = ... = y_{n-r}^0 = 1$. x_1^0 takes the greatest possible value, which is less than or equal to γ. Also $x_1^0 = \delta - n - r + 4 - x_2^0 \leq \delta - n - r + 2$,

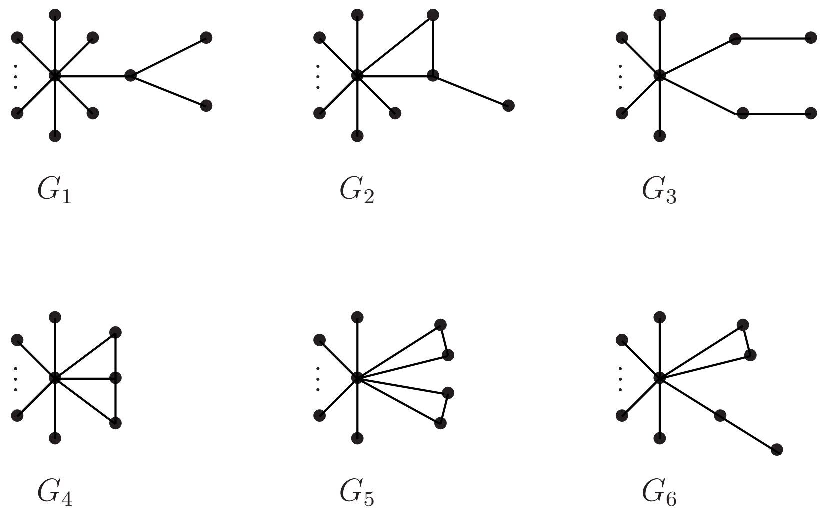


Figure 2.1: Six graphs of order n

which implies $x_1^0 = \min(\delta - n - r + 2, \gamma)$ and $x_2^0 = \delta - n - r + 4 - x_1^0$.
If $r \geq 5$ then $\delta - n - r + 2 \leq \delta - n - 3 \leq n - 3 \leq \gamma$, thus implying $x_1^0 = \delta - n - r + 2$ and $x_2^0 = 2$. ∎

Six graphs $G_1 - G_6$ of order n are represented in Figure 2.1. G_1 is the bistar $BS(n-4, 2)$. We will show that they are the next members completing the sequence $K_{1,n-1}$, $BS(n-3, 1)$, $K_{1,n-1}+e$ of graphs having smallest degree distances, provided $n \geq 15$.
By direct computations we deduce:

Lemma 2.1.4. *For every $n \geq 5$ we have*
$D'(G_1) = 3n^2 + n - 28$; $D'(G_2) = 3n^2 + n - 22$; $D'(G_3) = 3n^2 + n - 20$; $D'(G_4) = 3n^2 + n - 18$ *and* $D'(G_5) = D'(G_6) = 3n^2 + n - 16$.

We shall prove that unique graphs G of order n having $D'(G) \leq 3n^2 + n - 16$ are graphs $K_{1,n-1}, BS(n-3, 1)$, $K_{1,n-1} + e$ and graphs $G_1 - G_6$ from Figure 2.1 for $n \geq 15$.
This will be done by considering the cases when $diam(G) = 2, 3, 4$ or $diam(G) \geq 5$.

2.1.1 Graphs of Diameter Two

Lemma 2.1.5. *All graphs G of order $n \geq 11$ and diameter 2 having $D'(G) \leq 3n^2 + n - 16$ are $K_{1,n-1}$, $K_{1,n-1} + e$, G_4 and G_5.*

Proof. Let G be a graph of diameter 2 with $D'(G) \leq 3n^2 + n - 16$. It follows that every vertex x of G has $ecc(x) = 1$(or equivalently, $d(x) = n - 1$) or $ecc(x) = 2$. If r denotes the number of vertices having eccentricity 1, by Lemma 1.10.3 we get

$$D'(G) = r(n-1)^2 + \sum_{x \in V(G); ecc(x)=2} d(x)(2n - 2 - d(x)),$$

where the sum has $n - r$ terms. Suppose $r = 0$. If $x \in V(G)$ has $d(x) = 1$ then the unique vertex y which is adjacent to x has $ecc(y) = 1$, which contradicts the hypothesis. It follows that $2 \leq d(x) \leq n-2$ for every $x \in V(G)$, which implies that $d(x)(2n - 2 - d(x)) \geq 2(2n - 4)$. In this case $D'(G) \geq 2n(2n - 4) > 3n^2 + n - 16$ for every $n \geq 7$, which contradicts the hypothesis.

Hence G has $r \geq 1$ vertices of degree $n - 1$. The function $d(x)(2n - 2 - d(x))$ is strictly increasing for $d(x) = 1, ..., n - 1$ having a maximum equal to $(n - 1)^2$.

If $r \geq 2$ it follows that all vertices x have $d(x) \geq 2$, which implies

$D'(G) \geq 2(n-1)^2 + 2(n-2)(2n-4) > 3n^2 + n - 16$ for every $n \geq 5$, a contradiction.

This implies that $r = 1$ and G has a unique vertex z of degree $n - 1$, hence G is deduced from $K_{1,n-1}$ eventually adding some new edges. If we add at most two edges we get $K_{1,n-1}$, $K_{1,n-1} + e$, G_4 and G_5 from Figure 2.1.

We shall prove that if we add at least three edges then the resulting graph G will have $D'(G) > 3n^2 + n - 16$ for $n \geq 11$. Suppose that G is obtained from $K_{1,n-1}$ by adding exactly three edges, hence G has size $m = n + 2$. If $x_1, ..., x_{n-1}$ denote the degrees of the vertices adjacent to z, we obtain $x_i \geq 1$ for $1 \leq i \leq n - 1$, $\sum_{i=1}^{n-1} x_i = n + 5$ and

$$D'(G) = (n-1)^2 + \sum_{i=1}^{n-1} x_i(2n - 2 - x_i).$$

By Lemma 1.10.1 the minimum of the sum $S_{n+5,2n-2,n-2}$ in D_1 is reached for $x_1 = 7, x_2 = ... = x_{n-1} = 1$, which implies $D'(G) \geq (n-1)^2 + 7(2n-9) + (n-2)(2n-3) = = 3n^2 + 5n - 56 > 3n^2 + n - 16$ for $n \geq 11$. Since $S_{p,2n-2,n-2}$ is strictly increasing in $p \geq n+5$ the proof is done. ∎

2.1.2 Graphs of Diameter Three

Lemma 2.1.6. *The set of graphs G of order $n \geq 15$, diameter 3 and $D'(G) \leq 3n^2 + n - 16$ contains only four members: $BS(n-3,1), G_1, G_2$ and G_6.*

Proof. Let G be a connected graph of order $n \geq 15$, size $m \geq n-1$, diameter 3 and $D'(G) \leq 3n^2 + n - 16$. Since $diam(G) = 3$ it follows that $d(x) \leq n-2$ for every $x \in V(G)$. We shall divide the proof in three cases: A. $m = n-1$; B. $m = n$ and C. $m \geq n+1$.

A. Consider first the case when $m = n-1$, i.e., G is a tree. Since G has diameter 3 it follows that G is a bistar $BS(r, n-2-r)$, where $1 \leq r \leq (n-3)/2$. By direct computation we obtain

$$D'(G) = 3n^2 - 7n + 4 - 4(r^2 - rn + 2r).$$

It results that $D'(G)$ is strictly increasing in $r \leq (n-3)/2$; for $r = 3$ we get $D'(G) = 3n^2 + 5n - 56 > 3n^2 + n - 16$ for every $n \geq 11$.

For $r = 1$, the resulting graph is $BS(n-3,1)$ and for $r = 2$ we get G_1 from Figure 2.1. It remains to consider the case when $m \geq n$.

B. Suppose that $m = n$ and there is a vertex x such that $d(x) = n-2$. There exist a vertex w which is not adjacent to x and two edges which are not incident to x. Since $diam(G) = 3$ we have only three possibilities to build such a graph, getting graphs G_2, G_6 and a graph, say F, deduced by making w adjacent to two vertices which are adjacent to x. By Lemma 2.1.4 we have $D'(G_2), D'(G_6) \leq 3n^2 + n - 16$ and by direct computation $D'(F) = 3n^2 + 2n - 24 > 3n^2 + n - 16$ for every $n \geq 9$. Suppose that $m = n$ and $d(x) \leq n-3$ for every vertex $x \in V(G)$. In this case we shall prove that $D'(G) > 3n^2 + n - 16$. Let $p \geq 0$ denote as above the number of vertices x of G having $ecc(x) = 2$; it results $n \geq p + 2$. We consider first the case when $p \geq 5$. By Lemma 1.10.3 we deduce that

$$D'(G) \geq \sum_{i=1}^{p} x_i(2n - 2 - x_i) + \sum_{j=1}^{n-p} y_j(2n - 1 - y_j),$$

where $x_1, ..., x_p$ and $y_1, ..., y_{n-p}$ are the degrees of vertices of eccentricity 2 and 3, respectively. Since $m = n$ we have $\sum_{i=1}^{p} x_i + \sum_{j=1}^{p} y_j = 2n$. From the hypothesis it follows that $x_i \leq n - 3$ for $1 \leq i \leq p$ and $y_j \leq n - 3$ for $1 \leq j \leq n - p$. If u is a vertex of eccentricity 2 and $d(u) = 1$, then the vertex v adjacent to u must have $d(v) = n - 1$, which contradicts the property that $diam(G) = 3$. It follows that $x_i \geq 2$ for every $i = 1, ..., p$. Using Lemma 2.1.3 for $F(x_1, ..., x_p, y_1, ..., y_{n-p})$, where $\alpha = 2n - 2$ and $\beta = 2n - 1$, we find that F is minimum for $x_1 = n - p + 2, x_2 = ... = x_p = 2$ and $y_1 = ... = y_{n-p} = 1$, which implies that

$D'(G) \geq (n-p+2)(n+p-4) + 2(p-1)(2n-4) + (n-p)(2n-2) = 3n^2 + 2np - 8n - p^2$.

We have $3n^2 + 2np - 8n - p^2 > 3n^2 + n - 16$ if and only if $n(2p - 9) > p^2 - 16$. This inequality is satisfied for $p = 5$ and $n \geq 10$. If $p \geq 6$ we can use inequality $n \geq p + 2$; we get $n(2p - 9) \geq (p + 2)(2p - 9) = 2p^2 - 5p - 18$ and $2p^2 - 5p - 18 > p^2 - 16$ for any $p \geq 6$. Consequently, for $p \geq 5$ we have deduced that $D'(G) > 3n^2 + n - 16$. It remains to prove this inequality for $0 \leq p \leq 4$. If $p = 0$, $D'(G) \geq \sum_{j=1}^{n} y_j(2n - 1 - y_j)$, where $1 \leq y_j \leq n - 3$ for $1 \leq j \leq n$ and $\sum_{j=1}^{n} y_j = 2n$. Using Lemma 1.10.1 the minimum of $S_{2n,2n-1,n-3}$ is reached for $y_1 = n - 3, y_2 = 5, y_3 = ... = y_n = 1$ and is equal to $(n - 3)(n + 2) + 5(2n - 6) + (n - 2)(2n - 2) = 3n^2 + 3n - 32 > 3n^2 + n - 16$ for every $n \geq 9$. If $1 \leq p \leq 4$ we can write $\sum_{i=1}^{p} x_i(2n - 2 - x_i) + \sum_{j=1}^{n-p} y_j(2n - 1 - y_j)$

$= \sum_{i=1}^{p} x_i(2n - 2 - x_i) + \sum_{j=1}^{n-p} y_j(2n - 2 - y_j) + \sum_{j=1}^{n-p} y_j$

$\geq \sum_{i=1}^{p} x_i(2n - 2 - x_i) + \sum_{j=1}^{n-p} y_j(2n - 2 - y_j) + n - p$.

By redenoting $y_1 = x_{p+1}, ..., y_{n-p} = x_n$, we get $D'(G) \geq \sum_{i=1}^{n} x_i(2n - 2 - x_i) + n - p$, where $1 \leq x_i \leq n - 3$ for $1 \leq i \leq n$ and $\sum_{i=1}^{n} x_i = 2n$. By Lemma 1.10.1 we obtain that the minimum of $S_{2n,2n-2,n-3}$ is reached for $(n-3,5,1,...,1)$. But this sequence of degrees is not graphical. From Lemma 2.1.2 it follows that the next minimum of this function is reached for $(n-4,6,1,...,1)$ or for $(n-3,4,2,1,...,1)$. We have $S_{2n,2n-2,n-3}(n-4,6,1,...,1) = 3n^2+3n-50 > S_{2n,2n-2,n-3}(n-3,4,2,1,...,1) = 3n^2+n-26$ for every $n \geq 13$. Consequently, since $n-p \geq n-4$, $D'(G) \geq 3n^2+n-26+n-4 = 3n^2+2n-30 > 3n^2+n-16$ for every $n \geq 15$.

C. If $m = n+1$ and there is a vertex x such that $d(x) = n-2$, it follows that $ecc(x) = 2$ and $D'(x) = n(n-2)$ by Lemma 1.10.3. By denoting by $p \geq 1$ the number of vertices of eccentricity 2 of G, the number of vertices of eccentricity 3 will be $n-p$. Let $x_2, ..., x_p$ be the degrees of the vertices of eccentricity 2 of G which are different from x and $y_1, ..., y_{n-p}$ be the degrees of the vertices of eccentricity 3 of G, arranged in a decreasing order. One has $D'(G) \geq n(n-2) + \sum_{i=2}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-1-y_j) =$

$$= n(n-2) + \sum_{i=2}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-2-y_j) + \sum_{j=1}^{n-p} y_j$$

$\geq n(n-2) + \sum_{i=2}^{n} x_i(2n-2-x_i) + n - p$, by redenoting $y_1 = x_{p+1}, ..., y_{n-p} = x_n$.

We have $\sum_{i=2}^{n} x_i = n+4$. By Lemma 1.10.1 the minimum of $S_{n+4,2n-2,n-2}(x_1, ..., x_{n-1})$ is reached for $(6,1,...,1)$ and it is equal to $6(2n-8)+(n-2)(2n-3) = 2n^2+5n-42$. The extremities of a diametral path in G have eccentricities equal to 3, which implies $n \geq p+2$, or $n-p \geq 2$. It follows that $D'(G) \geq n(n-2)+2n^2+5n-42+2 = 3n^2+3n-40 > 3n^2+n-16$ for any $n \geq 13$. Because $S_{q,2n-2,n-2}(x_1, ..., x_{n-1})$ is increasing for $q \geq n+4$, we deduce that $D'(G) > 3n^2+n-16$ for any $m \geq n+1$ and $n \geq 13$ if there is a vertex x of degree $n-2$.

