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DISTANCE MEASURES IN GRAPHS

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by

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Dedicated to:

My wife Janet Mazorodze;

My colleagues and friends in the field of Mathematics.

Preface and Declaration

The study described in this thesis was carried out in the Faculty of Science, Department of Mathematics, University of Zimbabwe, during the period May 2012 to April 2016. This thesis was completed under the supervision of Professor S. Mukwembi and Professor A. G. R. Stewart.

This study represents original work by the author and has not been submitted in any form to another University. Where use was made of the work of others it has been duly acknowledged in the text.

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Publications arising from this thesis

1). Mazorodze, J.P., Mukwembi, S. & Vetrík, T. 2014, 'On the Gutman index and minimum degree', *Discrete Applied Mathematics.* vol.**173**, pp 77–82.

2). Mazorodze, J.P. & Mukwembi, S. 2015, 'Radius, diameter and the degree sequence of a graph', *Math. Slovaca.* vol. **65**, No. 6. pp 1–14.

3). Mazorodze, J.P., Mukwembi, S. & Vetrík, T. 'The Gutman index and the Edge-Wiener index of graphs with given vertex-connectivity', (to appear in the journal titled *Discussiones Mathematicae Graph Theory*).

4). Mazorodze, J.P., Mukwembi, S. & Vetrík, T. 'On the Gutman index, the Edge-Wiener index and the edge-connectivity in graphs', (submitted).

5). Ali, P., Mazorodze, J.P., Mukwembi, S. & Vetrík, T. 'On size, order, diameter and edge-connectivity', (submitted).

Abstract

This thesis details the results of an investigation of bounds on four distances measures, namely, radius, diameter, the Gutman index and the edge-Wiener index, in terms of other graph parameters, namely, order, irregularity index and the three classical connectivity measures, minimum degree, vertex-connectivity and edge-connectivity.

The thesis has six chapters. In Chapter 1, we define the most important terms used throughout the thesis and we also give a motivation for our research and provide background for relevant results. In this chapter we include the importance of the distance measures to be studied.

Chapter 2 focuses on the radius, diameter and the degree sequence of a graph. We give asymptotically sharp upper bounds on the radius and diameter of

(i) a connected graph,

(ii) a connected triangle-free graph,

(iii) a connected C_4-free graph of given order, minimum degree, and given number of distinct terms in the degree sequence of the graph.

We also give better bounds for graphs with a given order, minimum degree and maximum degree. Our results improve on old classical theorems by Erdös, Pach, Pollack and Tuza [24] on radius, diameter and minimum degree.

In Chapter 3, we deal with the Gutman index and minimum degree. We show

that for finite connected graphs of order n and minimum degree δ, where δ is a constant, $\mathrm{Gut}(G) \leq \frac{2^4 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4)$. Our bound is asymptotically sharp for every $\delta \geq 2$ and it extends results of Dankelmann, Gutman, Mukwembi and Swart [18] and Mukwembi [43], whose bound is sharp only for graphs of minimum degree 2.

In Chapter 4, we develop the concept of the Gutman index and edge-Wiener index in graphs given order and vertex-connectivity. We show that $\mathrm{Gut}(G) \leq \frac{2^4}{5^5 \kappa} n^5 + O(n^4)$ for graphs of order n and vertex-connectivity κ, where κ is a constant. Our bound is asymptotically sharp for every $\kappa \geq 1$ and it substantially generalizes the bound of Mukwembi [43]. As a corollary, we obtain a similar result for the edge-Wiener index of graphs of given order and vertex-connectivity.

Chapter 5 completes our study of the Gutman index, the edge-Wiener index and edge-connectivity. We study the Gutman index $\mathrm{Gut}(G)$ and the Edge-Wiener index $W_e(G)$ of graphs G of given order n and edge-connectivity λ. We show that the bound $\mathrm{Gut}(G) \leq \frac{2^4 \cdot 3}{5^5(\lambda+1)} n^5 + O(n^4)$ is asymptotically sharp for $\lambda \geq 8$. We improve this result considerably for $\lambda \leq 7$ by presenting asymptotically sharp upper bounds on $\mathrm{Gut}(G)$ and $W_e(G)$ for $2 \leq \lambda \leq 7$.