Note that for $m = n+1$ and $d(x) \leq n-3$ for every vertex $x \in V(G)$, the minimum of $S_{2n+2,2n-2,n-3}$ over D_1 is reached for $(n-3,7,1,...,1)$ and is equal to $3n^2+5n-60$. In this case $D'(G) \geq 3n^2+6n-64$ since $n-p \geq n-4$ and $3n^2+6n-64 > 3n^2+n-16$ for every $n \geq 10$. Since $S_{q,2n-2,n-3}$ is increasing for $q \geq 2n+2$, it follows that for $m \geq n+2$ and $d(x) \leq n-3$ for every vertex $x \in V(G)$, $D'(G) > 3n^2+n-16$ holds, which concludes the proof. ∎

2.1.3 Graphs of Diameter Four

Lemma 2.1.7. *There exists a unique graph G of order $n \geq 13$ having $diam(G) = 4$ and $D'(G) \leq 3n^2 + n - 16$, namely G_3.*

Proof. Suppose G is a graph of diameter 4, order $n \geq 13$ and $D'(G) \leq 3n^2 + n - 16$. It follows that $d(x) \leq n - 3$ for every $x \in V(G)$. We shall prove that if $m = n - 1$, i.e, G is a tree, then $G = G_3$. In this case the center of G consists of a single vertex w since the diameter is even. Denote by $p \geq 2$ the number of vertices x having $ecc(x) = 4$; it follows that $n - p - 1$ vertices y have eccentricity $ecc(y) = 3$, only w having eccentricity $ecc(w) = 2$. All vertices x with $ecc(x) = 4$ have $d(x) = 1$. It results that $\sum_{ecc(y)=3} d(y) = n - 1$ since $d(w) = n - p - 1$. Since $d(w) \geq 2$ it follows that $n \geq p + 3$. If $p = 2$ we deduce that $G = G_3$. Suppose that $p \geq 3$. Let $N_i(u) = \{v \in V(G) : d(u, v) = i\}$. If there is a vertex z of eccentricity 4 such that $|N_2(z)| = p$, by denoting by y the vertex of eccentricity 3 adjacent to z we obtain $d(y) = p + 1$. It results that y is adjacent to all vertices of G of eccentricity 4 which would imply that $diam(G) = 3$, a contradiction. Suppose that there exists a vertex z such that $ecc(z) = 4$ and $|N_2(z)| = p - 1$.

In this case there is a unique tree H illustrated in Figure 2.2 having these properties, where $d(w) = n - p - 1$ and $d(y) = p$. By direct computation we get $D'(H) = 3n^2 - 7n + 4np - 4p^2 - 4$. We have $D'(H) > 3n^2 + n - 16$ if and only if $n(4p - 8) > 4p^2 - 12$. For $p = 3$ this inequality holds for every ≥ 7. Let $p \geq 4$. Since $n \geq p + 3$ we deduce $n(4p - 8) \geq 4p^2 + 4p - 24 > 4p^2 - 12$ for any $p \geq 4$. The remaining situation is that when for every vertex z of eccentricity 4 we have $|N_2(z)| \leq p - 2$. We need a more careful evaluation of the lower bound for $D'(z)$. Since $d(z) = 1$ and $|N_3(z)| = n - p - 2$ we get $|N_2(z)| = n - 1 - (1 + n - p - 2) - |N_4(z)| = p - |N_4(z)|$. Since $|N_2(z)| \leq p - 2$ it follows that $|N_4(z)| \geq 2$. We can write $D'(G) = 1 + 2|N_2(z)| + 3(n - p - 2) + 4|N_4(z)| = 1 + 2p + 3(n - p - 2) + 2|N_4(z)| \geq 3n - p - 1$ since $|N_4(z)| \geq 2$.

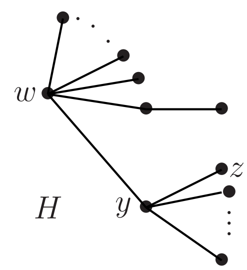


Figure 2.2: Tree H of diameter 4

Finally, $D'(G) \geq (n-p-1)(n+p-1) + \sum_{ecc(y)=3} d(y)(2n-1-d(y)) + 3np - p^2 - p$. The minimum value of $\sum_{ecc(y)=3} d(y)(2n-1-d(y))$ is realized, by Lemma 1.10.1 for $(p+1, \underbrace{1, ..., 1}_{n-p-2})$. But this sequence of degrees of vertices of eccentricity 3 cannot be realized by a tree of diameter 4 since a unique vertex has its degree greater than 1. By Lemma 2.1.2 the next minimum value of $S_{2n-2,2n-1,n-3}$ is realized for $(p, 2, \underbrace{1, ..., 1}_{n-p-3})$. It follows that

$D'(G) \geq (n-p-1)(n+p-1) + p(2n-1-p) + 2(2n-3) + (n-p-3)(2n-2) + 3np - p^2 - p = 3n^2 + 3np - 6n - 3p^2 + 1$.

$D'(G) > 3n^2 + n - 16$ holds if $n(3p-7) > 3p^2 - 17$. If $p \geq 3$ and $n \geq p+3$ the expression $n(3p-7)$ is greater than or equal to $3p^2 + 2p - 21$ and this polynomial is strictly greater than $3p^2 - 17$ for every $p \geq 3$.

Let now $m = n$. By Lemma 1.10.3 we deduce

$D'(G) \geq \sum_{ecc(x)=2} d(x)(2n-2-d(x)) + \sum_{ecc(y)=3} d(y)(2n-1-d(y)) + \sum_{ecc(z)=4} d(z)(2n+1-d(z))$.

Let u, a, t, b, v be a shortest path of length 4 between two vertices of eccentricity 4. It follows that $ecc(a), ecc(b) \geq 3$ and $d(a), d(b) \geq 2$. Since $d(y)(2n-1-d(y)) = d(y)(2n-2-d(y)) + d(y)$ and $d(z)(2n+1-d(z)) = d(z)(2n-2-d(z)) + 3d(z)$, it results that $D'(G) \geq \sum_{x \in V(G)} d(x)(2n-2-d(x)) + 10$, where $\sum_{x \in V(G)} d(x) = 2n$.

Since $diam(G) = 4$ we get $d(x) \leq n-3$ for any $x \in V(G)$. For $p = 2n, m = 2n-2$ and $t = n-3$, the minimum of $S_{2n,2n-2,n-3}(x_1, ..., x_n)$ in D_1 is realized for $x_1 = n-3, x_2 = 5, x_3 = ... = x_n = 1$. But the sequence $(n-3, 5, 1, ..., 1)$ is not graphical. By Lemma 2.1.2 the next minimum of $S_{2n,2n-2,n-3}$ is realized for $\mathbf{z}^1 = (n-4, 6, 1, ..., 1)$ or $\mathbf{z}^2 = (n-3, 4, 2, 1, ..., 1)$.
In the first case we get $D'(G) \geq 3n^2 + 3n - 40 > 3n^2 + n - 16$ for every $n \geq 13$ and in the second case $D'(G) = 3n^2 + n - 16$. Equality is reached only for $\mathbf{z}^2$, which has a unique graphical realization, having diameter 3, which contradicts the hypothesis. We can conclude that for $m = n$ for all graphs G of order n, size m and diameter 4 $D'(G)$ is strictly greater than $3n^2 + n - 16$.
Let $m = n + 1$. The minimum of $S_{2n+2,2n-2,n-3}$ is realized for $(n-3, 7, 1, ..., 1)$ and is equal to $3n^2 + 5n - 60$. We deduce $D'(G) \geq 3n^2 + 5n - 50 > 3n^2 + n - 16$ for $n \geq 9$. For $m \geq n + 2$, $S_{p,2n-2,n-3}$ being increasing in $p \geq 2n + 2$, the same conclusion holds. ∎

2.1.4 Graphs of Diameter At Least Five

Lemma 2.1.8. *Let G be a graph of order $n \geq 8$ and diameter $diam(G) \geq 5$. Then $D'(G) > 3n^2 + n - 16$.*

Proof. If G has diameter at least 5 it follows that for every $x \in V(G)$ we have $ecc(x) \geq 3$ since otherwise, by triangle inequality, we obtain $diam(G) \leq 4$. The same conclusion holds if there exists a vertex x having $d(x) \geq n-3$. It follows that $d(x) \leq n-4$ for every $x \in V(G)$. Since $ecc(x) \geq 3$, by Lemma 1.10.3 we obtain that $D'(x) \geq d(x)(2n-1-d(x))$, which implies that $D'(G) \geq \sum_{x \in V(G)} d(x)(2n-1-d(x))$. Suppose that G has diameter 5 and it is a tree, hence $m = n-1$. It follows that $D'(G) \geq S_{2n-2,2n-1,n-4}(x_1, ..., x_n)$, where $x_1, ..., x_n$ are the degrees of the vertices of G. By Lemma 1.10.1 it follows that the minimum of $S_{2n-2,2n-1,n-4}$ is reached in D_1 for $x_1 = n-4, x_2 = 4$ and $x_3 = ... = x_n = 1$ and is equal to $(n-4)(n+3) + 4(2n-5) + (n-2)(2n-2) = 3n^2 + n - 28$. Note that

$(n-4,4,1,...,1)$ has a unique graphical realization which has diameter 3. If G has diameter 5, let u,v be two diametral vertices of G and u,x,w,t,y,v be a shortest path between them. It follows that $ecc(u)=ecc(v)=5, ecc(x)\geq 4, ecc(y)\geq 4$ and $d(x),d(y)\geq 2$. This implies that $D'(u)\geq d(u)(2n+4-d(u))$ and the difference $d(u)(2n+4-d(u))-d(u)(2n-1-d(u))=5d(u)\geq 5$. In a similar way we get $D'(x)\geq d(x)(2n+1-d(x))$ and $d(x)(2n+1-d(x))-d(x)(2n-1-d(x))=2d(x)\geq 4$. It follows that we can write $D'(G)\geq 3n^2+n-28+2(5+4)=3n^2+n-10>3n^2+n-16$ for every n.

The inequality $D'(G)\geq \min_{x_1+...+x_n=2n-2} S_{2n-2,2n-1,n-4}(x_1,...,x_n)+18$ also holds if $diam(G)>5$ and the constant 18 may be improved by a similar argument. Since $S_{p,2n-1,n-4}$ is strictly increasing in $p\geq 2n-2$, it follows that $D'(G)>3n^2+n-16$ for any connected graph G of order n, size $m\geq n-1$ and diameter $diam(G)\geq 5$.
∎

Chapter 3

Unicyclic Connected Graphs Having Smallest Degree Distances

The motivation of this chapter is to continue the work of ordering connected graphs having small degree distances. In the previous chapter, we determined nine graphs having smallest degree distances. Here a list of four trees of order n having smallest degree distances is deduced from that list of nine graphs provided $n \geq 10$: one has diameter 2, two diameter 3 and one diameter 4. Since for trees the degree distance and the Wiener index are strongly related, it also follows that these trees have minimum Wiener index. Also four unicyclic connected graphs of order n having smallest degree distances are determined provided $n \geq 15$: one has diameter 2 and three diameter 3. Here again we will use the symmetric function

$$S_{p,m,t}(x_1, ..., x_n) = \sum_{i=1}^{n} x_i(m - x_i)$$

with the Lemmas 1.10.1 [41] and 2.1.2 [37]. Eventually applying several times T_1 we deduce:

Corollary 3.0.9. $\min\limits_{t \leq n-4} \min\limits_{(x_1,...,x_n) \in D_1} S_{2n,2n-2,t}(x_1, \ldots, x_n)$ *is reached only for* $(n-4, 6, 1, \ldots, 1)$.

Also we will consider other function which is also defined in chapter 1 as

$F(x_1, ..., x_r, y_1, ..., y_{n-r})$ (defined in [41, 37]). In the sequence of graphs described by Theorem 2.1.1, only $K_{1,n-1}$, $BS(n-3,1)$, $G_1 = BS(n-4,2)$ and G_3 are trees whereas $K_{1,n-1}+e$, G_2 and G_6 are unicyclic. In the next section we will show that these graphs are four trees having smallest degree distances (in the order mentioned above), provided $n \geq 10$, and in the last section we shall prove that the fourth graph in this sequence of unicyclic graphs is $H_{n,4}$ (which was also denoted by F in [37]) for $n \geq 15$.

3.1 Main Results

Two main results of this chapter are as follows.

Theorem 3.1.1. *The trees of order* $n \geq 10$ *having the smallest degree distances are (in this order):* $K_{1,n-1}$, $BS(n-3,1)$, $G_1 = BS(n-4,2)$, G_3, *where* $diam(K_{1,n-1}) = 2$, $diam(BS(n-3,1)) = diam(BS(n-4,2)) = 3$ *and* $diam(G_3) = 4$.

The relation between the Wiener index and the degree distance index [20] shows that trees of order $n \geq 10$ having the smallest Wiener index also are $K_{1,n-1}$, $BS(n-1,3)$, $G_1 = BS(n-4,2)$ and G_3.

Theorem 3.1.2. *The unicyclic connected graphs of order* $n \geq 15$ *having the smallest degree distances are* $K_{1,n-1}+e$, G_2, G_6 *and* $H_{n,4}$ *(in this order).*

By direct computations we have

Lemma 3.1.3. *[27, 37] For every* $n \geq 5$ *we have*
$D'(G_1 = BS(n-4,2)) = 3n^2+n-28$; $D'(G_3) = 3n^2+n-20$; $D'(K_{1,n-1}+e) = 3n^2-3n-6$; $D'(G_2) = 3n^2+n-22$; $D'(G_6) = 3n^2+n-16$ *and* $D'(H_{n,4}) = 3n^2+2n-24$.

3.1.1 Ordering Trees Having Small Degree Distances

We shall prove that all trees T of order n having $D'(T) \leq 3n^2+n-20$ are trees $K_{1,n-1}$, $BS(n-3,1)$, $G_1 = BS(n-4,2)$ and G_3 (from Figure 2.1) for $n \geq 10$.

For this we shall consider the cases when $diam(G) = 2, 3, 4$ or $diam(G) \geq 5$.
The following property is obvious.

Lemma 3.1.4. *The only tree T of order $n \geq 3$ and diameter 2 is $K_{1,n-1}$.*

Lemma 3.1.5. *The set of trees T of order $n \geq 10$, diameter 3 and $D'(T) \leq 3n^2 + n - 20$ contains only two members: $BS(n-3, 1)$ and $G_1 = BS(n-4, 2)$.*

Proof. Let T be a tree of order $n \geq 10$, diameter 3 and $D'(T) \leq 3n^2 + n - 20$. As T is a tree and T has diameter 3 it follows that T is a bistar $BS(r, n-2-r)$, where $1 \leq r \leq (n-3)/2$. By direct computation we obtain

$$D'(T) = 3n^2 - 7n + 4 + \varphi(r),$$

where $\varphi(r) = -4(r^2 - rn + 2r)$. It results that $D'(T)$ is strictly increasing in $r \leq (n-3)/2$; for $r = 3$ we get $D'(T) = 3n^2 + 5n - 56 > 3n^2 + n - 20$ for every $n \geq 10$.
Let $r \geq 4$. Inequality $D'(T) > 3n^2 + n - 20$ is equivalent to $n(4r-8) > 4r^2 + 8r - 16$. Since $n \geq 2r+3$ it follows that $n(4r-8) \geq (2r+3)(4r-8) = 8r^2 - 4r - 24$ and this expression is greater than $4r^2 + 8r - 16$ if $r(r-3) > 2$, which is true for every $r \geq 4$. For $r = 1$, the resulting graph is $BS(n-3, 1)$ and for $r = 2$ we get $G_1 = BS(n-4, 2)$ (from Figure 2.1). ∎

Lemma 3.1.6. *There exists a unique tree T of order $n \geq 6$ having $diam(T) = 4$ and $D'(T) \leq 3n^2 + n - 20$, namely G_3.*

Proof. Suppose T is a tree of diameter 4, order $n \geq 6$ and $D'(T) \leq 3n^2 + n - 20$. It follows that $d(x) \leq n - 3$ for every $x \in V(T)$. We shall prove that $T = G_3$. The center of T consists of a single vertex w, since its diameter is even. Let $p \geq 2$ denote the number of vertices x having $ecc(x) = 4$. It follows that $n - p - 1$ vertices y have eccentricity $ecc(y) = 3$, only w has $ecc(w) = 2$. We get that if $p = 2$ then $T = G_3$. For $p = 3$ we get two trees T_1 and T_2 of diameter 4, represented in Figure 3.1. By

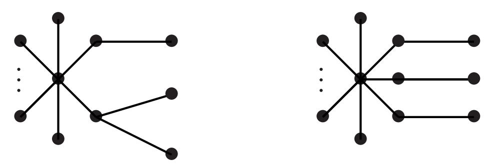


Figure 3.1: Two trees of diameter 4

direct computations we get $D'(T_1) = 3n^2 + 5n - 40 > 3n^2 + n - 20$ for $n \geq 6$ and $D'(T_2) = 3n^2 + 5n - 32 > 3n^2 + n - 20$ for $n \geq 4$.

Let now $p \geq 4$. By Lemma 1.10.3 we get

$$D'(T) \geq (n - p - 1)(n + p - 1) + \sum_{ecc(y)=3} d(y)(2n - 1 - d(y)) + 2np.$$

The minimum value of the sum is realized, by Lemma 1.10.1 for $(p + 1, \underbrace{1, ..., 1}_{n-p-2})$. This sequence of degrees of vertices of eccentricity 3 cannot be realized by a tree of diameter 4 since a unique vertex has its degree greater than 1, which would imply that T has diameter equal to 3.

The next minimum value of $S_{2n-2,2n-1,n-3}$ is realized, by Lemma 2.1.2 for $(p, 2, \underbrace{1, ..., 1}_{n-p-3})$. This sequence of degrees of the vertices of eccentricity 3, equal to $(p, 2, 1, ..., 1)$ is realized for a unique tree, H, represented in Figure 2.2, where $d(w) = n - p - 1$ and $d(y) = p$. For $p = 3$ H coincides with T_1. We can compute $D'(H) = 3n^2 - 7n + 4np - 4p^2 - 4$ and $D'(H) > 3n^2 + n - 20$ is equivalent to $n(4p - 8) > 4p^2 - 16$. Since $n \geq p + 3$ this inequality is valid for every $n \geq 6$ and $3 \leq p \leq n - 3$ since $n(4p - 8) \geq (p + 3)(4p - 8) > 4p^2 - 16$ for every $p \geq 3$. ∎

Lemma 3.1.7. *All trees T of order $n \geq 8$ and diameter $diam(T) \geq 5$ have $D'(T) > 3n^2 + n - 20$.*

Proof. If T has diameter at least 5 it follows that for every $x \in V(T)$ we have $ecc(x) \geq 3$ since otherwise, by the triangle inequality, we obtain $diam(T) \leq 4$. The same conclusion holds if there exists a vertex x having $d(x) \geq n-3$. It follows that $d(x) \leq n-4$ for every $x \in V(T)$. Since $ecc(x) \geq 3$, by Lemma 1.10.3 we obtain that $D'(x) \geq d(x)(2n-1-d(x))$, which implies that $D'(T) \geq \sum_{x \in V(T)} d(x)(2n-1-d(x))$. Suppose that T has diameter 5. It follows that $D'(T) \geq S_{2n-2,2n-1,n-4}(x_1, ..., x_n)$, where $x_1, ..., x_n$ are the degrees of the vertices of T. By Lemma 1.10.1 it follows that the minimum of $S_{2n-2,2n-1,n-4}$ is reached in D_1 for $x_1 = n-4, x_2 = 4$ and $x_3 = ... = x_n = 1$ and it is equal to $(n-4)(n+3)+4(2n-5)+(n-2)(2n-2) = 3n^2+n-28$. Note that $(n-4, 4, 1, ..., 1)$ has a unique graphical realization which has diameter 3. If T has diameter 5, let u, v be two diametral vertices of T and u, x, w, t, y, v be a shortest path between them. It follows that $ecc(u) = ecc(v) = 5, ecc(x) \geq 4, ecc(y) \geq 4$ and $d(x), d(y) \geq 2$. This implies that $D'(u) \geq d(u)(2n+4-d(u))$ and the difference $d(u)(2n+4-d(u)) - d(u)(2n-1-d(u)) = 5d(u) \geq 5$. In a similar way we get $D'(x) \geq d(x)(2n+1-d(x))$ and $d(x)(2n+1-d(x))-d(x)(2n-1-d(x)) = 2d(x) \geq 4$. It follows that we can write $D'(T) \geq 3n^2+n-28+2(5+4) = 3n^2+n-10 > 3n^2+n-20$ for every n.
By considering a diametral path of T it can be seen that the inequality $D'(T) \geq \min_{x_1+...+x_n=2n-2} S_{2n-2,2n-1,n-4}(x_1, ..., x_n) + 18$ also holds if $diam(T) > 5$, which concludes the proof. ∎

Note that the conclusions of Lemmas 3.1.6 and 3.1.7 can also be deduced after some calculations, from the characterization of trees with a fixed order and diameter which minimizes Wiener index [25, 30].

3.1.2 Ordering Unicyclic Graphs Having Small Degree Distances

In this section we shall prove that the fourth graph in this sequence of unicyclic graphs is $H_{n,4}$ (which was also denoted by F in [37]) for $n \geq 15$.

Lemma 3.1.8. *Let G be a unicyclic connected graph of order $n \geq 7$ and $diam(G) = 3$ such that $d(x) \leq n-3$ for any $x \in V(G)$. Let p be the number of vertices x of G having $ecc(x) = 2$. Then $2 \leq p \leq 3$.*

Proof. Since $n \geq 7$ it follows that $g(G) \in \{3, 4, 5\}$ and G belongs to one of the following families of graphs: $H(n, 3; \alpha, \beta, \gamma)$, where $\alpha, \beta, \gamma \geq 1$ and $\alpha + \beta + \gamma = n - 3$; $H(n, 3; \alpha, \beta, 0)$ with $\alpha, \beta \geq 2$; $H(n, 4; \alpha, \beta, 0, 0)$, where $\alpha, \beta \geq 1$; $H(n, 5; n - 5, 0, 0, 0, 0)$; $H(n, 5; \alpha, \beta, 0, 0, 0)$ with $\alpha, \beta \geq 1$ and $H_{n-\alpha,3}$, where a pendant vertex is adjacent to new $\alpha \geq 2$ pendant vertices.
One can easily verify that in all cases we have $2 \leq p \leq 3$. ∎

In this section, we will prove that all connected unicyclic graphs G of order n having $D'(G) \leq 3n^2 + 2n - 24$ are graphs $K_{1,n-1} + e$, G_2, G_6 from Figure 2.1 and $H_{n,4}$ for $n \geq 15$.
For this we shall consider the cases when $diam(G) = 2, 3, 4$ or $diam(G) \geq 5$.
The following property is obvious: If $diam(G) = 2$ and $n \geq 6$ then the unique unicyclic graph of order n is $K_{1,n-1} + e$.

Lemma 3.1.9. *The set of unicyclic connected graphs G of order $n \geq 15$, diameter 3 and $D'(G) \leq 3n^2 + 2n - 24$ contains only 3 members: G_2, G_6 and $H_{n,4}$.*

Proof. Let G be a connected unicyclic graph of order n and diameter $diam(G) = 3$. It follows that the number of edges of G is equal to n and $d(x) \leq n - 2$ for every $x \in V(G)$. Suppose that there is a vertex x such that $d(x) = n-2$. Then there exist a vertex w which is not adjacent to x and two edges which are not incident to x. Since $diam(G) = 3$ we have only three possibilities to build such a graph, yielding graphs G_2, G_6 and $H_{n,4}$, when w is adjacent to two vertices which are adjacent to x. By Lemma 3.1.3 we have $D'(G_2), D'(G_6), D'(H_{n,4}) \leq 3n^2+2n-24$ for every $n \geq 8$. Suppose that $d(x) \leq n-3$ for every vertex $x \in V(G)$. In this case we shall prove that $D'(G) > 3n^2+2n-24$ for $n \geq 15$. By Lemma 3.1.8 the number p of the vertices x of G having $ecc(x) = 2$ is equal to 2 or to 3. The number of vertices y of eccentricity $ecc(y) = 3$ will be equal to $n-p$ and by Lemma 1.10.3 we deduce that

$$D'(G) \geq \sum_{i=1}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-1-y_j),$$

where $x_1, ..., x_p$ and $y_1, ..., y_{n-p}$ are the degrees of vertices of eccentricity 2 and 3, respectively. Since G has n edges we obtain $\sum_{i=1}^{p} x_i + \sum_{j=1}^{n-p} y_j = 2n$. From the hypothesis it also follows that $1 \leq x_i, y_j \leq n-3$ for $1 \leq i \leq p$ and $1 \leq j \leq n-p$. We can write

$\sum_{i=1}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-1-y_j)$

$= \sum_{i=1}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-2-y_j) + \sum_{j=1}^{n-p} y_j$

$\geq \sum_{i=1}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-2-y_j) + n-p.$

By redenoting the degrees $y_1 = x_{p+1}, ..., y_{n-p} = x_n$, we get $D'(G) \geq \sum_{i=1}^{n} x_i(2n-2-x_i) + n-p$, where $1 \leq x_i \leq n-3$ for $1 \leq i \leq n$ and $\sum_{i=1}^{n} x_i = 2n$, or $D'(G) \geq S_{2n,2n-2,n-3}(x_1, \ldots, x_n) + n-3$ since $p \leq 3$. By Lemma 1.10.1 we deduce that the minimum of $S_{2n,2n-2,n-3}$ in D_1 is reached for $(n-3, 5, 1, ..., 1)$. But this sequence of degrees is not graphical. From Lemma 2.1.2 it follows that the next minimum of this function is reached for $(n-4, 6, 1, ..., 1)$ or for $(n-3, 4, 2, 1, ..., 1)$. We have $S_{2n,2n-2,n-3}(n-4, 6, 1, ..., 1) = 3n^2+3n-50 > S_{2n,2n-2,n-3}(n-3, 4, 2, 1, ..., 1) = 3n^2+n-26$ for every $n \geq 13$. We get $3n^2+3n-50+n-3 = 3n^2+4n-53 > 3n^2+2n-24$ for every $n \geq 15$, hence by Corollary 3.0.9 it is necessary to consider only values of $S_{2n,2n-2,n-3}(x_1, \ldots, x_n)$ for $(x_1, \ldots, x_n) \in D_1$ having the property $x_1 = n-3$. Denote by $D_{1,n-3} = \{(x_1, \ldots, x_n) : x_1, \ldots, x_n \in \mathbb{N}, x_1 \geq \ldots \geq x_n \geq 1, 1 \leq x_i \leq n-3$ for $1 \leq i \leq n, \sum_{i=1}^{n} x_i = 2n$ and $x_1 = n-3\}$.

$S_{2n,2n-2,n-3}$ has a unique minimum in $D_{1,n-3} \setminus \{(n-3, 5, 1, \ldots, 1)\}$ for $(n-$

$3, 4, 2, 1, \ldots, 1)$. The sequence $(n-3, 4, 2, 1, \ldots, 1)$ has a unique graphical realization, $H(n, 3; n-5, 2, 0)$ and $D'(H(n, 3; n-5, 2, 0)) = 3n^2 + 5n - 46 > 3n^2 + 2n - 24$ for $n \geq 8$.

The minimum of $S_{2n,2n-2,n-3}$ in $D_{1,n-3} \backslash \{(n-3, 5, 1, \ldots, 1), (n-3, 4, 2, 1, \ldots, 1)\}$ is realized for $(n-3, 3, 3, 1, \ldots, 1)$, which has a unique graphical realization, namely $H(n, 3; n-5, 1, 1)$ for which $D'(H(n, 3; n-5, 1, 1)) = 3n^2 + 5n - 42 > 3n^2 + 2n - 24$ for $n \geq 7$.

Similarly, in $D_{1,n-3} \backslash \{(n-3, 5, 1, \ldots, 1), (n-3, 4, 2, 1, \ldots, 1), (n-3, 3, 3, 1, \ldots, 1)\}$ the minimum of $S_{2n,2n-2,n-3}$ is realized for $(n-3, 3, 2, 2, 1, \ldots, 1)$, which has two graphical realizations, $H(n, 4; n-5, 1, 0, 0)$, of diameter equal to 3 and another graph of diameter equal to 4. We also have $D'(H(n, 4; n-5, 1, 0, 0)) = 3n^2 + 6n - 44 > 3n^2 + 2n - 24$ for $n \geq 6$.

Finally, in $D_{1,n-3} \backslash \{(n-3, 5, 1, \ldots, 1), (n-3, 4, 2, 1, \ldots, 1), (n-3, 3, 3, 1, \ldots, 1), (n-3, 3, 2, 2, 1, \ldots, 1)\}$ we get a unique minimum for $(x_1, \ldots, x_n) = (n-3, 2, 2, 2, 2, 1, \ldots, 1)$ (having a unique realization $H(n, 5; n-5, 0, 0, 0, 0)$).

But $S_{2n,2n-2,n-3}(n-3, 2, 2, 2, 2, 1, \ldots, 1) = 3n^2 + n - 20$. It follows that $D'(G) \geq 3n^2 + n - 20 + n - 3 = 3n^2 + 2n - 23 > 3n^2 + 2n - 24$ for any $n \in \mathbb{N}$. ∎

Lemma 3.1.10. *Let G be a unicyclic connected graph of order $n \geq 7$ having $diam(G) = 4$. Then $D'(G) > 3n^2 + 2n - 24$.*

Proof. Suppose G is a unicyclic connected graph of diameter 4 and order $n \geq 7$. It follows that $d(x) \leq n - 3$ for every $x \in V(G)$. By Lemma 1.10.3 we deduce $D'(G) \geq \sum_{ecc(x)=2} d(x)(2n-2-d(x)) + \sum_{ecc(y)=3} d(y)(2n-1-d(y)) + \sum_{ecc(z)=4} d(z)(2n+1-d(z))$, where $\sum_{x \in V(G)} d(x) = 2n$.

Let u, a, t, b, v be a shortest path of length 4 between two vertices of eccentricity 4. It follows that $ecc(a), ecc(b) \geq 3$ and $d(a), d(b) \geq 2$. By denoting by p the number of vertices of eccentricity 2 it follows that $n \geq p + 4$. Also $d(z)(2n+1-d(z)) =$

$d(z)(2n-1-d(z))+2d(z) \geq d(z)(2n-1-d(z))+2$, which implies

$$D'(G) \geq \sum_{i=1}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-1-y_j) + 4, \tag{3.1}$$

where $\sum_{i=1}^{p} x_i + \sum_{j=1}^{n-p} y_j = 2n, 1 \leq x_i \leq n-3, 1 \leq y_j \leq n-3$. If a vertex u has $ecc(u) = 2$ and $d(u) = 1$ it follows that the vertex v which is adjacent to u has $d(v) = n-1$, which implies $diam(G) = 2$, which contradicts the hypothesis. Consequently, we have $2 \leq x_i \leq n-3$ for every $1 \leq i \leq p$. We deduced that $D'(G) \geq F(x_1, \ldots, x_p, y_1, \ldots, y_{n-p}) + 4$. By Lemma 2.1.3 for $p \geq 5$ we get that the minimum of $F(x_1, \ldots, x_p, y_1, \ldots, y_{n-p})$ is reached for $x_1 = n-p+2, x_2 = \ldots = x_p = 2, y_1 = \ldots = y_{n-p} = 1$, which implies
$D'(G) \geq (n-p+2)(n+p-4)+(2p-2)(2n-4)+(n-p)(2n-2)+4 = 3n^2+2np-8n-p^2+4$ and $3n^2+2np-8n-p^2+4 > 3n^2+2n-24$ is equivalent to $n(2p-10) > p^2-28$. This inequality is verified for $p = 5$ and for $p \geq 6$, using the inequality $n \geq p+4$ we deduce that $n(2p-10) \geq (p+4)(2p-10) = 2p^2-2p-40 > p^2-28$ for any $p \geq 5$. It remains to consider the case $0 \leq p \leq 4$. From (1) we get
$D'(G) \geq \sum_{i=1}^{p} x_i(2n-2-x_i) + \sum_{j=1}^{n-p} y_j(2n-2-y_j) + \sum_{j=1}^{n-p} y_j + 4 \geq \sum_{i=1}^{n} x_i(2n-2-x_i) + n-p+4$, by redenoting $y_1 = x_{p+1}, \ldots, y_{n-p} = x_n$. Since $n-p+4 \geq n$ we get $D'(G) \geq S_{2n,2n-2,n-3}(x_1, \ldots, x_n)+n$. Now the proof is similar to the case when $diam(G) = 3$, since $S_{2n,2n-2,n-3}(n-3,3,3,1,\ldots,1)+n = 3n^2+2n-24$, but the sequence $(n-3,3,3,1,\ldots,1)$ has a unique graphical realization of diameter equal to 3. Finally, $S_{2n,2n-2,n-3}(n-3,3,2,2,1,\ldots,1)+n = 3n^2+2n-22 > 3n^2+2n-24$. ∎

Lemma 3.1.11. *Let G be a unicyclic connected graph of order $n \geq 10$ and diameter $diam(G) \geq 5$. Then $D'(G) > 3n^2+2n-24$.*

Proof. If G is a graph satisfying the requirements of the statement then for every $x \in V(G)$ we have $ecc(x) \geq 3$ since otherwise, by the triangle inequality, we deduce $diam(G) \leq 4$. The same conclusion holds if there exists a vertex x having $d(x) \geq$

$n-3$. It follows that $d(x) \leq n-4$ for every $x \in V(G)$. By Lemma 1.10.3 we obtain that $D'(G) > \sum_{x\in V(G)} d(x)(2n-1-d(x))$, where $\sum_{x\in V(G)} d(x) = 2n$, or $D'(G) > S_{2n,2n-1,n-4}(x_1,\ldots,x_n)$.

By Lemma 1.10.1 it follows that the minimum of $S_{2n,2n-1,n-4}$ is reached in D_1 for $x_1 = n-4, x_2 = 6$ and $x_3 = \ldots = x_n = 1$ and is equal to $(n-4)(n+3)+6(2n-7)+(n-2)(2n-2) = 3n^2+5n-50 > 3n^2+2n-24$ for any $n \geq 9$. ∎

Chapter 4

Bounds for Degree Distance of a Graph

In this chapter, lower and upper bounds on degree distance index of connected simple graphs are obtained in terms of different graphical parameters like first Zagreb index, order, size, diameter, radius, minimum degree, and graphs for which these bounds are attained are characterized.

4.1 Upper Bounds on Degree Distance

In this section, we establish results that give us upper bounds for degree distance of graph G in terms of several graphical parameters mentioned above.

Lemma 4.1.1. *Let G be a connected graph of order n and $x \in V(G)$ such that $ecc(x) = p$. Then:*

$$D'(x) \geq d(x)(2n - d(x) + \frac{p^2 - 3p}{2} - 1); \quad (4.1)$$

$$D'(x) \leq d(x)(d(x) + p(n - d(x)) - \frac{p^2 - p}{2} - 1). \quad (4.2)$$

Equality holds in (4.1) if and only if:

$p = 1$ or $p = 2$ or $p \geq 3$ and $|N_3(x)| = \ldots = |N_p(x)| = 1$.

Equality holds in (4.2) if and only if: $p = 1$ *or* $p = 2$ *or* $p \geq 3$ *and* $|N_2(x)| = \ldots = |N_{p-1}(x)| = 1$.

Proof. For $p = 1$ and $p = 2$ we have $D'(x) = (n-1)^2$ and $D'(x) = d(x)(2n - 2 - d(x))$, respectively, and both (4.1) and (4.2) are equalities.
Let $p \geq 3$. The minimum value of $D'(x)$ is reached only for $|N_2(x)| = n - d(x) - p + 1$ and $|N_i(x)| = 1$ for every $3 \leq i \leq p$, thus giving $D'(x) \geq d(x)(d(x) + 2(n - d(x) - p + 1) + 3 + 4 + \ldots + p) = d(x)(2n - d(x) + \frac{p^2-3p}{2} - 1)$.
The maximum value is attained only for $|N_p(x)| = n - d(x) - p + 1$ and $|N_i(x)| = 1$ for every $2 \leq i \leq p - 1$.
In this case $D'(x) = d(x)(d(x) + 2 + 3 + \ldots + (p-1) + p(n - p - d(x) + 1)) = d(x)(d(x) + p(n - d(x)) - \frac{p^2-p}{2} - 1)$. ∎

Note that inequality (4.1) was used in [41, 37]. Since in a shortest path of length $ecc(x)$ starting from x there are $ecc(x)+1$ vertices, it follows that $ecc(x)+1+d(x)-1 \leq n$, or

$$ecc(x) + d(x) \leq n \tag{4.3}$$

holds for every vertex $x \in V(G)$. We need the following result.

Lemma 4.1.2. *For any connected graph* G *of order* n*, we have*

$$diam(G) + \Delta(G) \leq n + 1. \tag{4.4}$$

Proof. Let $x \in V(G)$ such that $\Delta(G) = d(x)$. Let $diam(G) = d$ so there exists at least one diametral path P in G of length d. We have the following three possibilities for x:

(a) x is an end of P.

(b) x lies on P but is not an end.

(c) x does not lie on P.

(a) When x is an end of the diametral path P, then $ecc(x) = d$ and since in a shortest path of length d starting from x there are $d + 1$ vertices, it follows that

$d+1+\Delta(G)-1 \le n$ or $d+\Delta(G) \le n$. So we are done in this case.
(b) In this case x lies on P but is not an end of P, so x is adjacent to exactly two vertices on P as otherwise diameter d will decrease, so $\Delta(G) \le n-(d+1)+2$, or $\Delta(G)+d \le n+1$, as desired.
(c) When x does not lie on P then it can only be adjacent to at most 3 (consecutive) vertices on P, so $\Delta(G) \le n-(d+1-3)-1$, or $\Delta(G)+d \le n+1$. ∎

Theorem 4.1.3. *Let G be a connected graph of order n, size m and diameter equal to d. We have*

$$D'(G) \le (1-d)Zg(G)+2mnd-(d^2-d+2)m. \tag{4.5}$$

Equality holds if and only if G is K_n or a graph of diameter 2.

Proof. Denote

$$\varphi(z) = -\frac{z^2}{2}+z(n-d(x)+\frac{1}{2})-1. \tag{4.6}$$

This function is strictly increasing for $z \in [1, n-d(x)+\frac{1}{2}]$. For integer values of z it takes two equal maximum values for $z=n-d(x)$ and $z=n-d(x)+1$. Lemma 4.1.2 implies that for every vertex x we have $d+d(x) \le d+\Delta(G) \le n+1$, or $d \le n-d(x)+1$ for all $x \in V(G)$. Since $ecc(x) \le d$ for every $x \in V(G)$ this gives us $\varphi(ecc(x)) \le \varphi(d)$ for every vertex $x \in V(G)$.
From (4.2) we get

$$D'(x) \le d(x)(d(x)+d(n-d(x))-\frac{d^2-d}{2}-1). \tag{4.7}$$

Finally, from (4.7) we deduce

$$D'(G) = \sum_{x\in V(G)} D'(x) \le \sum_{x\in V(G)} d^2(x)(1-d)+\sum_{x\in V(G)} d(x)(nd-\frac{d^2-d}{2}-1),$$

which implies (4.5) since $\sum_{x\in V(G)} d(x) = 2m$. Suppose that equality holds in (4.5). Since (4.7) is an equality for every $x \in V(G)$ it follows that vertices of G have equal eccentricities $ecc(x)=d$ and by Lemma 4.1.1, if $d \ge 3$ then $|N_2(x)| = \ldots =$

$|N_{d-1}(x)| = 1$ for every $x \in V(G)$.

If $d \geq 4$ consider a shortest path $x_1, x_2, \ldots, x_5$ in G. In this case $d(x_3, x_1) = d(x_3, x_5) = 2$, hence $|N_2(x_3)| \geq 2$, a contradiction. It follows that $1 \leq d \leq 3$. Suppose that $d = 3$ and let x_1, x_2, x_3, x_4 be a shortest path of length 3 in G.

Since $N_2(x_1) = \{x_3\}$, it follows that $ecc(x_2) = 2$, a contradiction. The remaining cases are $d = 1$, when G is K_n or $d = 2$, when G is a graph of diameter 2.

If $d =$ 1 or 2 (4.7) is an equality for every $x \in V(G)$, which implies that (4.5) is also an equality. ∎

Corollary 4.1.4. *Let G be a connected graph of order n, size m and diameter d. Then*

$$D'(G) \leq 2mnd - (d-1)\frac{4m^2}{n} - (d^2 - d + 2)m. \tag{4.8}$$

Equality holds if and only if G is K_n or a regular graph of diameter 2.

Proof. Since (4.5) holds, by the Cauchy- Schwarz inequality we have $nZg(G) = n\sum_{x \in V(G)} d^2(x) \geq 4m^2$, *i.e.*, $Zg(G) \geq \frac{4m^2}{n}$. Since $1 - d \leq 0$ this implies $(1 - d)Zg(G) \leq (1-d)\frac{4m^2}{n}$ and (4.8) is proved.

Suppose that equality holds in (4.8). In this case the equality in Cauchy- Schwarz inequality holds if and only if G is regular. But from Theorem 4.1.3 G is K_n, which is regular, or a graph of diameter 2 which must be also regular. ∎

Theorem 4.1.5. *If G is a connected graph of order n, size m and minimum degree $\delta(G) = \delta$, then*

$$D'(G) \leq m(n^2 + n + 2) + n\delta(\frac{\delta^2}{2} - n\delta + \frac{\delta}{2}). \tag{4.9}$$

Equality holds if and only if G is K_n or n is even and G is deduced from K_n by deleting the edges of a perfect matching.

Proof. The maximum value of $\varphi(z)$ defined by (4.6) for integer values of z is equal to

$$\varphi(n - d(x)) = \frac{n^2}{2} + \frac{n}{2} - 1 + \frac{d^2(x)}{2} - nd(x) - \frac{d(x)}{2}.$$

From (4.2) and (4.3) we get

$$D'(x) \leq d(x)(\frac{n^2}{2} + \frac{n}{2} - 1 + \frac{d^2(x)}{2} - nd(x) + \frac{d(x)}{2}). \tag{4.10}$$

Since the function

$$\psi(z) = \frac{z^3}{2} - z^2(n - \frac{1}{2})$$

is strictly decreasing for $z \in [1, n-1]$, it follows that

$$d(x)(\frac{d^2(x)}{2} - nd(x) + \frac{d(x)}{2}) \leq \delta(\frac{\delta^2}{2} - n\delta + \frac{\delta}{2})$$

for every $x \in V(G)$. Finally, from (4.10) we deduce

$$D'(G) = \sum D'(x) \leq (\frac{n^2}{2} + \frac{n}{2} - 1) \sum_{x \in V(G)} d(x) + n\delta(\frac{\delta^2}{2} - n\delta + \frac{\delta}{2})$$

$$= m(n^2 + n - 2) + n\delta(\frac{\delta^2}{2} - n\delta + \frac{\delta}{2}).$$

Suppose that equality holds in (4.9). In this case $d(x) = \delta$ for every $x \in V(G)$ i.e., G is δ-regular and $ecc(x) = n - d(x)$, or $ecc(x) + d(x) = n$ for every vertex $x \in V(G)$. It follows that vertices of G have equal eccentricities $ecc(x) = p = n - \delta$ and by Lemma 4.1.1 if $p \geq 3$ then $|N_2(x)| = \ldots = |N_{p-1}(x)| = 1$ for every $x \in V(G)$.
If $p \geq 4$ consider a shortest path $x_1, x_2, \ldots, x_5$ in G. In this case $d(x_3, x_1) = d(x_3, x_5) = 2$, hence $|N_2(x_3)| \geq 2$, a contradiction. It follows that $1 \leq p \leq 3$. Suppose that $p = 3$ and let x_1, x_2, x_3, x_4 be a shortest path of length 3 in G.
Since $N_2(x_1) = \{x_3\}$ it follows that $ecc(x_2) = 2 < p$, a contradiction. The remaining cases are $p = 1$, when G is K_n or $p = 2$. In the last case it follows that $d(x) = n - 2$ for every $x \in V(G)$, which implies that n is even and G is deduced from K_n by deleting the edges of a perfect matching. ∎

If G is a connected graph of order n, size m and diameter $d = 2$, then $D'(G) = 2m(2n-2) - Zg(G)$ and Corollary 4.1.4 yields

$$D'(G) \leq 2m(2n-2) - \frac{4m^2}{n}. \tag{4.11}$$

Equality holds in (4.11) if and only if G is a regular graph.

Since almost all graphs of order n have diameter equal to 2 as $n \to \infty$ [3], the following corollary holds.

Corollary 4.1.6. *For almost all connected graphs G of order n and size m the following inequality holds as $n \to \infty$:*

$$D'(G) \leq 2m(2n-2) - \frac{4m^2}{n}.$$

4.2 Example

For complete graph K_n, there are n vertices each having degree $n-1$ and distance 1 from every other vertex, so using definition of degree distance $D'(K_n) = n(n-1)\{\underbrace{1+1+\ldots+1}_{n-1-times}\}$, which gives $D'(K_n) = n(n-1)^2$. This verifies the claim of above Theorem as $m = \frac{n(n-1)}{2}$ and $\delta(K_n) = n-1$, so the right hand side in (4.9) is $\frac{n(n-1)}{2}(n^2+n+2) + n(n-1)(\frac{(n-1)^2}{2} - n(n-1) + \frac{n-1}{2}) = n(n-1)^2$. Now look at K_{2n} after deleting the n edges of a perfect matching (say G) (as shown in Figure 1.4, where K_6 and also $K_6 - \{$edges of a perfect matching$\}$ are drawn there). So by using definition of degree distance, we get $D'(G) = 2n(2n-2)\{\underbrace{1+1+\ldots+1}_{2n-2-times}+2\}$, hence we deduce $D'(G) = 8n^2(n-1)$. The upper bound provided by Theorem 4.1.5, since the number of vertices is $2n$, $m = \frac{2n(2n-1)}{2} - n$ and $\delta(G) = 2n-2$, is also $8n^2(n-1)$. Hence upper bound given by the above Theorem is also attained by $G = K_n - \{$edges of a perfect matching$\}$.

4.3 Lower Bound on Degree Distance

In this section, we establish a result that gives us a lower bound for degree distance of a graph G in terms of order, size and its radius.

Theorem 4.3.1. *Let G be a connected graph of order n, size m and radius equal to r. We have*

$$D'(G) \geq m(2n - 2 + r^2 - r). \tag{4.12}$$

Equality holds if and only if G is K_n or n is even and G is obtained from K_n by deleting the edges of a perfect matching.

Proof. Since (4.3) holds it follows that $n - d(x) \geq ecc(x)$, and from (4.1) we deduce that $D'(x) \geq d(x)(n - 1 + (ecc(x)^2 - ecc(x))/2) \geq d(x)(n - 1 + (r^2 - r)/2)$, thus implying $D'(G) \geq m(2n - 2 + r^2 - r)$.

Suppose that equality holds in (4.12). It follows that equality holds in (4.1), or $n - d(x) = ecc(x)$ and also $ecc(x) = r$ for every $x \in V(G)$, i.e., G is regular of degree $n - r$ and has diameter equal to r. Moreover, if $r \geq 3$ then $|N_3(x)| = \ldots = |N_r(x)| = 1$ holds for every $x \in V(G)$. We also have $|N_2(x)| = n - r - d(x) + 1 = 1$ for every $x \in V(G)$. By an argument similar to that used in the proof of Theorem 4.1.3 we deduce that $r \leq 3$. If $r = 3$ let x, u_1, u_2, u_3 be a shortest path in G. It follows that $N_2(x) = \{u_2\}, N_3(x) = \{u_3\}$. As above, we get $ecc(u_1) = 2$, a contradiction.

Finally, we have $r = 1$ or $r = 2$. For $r = 1$ G is K_n and for $r = 2$ G is $(n-2)$-regular, hence n is even and G may be obtained from K_n by deleting the edges of a perfect matching. ∎

Chapter 5

Ordering Trees Having Small General Sum-Connectivity Index

The aim of this chapter is twofold. We determine the minimum value of the general sum-connectivity index:

(i) for trees of order $n \geq 3$ and diameter d, $2 \leq d \leq n-1$ and of trees of order $n \geq 5$ having p pendant vertices, $3 \leq p \leq n-2$ and the corresponding extremal trees for $-1 \leq \alpha < 0$ and

(ii) for connected multigraphs of order $n \geq 3$ and size m, $m \geq n-1$ and the corresponding extremal multigraphs for $-3 \leq \alpha < 0$. Further, for n sufficiently large and $-1 \leq \alpha < 0$, we characterize five n-vertex trees having smallest values of χ_α.

5.1 Graph Transformations

In this section we shall define some graph transformations which strictly decrease the general sum-connectivity index in the case $-1 \leq \alpha < 0$. First we need a technical lemma.

Lemma 5.1.1. *For every $-1 \leq \alpha < 0$ the function*

$$f(x) = x(x+2)^\alpha - x(x+3)^\alpha - (x+4)^\alpha$$

defined on the interval $[0,\infty)$ *is strictly increasing.*

Proof. It is necessary to show that $f'(x) > 0$ for every $x \in [0,\infty)$. By induction we easily deduce that the n-th derivative of f equals

$$f^{(n)}(x) = (\alpha)_{n-1}[(x+2)^{\alpha-n}((\alpha+1)x+2n)-(x+3)^{\alpha-n}((\alpha+1)x+3n)-(\alpha-n+1)(x+4)^{\alpha-n}],$$

where $(\alpha)_n = \alpha(\alpha-1)\dots(\alpha-n+1)$ and $(\alpha)_0 = 1$.

The function $(x+2)^\alpha - (x+3)^\alpha$ defined on $[0,\infty)$ is strictly decreasing for $\alpha < 0$ since its derivative equals $\alpha((x+2)^{\alpha-1} - (x+3)^{\alpha-1}) < 0$.

It follows that $(x+2)^{\alpha-n} - (x+3)^{\alpha-n} > (x+3)^{\alpha-n} - (x+4)^{\alpha-n}$, which implies that $\frac{f^{(n)}(x)}{(\alpha)_{n-1}} > (x(\alpha+1)+n)(x+3)^{\alpha-n} - ((\alpha+1)x+\alpha+n+1)(x+4)^{\alpha-n}$. Since $\alpha+1 \geq 0$, $\frac{f^{(n)}(x)}{(\alpha)_{n-1}} > 0$ is equivalent to

$$\left(\frac{x+3}{x+4}\right)^{\alpha-n} > \frac{(\alpha+1)x+\alpha+n+1}{(\alpha+1)x+n}.$$

There exists an index n_0 such that this inequality is true, since for a fixed $x \geq 0$ we have $\lim_{n\to\infty}(\frac{x+3}{x+4})^{\alpha-n} = \infty$ and the right-hand side tends to 1 as $n \to \infty$. We also deduce $\lim_{n\to\infty} f^{(n)}(x) = 0$ for any $n \in \mathbb{N}$. Suppose that n_0 is even. Then $(\alpha)_{n_0-1}$ is negative, which implies that $f^{(n_0)}(x) < 0$ for any $x \in [0,\infty)$. We deduce that $f^{(n_0-1)}(x)$ is strictly decreasing and since $\lim_{n\to\infty} f^{(n_0-1)}(x) = 0$ this implies that $f^{(n_0-1)}(x) > 0$ for $x \in [0,\infty)$. By induction we deduce that for any $n \leq n_0$, $f^{(n)}(x) > 0$ for odd n and $f^{(n)}(x) < 0$ for even n for any $x \in [0,\infty)$. In particular, $f'(x) > 0$. The same conclusion follows if n_0 is odd. ∎

Let u and v be two adjacent vertices of a graph G such that $N(u) = \{v, z_1, \dots, z_p\}$, $N(v) = \{u, w_1, \dots, w_s\}$, where $\{z_1, \dots, z_p\} \cap \{w_1, \dots, w_s\} = \emptyset$, $p \geq 0$ and $s \geq 1$. We define a graph denoted by $t_1(G)$ by removing edges $vw_1, vw_2, \dots, vw_s$ and adding new edges $uw_1, uw_2, \dots, uw_s$. We say that $t_1(G)$ is a t_1- transform of G (see Fig. 5.1).

Lemma 5.1.2. *[14] For a graph* G *denote* $G' = t_1(G)$. *If* $\alpha < 0$ *then* $\chi_\alpha(G') < \chi_\alpha(G)$ *and if* $\alpha > 0$ *then the inequality is reversed.*

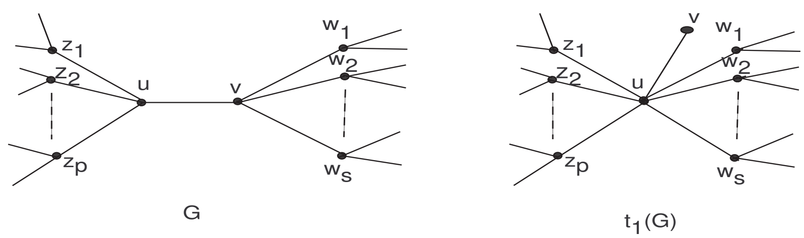


Figure 5.1: t_1- transform applied to G at vertex v

Proof. We have $d_{G'}(u) = d_G(u) + s > d_G(u)$ and $d_{G'}(u) + d_{G'}(v) = d_G(u) + d_G(v) = p + s + 2$. Since $\alpha < 0$ we get
$\chi_\alpha(G') - \chi_\alpha(G) = \sum_{i=1}^{p}[(d_G(z_i) + d_G(u) + s)^\alpha - (d_G(z_i) + d_G(u))^\alpha] + \sum_{i=1}^{s}[(d_G(w_i) + d_G(u) + s)^\alpha - (d_G(w_i) + s + 1)^\alpha] < 0$, since $\alpha < 0$ and the degrees of the vertices $z_1, \ldots, z_p, w_1, \ldots, w_s$ remain unchanged. ∎

Other transformations are described below.

Lemma 5.1.3. *For trees G and G' from Fig. 5.2, where $d_G(w,t) \geq 1$ we have $\chi_\alpha(G) > \chi_\alpha(G')$ for any p, q, $r \geq 1$ and $-1 \leq \alpha < 0$.*

Proof. It is easily seen that:
$\chi_\alpha(G) - \chi_\alpha(G') = p(p+2)^\alpha + r(r+3)^\alpha + (r+q+3)^\alpha - (p+r)(p+r+2)^\alpha - (q+3)^\alpha = r(r+3)^\alpha + F(p) + G(q)$, where $F(p) = p(p+2)^\alpha - (p+r)(p+r+2)^\alpha$ and $G(q) = (r+q+3)^\alpha - (q+3)^\alpha$.
We obtain $F'(p) = (p+2+p\alpha)(p+2)^{\alpha-1} - (p+r+\alpha(p+r)+2)(p+r+2)^{\alpha-1} =$

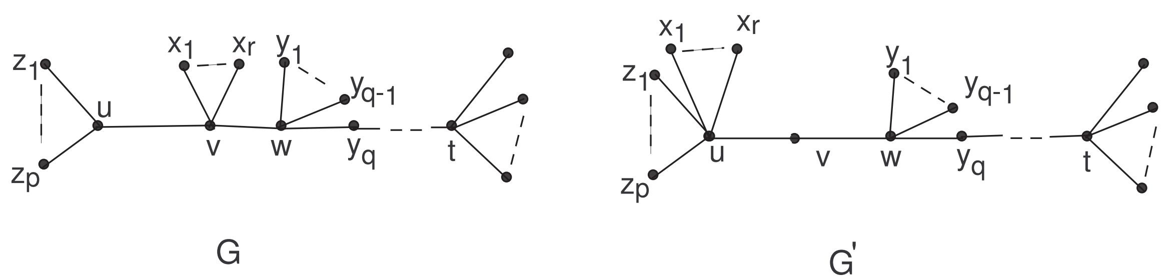


Figure 5.2: Swaping pendant edges at one end of a diametral path of G

$g(p) - g(p+r)$, by denoting $g(x) = (x + \alpha x + 2)(x+2)^{\alpha-1}$.
Also $g'(x) = \alpha(x+2)^{\alpha-2}(x(\alpha+1)+4) < 0$ for every $x > 0$ and $-1 \le \alpha < 0$. It follows that $F'(p) > 0$, which implies that $F(p)$ is strictly increasing. Since $G'(q) = \alpha[(r+q+3)^{\alpha-1} - (q+3)^{\alpha-1}] > 0$ for $\alpha < 0$ we get that $G(q)$ is also strictly increasing.
We can write $\chi_\alpha(G) - \chi_\alpha(G') \ge r(r+3)^\alpha + F(1) + G(1) = (r+4)^\alpha - (r+3)^\alpha + 3^\alpha - 4^\alpha$. Consider the function $h(x) = (x+4)^\alpha - (x+3)^\alpha$. We get $h'(x) = \alpha[(x+4)^{\alpha-1} - (x+3)^{\alpha-1}] > 0$, which implies $h(r) \ge h(1) = 5^\alpha - 4^\alpha$ for $x \ge 1$.
It remains to show that $5^\alpha + 3^\alpha > 2 \cdot 4^\alpha$. This inequality can be deduced by Jensen's inequality since the function x^α is strictly convex for $-1 \le \alpha < 0$. ∎

Lemma 5.1.4. *Consider two trees G and G' from Fig. 5.3, where $d_G(u,v) = d_{G'}(u,v) \ge 2$ and $d_G(w,t) = d_{G'}(w,t) \ge 0$. If $p,q,r \ge 1$ and $-1 \le \alpha < 0$ then $\chi_\alpha(G) > \chi_\alpha(G')$.*

Proof. As for the previous lemma we get:
$\chi_\alpha(G) - \chi_\alpha(G') = p(p+2)^\alpha + (p+3)^\alpha + r(r+3)^\alpha + (r+4)^\alpha + (r+q+3)^\alpha - (p+r)(p+r+2)^\alpha - (p+r+3)^\alpha - (q+3)^\alpha - 4^\alpha$.
By denoting $f(p) = (p+3)^\alpha - (p+r+3)^\alpha + p(p+2)^\alpha - (p+r)(p+r+2)^\alpha$ and $g(q) = (r+q+3)^\alpha - (q+3)^\alpha$, it follows that

$$\chi_\alpha(G) - \chi_\alpha(G') = f(p) + g(q) + (r+4)^\alpha + r(r+3)^\alpha - 4^\alpha. \qquad (5.1)$$

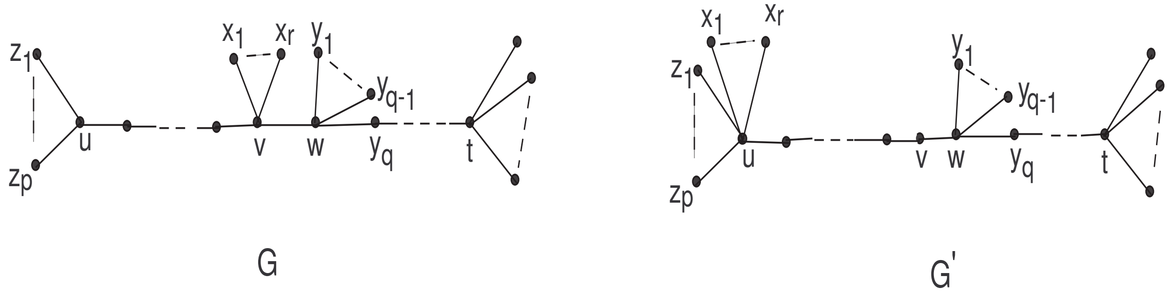


Figure 5.3: Swaping pendant edges at one end of a diametral path of G

Since $g'(q) > 0$ for any $-1 \leq \alpha < 0$ we can write $g(q) \geq g(1) = (r+4)^\alpha - 4^\alpha$. For $f(p)$ we get $f'(p) = h(p) - h(p+r)$ by denoting $h(p) = \alpha(p+3)^{\alpha-1} + (p+2)^\alpha + \alpha p(p+2)^{\alpha-1}$. We obtain $h'(p) = \alpha[(\alpha-1)(p+3)^{\alpha-2} + (4+(\alpha+1)p)(p+2)^{\alpha-2}]$. The expression $(\alpha-1)(p+3)^{\alpha-2} + (4+(\alpha+1)p)(p+2)^{\alpha-2} \geq (\alpha-1)(p+3)^{\alpha-2} + 4(p+3)^{\alpha-2} = (\alpha+3)(p+3)^{\alpha-2} > 0$, thus implying $h'(p) < 0$. We have deduced $f'(p) > 0$, hence $f(p) \geq f(1) = 4^\alpha - (r+4)^\alpha + 3^\alpha - (r+1)(r+3)^\alpha$.
From (5.1) we can write

$$\chi_\alpha(G) - \chi_\alpha(G') \geq (r+4)^\alpha - (r+3)^\alpha + 3^\alpha - 4^\alpha > 0$$

since $r \geq 1$ function $(r+4)^\alpha - (r+3)^\alpha$ is strictly increasing for $r \geq 0$ and $\alpha \geq -1$.
■

Lemma 5.1.5. *Let G and G' be trees from Fig. 5.4, where $d_G(u,v) \geq 1$. If $-1 \leq \alpha < 0$ and $p \geq q \geq 2$ then $\chi_\alpha(G) > \chi_\alpha(G')$.*

Proof. If $d_G(u,v) = 1$ then $d_{G'}(u) + d_{G'}(v) = d_G(u) + d_G(v) = p+q+2$, and $\chi_\alpha(G) - \chi_\alpha(G') = p(p+2)^\alpha + q(q+2)^\alpha - (p+1)(p+3)^\alpha - (q-1)(q+1)^\alpha$.
By denoting $p = q+r$, where $r \geq 0$, it is necessary to prove that

$$(q+r)(q+r+2)^\alpha - (q+r+1)(q+r+3)^\alpha + q(q+2)^\alpha - (q-1)(q+1)^\alpha > 0, \quad (5.2)$$

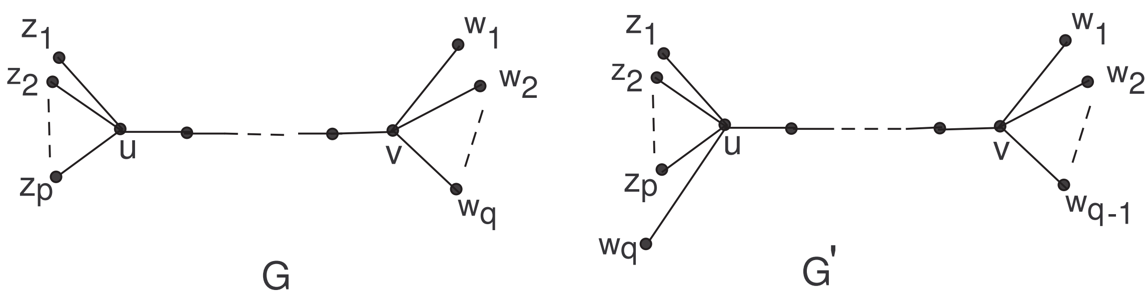


Figure 5.4: Swaping a pendant edge between ends of a diametral path.

or $g(q) > g(q+r+1)$, where $g(q) = q(q+2)^{\alpha} - (q-1)(q+1)^{\alpha}$.

We deduce $g'(q) = (q+2+\alpha q)(q+2)^{\alpha-1} - (q+1+\alpha(q-1))(q+1)^{\alpha-1} = h(q) - h(q-1)$, where $h(q) = (q+2+\alpha q)(q+2)^{\alpha-1}$.

Finally, $h'(q) = (4\alpha + \alpha(1+\alpha)q)(q+2)^{\alpha-2} < 0$ since $-1 \leq \alpha < 0$.

Consequently, $h(q) - h(q-1) < 0$, which implies $g'(q) < 0$. Since g' is strictly decreasing we have $g(q) > g(q+r+1)$ and (5.2) is proved.

If $d_G(u, v) \geq 2$ then $\chi_{\alpha}(G) - \chi_{\alpha}(G') = p(p+2)^{\alpha} - p(p+3)^{\alpha} - (p+4)^{\alpha} - (q-1)(q+1)^{\alpha} + (q-1)(q+2)^{\alpha} + (q+3)^{\alpha} = f(p) - f(q-1)$, where $f(x) = x(x+2)^{\alpha} - x(x+3)^{\alpha} - (x+4)^{\alpha}$. By Lemma 5.1.1 $f(x)$ is strictly increasing for $x \geq 0$, which implies $f(p) > f(q-1)$. ∎

5.2 Minimum Value of $\chi_{\alpha}\,(-1 \leq \alpha < 0)$ for Trees of Given Diameter

Let $d \geq 3$. We shall denote by $MS(n_1, n_2, \ldots, n_{d-1})$ where $n_1, n_{d-1} \geq 1$ and $n_i \geq 0$ for $2 \leq i \leq d-2$, the caterpillar consisting of a path $v_1, v_2, \ldots, v_{d-1}$ of length $d-2$ with n_i pendant vertices attached at v_i for $1 \leq i \leq d-1$. It has diameter equal to d. This multistar may also be obtained by joining by edges the centers of stars $K_{1,n_1}, K_{1,n_2}, \ldots, K_{1,n_{d-1}}$. Note that every tree of order n and diameter three is a bistar $MS(n_1, n_2)$ (denoted by $BS(n_1, n_2)$ in [37]), where $n_1, n_2 \geq 1$ and $n_1 + n_2 = n - 2$. Observe that $MS(n_1, n_2, \ldots, n_{d-1})$ is isomorphic to $MS(n_{d-1}, n_{d-2}, \ldots, n_1)$. The multistar with $d = n - p + 1$, $n_1 = p - 1$, $n_2 = \ldots = n_{d-2} = 0$ and $n_{d-1} = 1$ has p pendant vertices and order n and was denoted by $S_{n,p}$ in [48]. Equivalently, for every integers n, p with $2 \leq p \leq n - 1$, $S_{n,p}$ is the tree formed by attaching $p - 1$ pendant vertices to an end vertex of the path P_{n-p+1}. We have $S_{n,2} = P_n$ and $S_{n,n-1}$ is the star $K_{1,n-1}$. $S_{n,p}$ has diameter equal to $n - p + 1$.

Theorem 5.2.1. *For every $-1 \leq \alpha < 0$ in the set of trees T having order $n \geq 3$ and $diam(T) = d$ $(2 \leq d \leq n - 1)$, $\chi_\alpha(T)$ is minimum if and only if $T = S_{n,n-d+1}$.*

Proof. Using the t_1- transform in Lemma 5.1.2 at vertices not belonging to a diametral path of T, we can deduce that among n-vertex trees T with diameter d, the minimum of $\chi_\alpha(T)$ is achieved exactly in the set of multistars $MS(n_1, n_2, \ldots, n_{d-1})$. Applying transformations described in Lemmas 5.1.3-5.1.5 it follows that minimum of $\chi_\alpha(T)$ is achieved only for $n_1 = n - d$, $n_2 = n_3 = \ldots = n_{d-2} = 0$ and $n_{d-1} = 1$, *i.e.*, for $S_{n,n-d+1}$. ∎

Corollary 5.2.2. *Let $-1 \leq \alpha < 0$. (a) In the set of trees T of order n we have*

$$\min_{diam(T)=i} \chi_\alpha(T) < \min_{diam(T)=j} \chi_\alpha(T)$$

if $2 \leq i < j \leq n - 1$.
(b) In the set of trees T of order n and diameter d with $3 \leq d \leq n - 2$ the trees having smallest general sum-connectivity index $\chi_\alpha(T)$ are (in this order):
$MS(n-d, 0, \ldots, 0, 1)$, $MS(n-d-1, 0, \ldots, 0, 2)$, $\ldots$, $MS(\lceil \frac{n-d+1}{2} \rceil, 0, \ldots, 0, \lfloor \frac{n-d+1}{2} \rfloor)$.

Proof. (a) This inequality follows from Lemma 5.1.2 since $MS(n-i, 0, \ldots, 0, 1)$ can be obtained from $MS(n - j, 0, \ldots, 0, 1)$ applying several times the t_1- transform.
(b) This ordering can be deduced using Lemmas 5.1.2, 5.1.4 and then making use of Lemma 5.1.5 to multistars of order n $MS(p, 0, \ldots, 0, q)$ with $p + q = n - d + 1$. ∎

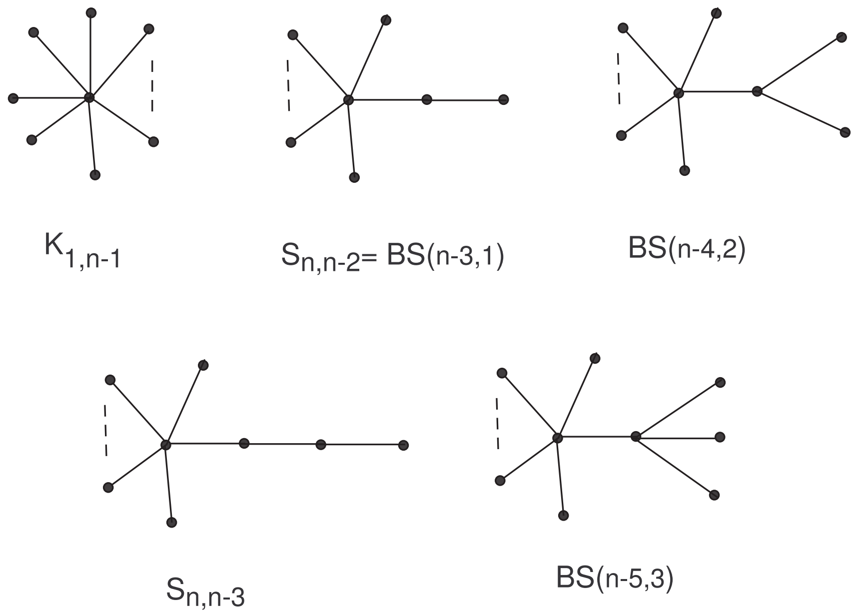


Figure 5.5: Five trees T having smallest $\chi_\alpha(T)$ for $-1 \le \alpha < 0$.

Theorem 5.2.3. *For every $-1 \le \alpha < 0$ there exists $n_0(\alpha) > 0$ such that for every $n \ge n_0(\alpha)$ the trees T having the smallest $\chi_\alpha(T)$ are $K_{1,n-1}$, $BS(n-3,1)$, $BS(n-4,2)$, $S_{n,n-3}$ and $BS(n-5,3)$ (in this order). Also we have $n_0(-1) = 16$.*

Proof. The unique tree having diameter two is the star $K_{1,n-1}$ and by Corollary 5.2.2 it reaches the minimum of χ_α. The second minimum value of χ_α is achieved for $S_{n,n-2} = BS(n-3,1)$, which minimizes this index in the set of trees of diameter three.

The next minimum values in the set of trees of diameter three are reached by $BS(n-4,2)$ (which coincides to $BS(n-3,1)$ for $n = 5$) and $BS(n-5,3)$ and the minimum value of χ_α in the set of trees of diameter four by $S_{n,n-3}$.

We get $\chi_\alpha(BS(n-4,2)) < \chi_\alpha(S_{n,n-3})$ since $BS(n-4,2)$ can be obtained from $S_{n,n-3}$ by a t_1- transform. It follows that for every $n \ge 6$ the trees having minimum values of χ_α are $K_{1,n-1}$, $BS(n-3,1)$ and $BS(n-4,2)$.

In order to obtain the fourth term in this sequence it is necessary to compare

$\chi_\alpha(BS(n-5,3))$ with $\chi_\alpha(S_{n,n-3})$. We get $\chi_\alpha(BS(n-5,3))-\chi_\alpha(S_{n,n-3}) = (n-5)(n-3)^\alpha + n^\alpha - (n-4)(n-2)^\alpha - (n-1)^\alpha + 3\cdot 5^\alpha - 4^\alpha - 3^\alpha$ and $\lim_{n\to\infty}((n-5)(n-3)^\alpha + n^\alpha - (n-4)(n-2)^\alpha - (n-1)^\alpha) = 0$ since $\alpha < 0$. We shall prove that $3\cdot 5^\alpha - 4^\alpha - 3^\alpha \geq \frac{1}{60}$.

For this consider the function $\varphi(x) = 3\cdot 5^x - 4^x - 3^x$ defined for $-1 \leq x < 0$. Since

$$\varphi^{(n)}(x) = (\ln 5)^n[3\cdot 5^x - 4^x\left(\frac{\ln 4}{\ln 5}\right)^n - 3^x\left(\frac{\ln 3}{\ln 5}\right)^n],$$

there exists an index m such that $\varphi^{(m)}(x) > 0$.

This means that $\varphi^{(m-1)}(x)$ is strictly increasing on $[-1,0)$, hence $\varphi^{(m-1)}(x) > \varphi^{(m-1)}(-1) = \frac{3}{5}(\ln 5)^{m-1} - \frac{1}{4}(\ln 4)^{m-1} - \frac{1}{3}(\ln 3)^{m-1} > (\ln 5)^{m-1}(\frac{3}{5} - \frac{1}{4} - \frac{1}{3}) > 0$. By induction it follows that $\varphi(x)$ is strictly increasing for $x \in [-1,0)$ and we deduce that $\varphi(x) \geq \varphi(-1) = \frac{3}{5} - \frac{1}{4} - \frac{1}{3} = \frac{1}{60}$. It follows that $\lim_{n\to\infty}(\chi_\alpha(BS(n-5,3)) - \chi_\alpha(S_{n,n-3})) = 3\cdot 5^\alpha - 4^\alpha - 3^\alpha \geq \frac{1}{60}$, which means that there exists $n_0(\alpha)$ such that $\chi_\alpha(BS(n-5,3)) > \chi_\alpha(S_{n,n-3}))$ for every $n \geq n_0(\alpha)$.

If $\alpha = -1$ (corresponding to the harmonic index), the difference

$$\chi_{-1}(BS(n-5,3)) - \chi_{-1}(S_{n,n-3}) = \frac{n-5}{n-3} - \frac{n-4}{n-2} - \frac{1}{n(n-1)} + \frac{1}{60}$$

is negative for $n \leq 15$ but becomes positive for $n \geq 16$.

We also have

$$\chi_\alpha(BS(n-5,3)) - \chi_\alpha(MS(n-5,0,2)) = n^\alpha - (n-2)^\alpha + 2(5^\alpha - 4^\alpha) < 0$$

for every $n \geq 3$ and $\alpha < 0$, where $MS(n-5,0,2)$ realizes the second minimum value of χ_α in the set of trees of diameter four after $S_{n,n-3}$. Using a t_1- transform it can be easily seen that the tree $MS(n-5,0,0,1)$, reaching minimum of χ_α in the set of trees of diameter five obeys $\chi_\alpha(MS(n-5,0,0,1)) > \chi_\alpha(MS(n-5,0,2))$, which concludes the proof. ■

Note that for $\alpha = -1/2$ first three trees from Fig. 5.5 having smallest χ_α index were found in [48]. Another extremal property of the tree $S_{n,p}$ is the following, which extends the corresponding property given in [48] from $\alpha = -1/2$ to $-1 \leq \alpha < 0$.

Theorem 5.2.4. *Let T be a tree with $n \geq 5$ vertices and p pendant vertices, where $3 \leq p \leq n-2$ and $-1 \leq \alpha < 0$. Then*

$$\chi_\alpha(T) \geq (p-1)(p+1)^\alpha + (p+2)^\alpha + 3^\alpha + (n-p-2)4^\alpha$$

with equality if and only if $T = S_{n,p}$.

Proof. First we shall prove that under the assumption of the theorem, if u is a pendant vertex being adjacent to v, then

$$\chi_\alpha(T) - \chi_\alpha(T-u) \geq (p-2)(p+1)^\alpha + (p+2)^\alpha - (p-2)p^\alpha$$

with equality if and only if $T = S_{n,p}$ and $d(v) = p$.

Note that $N(v) \setminus \{u\}$ contains some vertex w_0 of degree $d(w_0) \geq 2$ since otherwise T is a star with center v having $p = n-1$ pendant vertices, which contradicts the hypothesis. We obtain

$\chi_\alpha(T) - \chi_\alpha(T-u) = (d(v)+1)^\alpha - \sum\limits_{w \in N(v)\setminus\{u\}} [(d(v)+d(w)-1)^\alpha - (d(v)+d(w))^\alpha]$.

Since the function $f(x) = (x-1)^\alpha - x^\alpha$ is strictly decreasing for $x \geq 1$ and $\alpha < 0$ we have $(d(v)+d(w_0)-1)^\alpha - (d(v)+d(w_0))^\alpha \leq (d(v)+1)^\alpha - (d(v)+2)^\alpha$ and for all other $d(v)-2$ vertices $w \in N(v) \setminus \{u, w_0\}$ we deduce $(d(v)+d(w)-1)^\alpha - (d(v)+d(w))^\alpha \leq d(v)^\alpha - (d(v)+1)^\alpha$ because $d(w) \geq 1$. It follows that $\chi_\alpha(T) - \chi_\alpha(T-u) \geq (d(v)+1)^\alpha - [(d(v)+1)^\alpha - (d(v)+2)^\alpha] - (d(v)-2)[d(v)^\alpha - (d(v)+1)^\alpha] =$
$= (d(v)+2)^\alpha + (d(v)-2)(d(v)+1)^\alpha - (d(v)-2)d(v)^\alpha$.

We also have $d(v) \leq p$ since $T-v$ consists of $d(v)$ trees. Making use of Lemma 5.1.1 the function $g(x) = (x+2)^\alpha + (x-2)(x+1)^\alpha - (x-2)x^\alpha$ is strictly decreasing for $-1 \leq \alpha < 0$ and $x \geq 2$ since $-g(x)$ is strictly increasing. Since $2 \leq d(v) \leq p$ this implies

$$\chi_\alpha(T) - \chi_\alpha(T-u) \geq (p-2)(p+1)^\alpha + (p+2)^\alpha - (p-2)p^\alpha.$$

Equality holds if and only if we have $d(v) = p$, one neighbor of v has degree two, and others are pendant vertices, *i.e.*, $T = S_{n,p}$ and u is adjacent to the vertex of degree p of $S_{n,p}$.

Now the proof of the theorem follows by induction on n. For $n = 5$ we get $p = 3$ and $S_{5,3} = BS(1,2)$ from Fig. 5.5 is a single tree of order five having three pendant vertices.

Let $n \geq 6$ and suppose that the theorem is true for all trees of order $n-1$ having p pendant vertices, where $3 \leq p \leq n-3$. Let u be a pendant vertex adjacent to the vertex v. We shall consider two subcases: A. $d(v) = 2$ and B. $d(v) \geq 3$.

A. In this case the unique vertex w adjacent to v has $d(w) \geq 2$, which implies $\chi_\alpha(T) - \chi_\alpha(T-u) = (d(w)+2)^\alpha + 3^\alpha - (d(w)+1)^\alpha \geq 4^\alpha$ since the function $(x+2)^\alpha - (x+1)^\alpha$ is strictly increasing for $x \geq 0$.

Equality holds if and only if $d(w) = 2$. In this case $T-u$ has p pendant vertices. By the induction hypothesis, for $p \leq n-3$ we have $\chi_\alpha(T-u) \geq \chi_\alpha(S_{n-1,p})$ with equality if and only if $T-u = S_{n-1,p}$. In this case

$$\chi_\alpha(T) \geq \chi_\alpha(T-u) + 4^\alpha \geq \chi_\alpha(S_{n-1,p}) + 4^\alpha = \chi_\alpha(S_{n,p})$$

and equality holds if and only if $T-u = S_{n-1,p}$ and $d(v) = d(w) = 2$, *i.e.*, $T = S_{n,p}$. If $p = n-2$, $T-u$ has $n-1$ vertices, and $n-2$ pendant vertices, *i.e.*, $T-u = K_{1,n-1}$ and $T = S_{n,n-2} = S_{n,p}$.

B. If $d(v) \geq 3$ then $T-u$ has $n-1$ vertices and $p-1$ pendant vertices. Using the induction hypothesis for $T-u$ and the above property we get $\chi_\alpha(T) \geq \chi_\alpha(T-u) + (p-2)(p+1)^\alpha + (p+2)^\alpha - (p-2)p^\alpha \geq \chi_\alpha(S_{n-1,p-1}) + (p-2)(p+1)^\alpha + (p+2)^\alpha - (p-2)p^\alpha = \chi_\alpha(S_{n,p})$. Equality holds if and only if $T-u = S_{n-1,p-1}$ and $d(v) = p$, *i.e.*, $T = S_{n,p}$. ∎

5.3 Minimum Value of χ_α $(-3 \leq \alpha < 0)$ for Multigraphs

The index $\chi_\alpha(G)$ may be defined in the same way when G is a multigraph containing parallel edges.

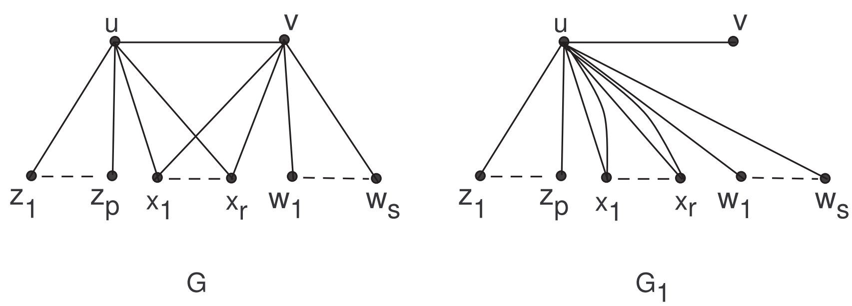


Figure 5.6: $G_1 = t_2(G)$

Theorem 5.3.1. *Let $m, n \in \mathbb{N}$ such that $n \geq 3$, $m \geq n-1$ and $-3 \leq \alpha < 0$. If G is a connected multigraph with n vertices and m edges, then*

$$\chi_\alpha(G) \geq (n-2)(m+1)^\alpha + (m-n+2)(2m-n+2)^\alpha$$

with equality if and only if G is $K_{1,n-1}$ having one edge of multiplicity $m-n+2$ and $n-2$ edges of multiplicity 1.

Proof. For any multigraph G we shall define the t_2- transform relatively to the pair $\{u, v\}$ of adjacent vertices from $V(G)$ such that $N(u) \neq \{v\}$ and $N(v) \neq \{u\}$. Suppose that $N(u) \setminus N(v) = \{v\} \cup \{z_1, \ldots, z_p\}$; $N(v) \setminus N(u) = \{u\} \cup \{w_1, \ldots, w_s\}$ and $N(u) \cap N(v) = \{x_1, \ldots, x_r\}$, where $p, r, s \geq 0$ and $p + r \geq 1$, $s + r \geq 1$.
We swap all edges $x_1 v, \ldots, x_r v, w_1 v, \ldots, w_s v$ incident to v from v to u, making them incident to u and preserving their multiplicities. If $m_G(xy)$ denotes the multiplicity of an edge xy in G, this means that in the graph $G_1 = t_2(G)$ thus obtained v is adjacent only to u and $m_{G_1}(uw_i) = m_G(vw_i)$ for every $1 \leq i \leq s$, $m_{G_1}(ux_i) = m_G(ux_i) + m_G(vx_i)$ for every $1 \leq i \leq r$.
We have $d_{G_1}(v) = m_G(uv)$, $m_{G_1}(uv) = m_G(uv)$, hence $d_{G_1}(u) + d_{G_1}(v) = d_G(u) + d_G(v)$.
This transformation is illustrated in Fig. 5.6 when G does not contain parallel edges. By this transformation only degrees of vertices u and v are changed. We can write $d_G(u) \geq m_G(uv) + p + r \geq m_G(uv) + 1$.

We deduce $d_{G_1}(u) = d_G(u) + d_G(v) - m_G(uv) \geq d_G(v) + 1$ and also $d_{G_1}(u) \geq d_G(u)$. It follows that for all edges xy, invariant or transformed, the sum of degrees increases or remains constant in G_1 and for at least one edge the increment is positive. We get $\chi_\alpha(G) > \chi_\alpha(G_1)$.

Let G be a connected multigraph of order n and size $m \geq n-1$ such that $\chi_\alpha(G)$ is minimum and let $uv \in E(G)$. If $N(u) \neq \{v\}$ and $N(v) \neq \{u\}$ we have seen that $\chi_\alpha(G)$ cannot be minimum, thus yielding $N(u) = \{v\}$ or $N(v) = \{u\}$. Suppose that $N(v) = \{u\}$; for any edge uz of G incident to u we also have $N(z) = \{u\}$. Since G is connected we obtain that G is $K_{1,n-1}$ containing some parallel edges, such that the size of G is m. Let w be the center of $K_{1,n-1}$. If there exist two vertices $u, v \neq w$ such that $m(uw) = p$, $m(vw) = q$ and $p \geq q \geq 2$, we shall prove that $\chi_\alpha(G)$ cannot be minimum. For this we shall define another graph G_2 which is obtained by transforming one parallel edge between w and v into a parallel edge between w and u, such that $d_{G_2}(u) = p+1$, $d_{G_2}(v) = q-1$ and other degrees remain unchanged. If $d(w) = p+q+s$ and $s \geq 0$ we get

$$\chi_\alpha(G_2) - \chi_\alpha(G) = (p+1)(2p+q+s+1)^\alpha + (q-1)(p+2q+s-1)^\alpha - p(2p+q+s)^\alpha - q(p+2q+s)^\alpha.$$

We shall prove that if $-3 \leq \alpha < 0$ then $\chi_\alpha(G_2) - \chi_\alpha(G) < 0$, which is equivalent to

$$(p+1)(2p+q+s+1)^\alpha - p(2p+q+s)^\alpha < q(p+2q+s)^\alpha - (q-1)(p+2q+s-1)^\alpha. \quad (5.3)$$

Consider the function $f(x) = (x+1)(x+a+1)^\alpha - x(x+a)^\alpha$, where $x > 0$ and $a > x$. We have $f'(x) = \varphi(x+1) - \varphi(x)$, where $\varphi(x) = (x+a+\alpha x)(x+a)^{\alpha-1}$. Since $-3 \leq \alpha < 0$ and $a > x$ one obtains $\varphi'(x) = \alpha(x+a)^{\alpha-2}(2a+x+\alpha x) < 0$, thus implying that φ is strictly decreasing on $(0, \infty)$, hence $f'(x) < 0$, or $f(x)$ is strictly decreasing on $(0, \infty)$.

Consequently, $f(p) < f(q-1)$ for any $a > p$ since $p > q-1$ and we can write $(p+1)(p+a+1)^\alpha - p(p+a)^\alpha < q(q+a)^\alpha - (q-1)(q-1+a)^\alpha$. Letting $a = p+q+s > p$ this inequality becomes (5.3).

Consequently, if $\chi_\alpha(G)$ is minimum then only one vertex different from w has degree equal to $m-n+2$ and other non-central vertices have degree equal to 1, whenever

$$\chi_\alpha(G) = (n-2)(m+1)^\alpha + (m-n+2)(2m-n+2)^\alpha.$$

∎

If $m = n-1$ then G is a tree and $\min \chi_\alpha(G)$ is reached if and only if G is $K_{1,n-1}$, which does not contain parallel edges. This result holds for trees in a more general setting when $\alpha < 0$ [49].

Denote by $M_{k,m}(K_{1,n-1})$ the set of multigraphs of size $m \geq n+k-1$ deduced from $K_{1,n-1}$ by considering k multiple edges and $n-1-k$ simple edges for $1 \leq k \leq n-1$. Denote also by $(d_1, \ldots, d_k, 1, \ldots, 1)$ with $d_1 \geq d_2 \geq \ldots \geq d_k \geq 2$ the vector of degrees of non-central vertices, where $\sum_{i=1}^{k} d_i = m-n+k+1$.

From this proof it follows that if $m \geq n+k-1$ then the multigraph G of order n and size m having k multiple edges and minimum general sum-connectivity index belongs to $M_{k,m}(K_{1,n-1})$, it is unique and has the vector of degrees $(m-n-k+3, \underbrace{2, \ldots, 2}_{k-1}, \underbrace{1, \ldots, 1}_{n-k-1})$. Also

$$\min_{G \in M_{k,m}(K_{1,n-1})} \chi_\alpha(G) < \min_{G \in M_{k+1,m}(K_{1,n-1})} \chi_\alpha(G) \tag{5.4}$$

holds for any $1 \leq k \leq n-2$ provided $m \geq n+k$.

Corollary 5.3.2. *Suppose that $-3 \leq \alpha < 0$. For fixed $n \geq 3$ and $m \geq n+3$, among the connected multigraphs of order n and size m the multigraphs having the minimum, the second and the third minimum general sum-connectivity index are deduced from $K_{1,n-1}$ having the vectors of degrees of non-central vertices equal to $(m-n+2, 1, \ldots, 1)$, $(m-n+1, 2, 1, \ldots, 1)$ and $(m-n, 3, 1, \ldots, 1)$, respectively.*

Proof. We have seen that $(m-n+2, 1, \ldots, 1)$ corresponds to the multigraph reaching $\min \chi_\alpha(G)$; in this case $k = 1$.

If $k = 2$ the minimum is reached for $(m-n+1, 2, 1, \ldots, 1)$ and the second minimum is achieved for $(m-n, 3, 1, \ldots, 1)$.

For $k = 3$ the minimum is reached for $(m - n, 2, 2, 1, \ldots, 1)$. The value of χ_α corresponding to this vector is greater than the value corresponding to $(m - n, 3, 1, \ldots, 1)$, as we have seen in the proof of Theorem 5.2.4. Since (5.4) holds, the conclusion follows. $\blacksquare$

Chapter 6

Comments and Open Problems

6.1 Comments

The threshold $n \geq 15$ is necessary in Theorem 3.1.2 giving the first nine connected graphs having smallest degree distances. For example, for $n = 7$ this ordering does not hold. In this case between G_4 and G_5 it is necessary to insert graphs G_7 and $H_{7,4}$(in this order) shown in Figure 6.1, where graph G_7 is a new graph containing a $3-$ cycle and two pairs of pendant vertices, each pair being adjacent to 2 different vertices of this cycle. Indeed, we have:
$D'(K_{1,6}) = 102$, $D'(BS(4,1)) = 118$, $D'(K_{1,6} + e) = 120$, $D'(BS(3,2)) = 126$, $D'(G_2) = 132$, $D'(G_3) = 134$, $D'(G_4) = 136$, $D'(G_7) = 136$, $D'(H_{7,4}) = 137$, $D'(G_5) = D'(G_6) = 138$.

6.2 Open Problems

In [14] the minimum general sum-connectivity index of unicyclic graphs was determined. Extremal graphs G have girth $g(G) = 3$. It would be interesting to find minimum general sum-connectivity index of unicyclic graphs G with given girth $g(G) = g \geq 4$. There are several well known chemical Indices in Graph theory like:

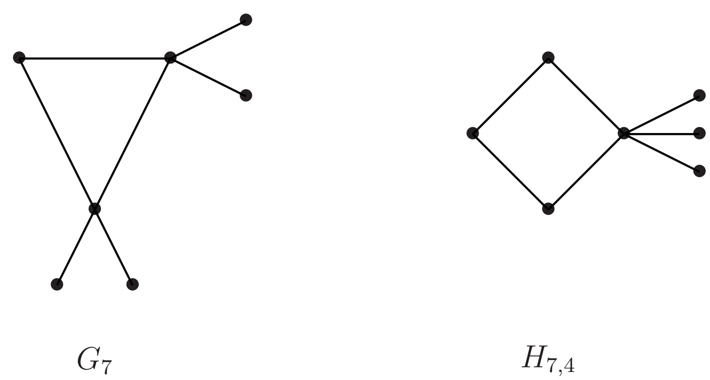


Figure 6.1: Graphs G_7 and $H_{7,4}$

1. Additive Zagreb indices
2. Multiplicative Zagreb indices
3. Harary Index
4. Estrada Index
5. Shultz Molecular Topological Index
6. Balaban's Index
7. Randić Index

So it would be interesting to give an ordering for graphs with respect to these indices (considering one family of graphs and one index at a time). No doubt Indices in Chemical graph theory is a vast subject for research and it has far reaching applications in various sciences.

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Bibliography

[1] V. K. Balakrishnan, *Schaum's Outline of Theory and Problems of Graph Theory*, Tata Mc Graw-Hill Publishing Company LTD, New Delhi, 2004.

[2] B. Bollobás, P. Erdös, Graphs of extremal weights, *Ars Combin.* **50** (1998) 225–233.

[3] B. Bollobás, *Modern Graph Theory*, Graduate Texts in Mathematics 184, Springer−Verlag New York, 1998.

[4] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, 2008.

[5] O. Bucicovski, S. M. Cioabă, The minimum degree distance of graphs of given order and size, *Discr. Appl. Math.* **156** (2008) 3518–3521.

[6] F. Buckley, F. Harary, *Distance in graphs*, Addison- Wesley, 1989.

[7] G. Chartrand, P. Zhang, *Introduction to graph theory*, Mc Graw Hill, 2005.

[8] A. Chen, *Ordering unicyclic graphs by their degree distance*, *J. of Fuzhou Univ. Nat. Sci.* **32**(2004) 664–668.

[9] P. Dankelmann, I. Gutman, S. Mukwembi, H. C. Swart, On the degree distance of a graph, *Discr. Appl. Math.* **157** (2009) 2773–2777.

[10] J. Devillers, A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach, Amsterdam, 1999.

[11] R. Diestel, *Graph Theory*, Springer-Verlag, NewYork, 2000.

[12] M. V. Diudea, I. Gutman, L. Jäntschi, *Molecular Topology*, Nova, New York, 2001.

[13] A. A. Dobrynin, A. A. Kochetova, Degree distance of a graph: a degree analogue of the Wiener index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1082–1086.

[14] Z. Du, B. Zhou, N. Trinajstić, Minimum general sum-connectivity index of unicyclic graphs, *J. Math. Chem.* **48** (2010) 697–703.

[15] Z. Du, B. Zhou, N. Trinajstić, On the general sum-connectivity index of trees, *Appl. Math. Letters* **24** (2011) 402–405.

[16] S. Fajtlowicz, On conjectures of Graffiti - II, *Congr. Numer.* **60** (1987) 187–197.

[17] R. Garcia - Domenech, J. Gálvez, J. V. de Julián - Ortiz, L. Pogliani, Some new trends in chemical graph theory, *Chem. Rev* **108** (2008) 1127–1169.

[18] I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors − Theory and Applications vols. I−II*, Univ. Kragujevac, Kragujevac, 2010.

[19] I. Gutman, B. Furtula (Eds.), *Recent Results in the Theory of Randić Index*, Univ. Kragujevac, Kragujevac, 2008.

[20] I. Gutman, Selected properties of the Schultz molecular topological index, *J. Chem. Inf. Comput. Sci.* **34** (1994) 1087–1089.

[21] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals III. Total $\pi-$ electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **17** (1972) 535–538.

[22] J. L. Gross, J. Yellen, *Graph theory and its applications*, Chapman- Hall, 2006.

[23] N. Hartsfield, *Pearls in graph theory*, Academic Press, London and New York , 1996.

[24] Y. Hou, A. Chang, The unicyclic graphs with maximum degree distance, *J. Math. Study* **39** (2006) 18–24.

[25] A. Ilić, A. Ilić, D. Stevanović, On the Wiener index and Laplacian coefficients of graphs with given diameter or radius, *MATCH Commun. Math. Comput. Chem.* **63**(2010) 91−100.

[26] A. Ilić, S. Klavžar, D. Stevanović, Calculating the degree distance of partial Hamming graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 411–424.

[27] A. Ilić, D. Stevanović, L. Feng, G. Yu, P. Dankelmann, Degree distance of unicyclic and bicyclic graphs, *Discr. Appl. Math.* **159** (2011) 779–788.

[28] L. B. Kier, L. H. Hall, *Molecular Connectivity in Structure - Activity Analysis*, Wiley, New York, 1986.

[29] S. Kanwal, I. Tomescu, Bounds for degree distance of a graph, submitted.

[30] H. Liu, X. F. Pan, On the Wiener index of trees with fixed diameter, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 85–94.

[31] B. Lučić, N. Trinajstić, B. Zhou, Comparison between the sum-connectivity index and product-connectivity index for benzenoid hydrocarbons, *Chem. Phys. Lett.* **475** (2009) 146–148.

[32] L. Pogliani, From molecular connectivity indices to semiempirical connectivity terms: recent trends in graph theoretical descriptors, *Chem. Rev.* **100** (2000) 3827–3858.

[33] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[34] H. P. Schultz, Topological organic chemistry. I. Graph theory and topological indices of alkanes, *J. Chem. Inf. Comput. Sci.* **29** (1989) 227–228.

[35] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.

[36] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley-VCH, Weinheim, 2009.

[37] I. Tomescu, S. Kanwal, Ordering connected graphs having small degree distances II., *MATCH Commun. Math. Comput. Chem.* **67** (2012) 425−437.

[38] I. Tomescu, S. Kanwal, Ordering trees having small general-sum connectivity index., *MATCH Commun. Math. Comput. Chem.* , to appear.

[39] I. Tomescu, S. Kanwal, Unicyclic connected graphs having smallest degree distances., *Utilitas Math.*, to appear.

[40] A. I. Tomescu, Minimal graphs with respect to the degree distance, *Technical Report, University of Bucharest*, 2008. Available online at: http://sole.dimi.uniud.it/-alexandru.tomescu/files/dd-distance.pdf.

[41] I. Tomescu, Ordering connected graphs having small degree distances, *Discr. Appl. Math.* **158** (2010) 1714–1717.

[42] I. Tomescu, Properties of connected graphs having minimum degree distance, *Discr. Math.* **309** (2009) 2745–2748.

[43] I. Tomescu, Some extremal properties of the degree distance of a graph, *Discr. Appl. Math.* **98** (1999) 159–163.

[44] A. I. Tomescu, Unicyclic and bicyclic graphs having minimum degree distance, *Discr. Appl. Math.* **156** (2008) 125–130.

[45] D. B. West, *An introduction to graph theory*, Prentice Hall, 1996.

[46] R. J. Wilson, *Introduction to graph theory*, Longman, London, 1972.

[47] L. Zhong, The harmonic index for graphs, *Appl. Math. Letters.* **25** (2012) 561–566.

[48] B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **46** (2009) 1252–1270.

[49] B. Zhou, N. Trinajstić, On general sum-connectivity index, *J. Math. Chem.* **47** (2010) 210–218.

[50] B. Zhou, N. Trinajstić, On reverse degree distance, *J. Math. Chem.* **47** (2010) 268−275.