We complete our study in Chapter 6 in which we use techniques introduced in Chapter 5 to solve new problems on size. We give asymptotically sharp upper bounds on the size, m of

(i) a connected triangle-free graph in terms of order, diameter and minimum degree,

(ii) a connected graph in terms of order, diameter and edge-connectivity,

(iii) a connected triangle-free graph in terms of edge-connectivity, order and diameter.

The result is a strengthening of an old classical theorem of Ore [49] if edge-connectivity is prescribed and constant.

Contents

0.1 Index for notation

$G = (V, E)$	graph G with vertex set V and edge set E.
$\mathrm{deg_G}(v)$	degree of a vertex $v \in V$.
$d_G(u, v)$	distance between $u, v \in V$ in G.
$d_G(f, g)$	distance between $f, g \in E$ in G.
$\mathrm{rad}(G)$	radius of G.
$\mathrm{diam}(G)$	diameter of G.
$ec_G(v)$	eccentricity of vertex $v \in V$.
$N[v]$	(closed) neighbourhood of vertex $v \in V$.
$N^k[v]$	closed $k^{th}-$neighbourhood of a vertex u of G.
$N(v)$	open neighbourhood of vertex $v \in V$.
$N_S(v)$	set of neighbours of v in S or $N(v) \cap S$, $S \subset V$.
$N_i(v)$	i-th distance layer of v.
$k_i(v)$	cardinality of the i-th distance layer of v.
$N_{\leq i}(v)$	i-th neighbourhood of v, namely $\cup_{0 \leq j \leq i} N_j$.
$N_{\geq i}(v)$	$\cup_{i \leq j \leq ec_G(v)} N_j(v)$.
$N[S]$	closed neighbourhood of subset $S \subseteq V$.
$N(S)$	open neighbourhood of subset $S \subseteq V$.
$E(V_1, V_2)$	$\{xy \in E(G) \mid x \in V_1, y \in V_2\},\ V_1, V_2 \subset V$.
$t(G)$	number of distinct terms in a degree sequence of G.
$\delta(G)$	minimum degree of G.
$\Delta(G)$	maximum degree of G.
$\lambda(G)$	edge-connectivity of G.
$\kappa(G)$	vertex-connectivity of G.
$G[S]$	subgraph induced by S in G, $S \subseteq V$.
$G_1 \cup G_2$	union of graphs G_1 and G_2.
$G_1 + G_2$	join of graphs G_1, G_2.
$G_1 + G_2 + \cdots + G_k$	sequential join of graphs $G_1, G_2, \cdots, G_k$.
$\lceil b \rceil$	the smallest integer greater than or equal to b.
$\lfloor b \rfloor$	the biggest integer less than or equal to b.

Chapter 1

Introduction and Preliminaries

1.1 Introduction

The purpose of this chapter is to present motivation as well as to provide relevant background to the study. We define the most important terms that will be used in this thesis. Terms not defined in this chapter will be defined in subsequent chapters, as the need arises.

1.2 Graph Theory Terminology

A *graph* $G = (V, E)$ consists of a finite non-empty set V of elements called vertices, and a (possibly empty) set E of edges. The *order* of G is defined as the number of elements in V, denoted by $|V(G)| = n$ and the number of elements m in E is called the *size* of G.

The *neighbourhood* $N_G(v)$ of a vertex $v \in V$ is the set of all vertices adjacent to v in G and the *closed neighbourhood* $N_G[v]$ is the union of $\{v\}$ and its neighbourhood, that is, $N_G[v] = \{v\} \cup N_G(v)$. If $S \subseteq V(G)$, then $N_G(S) = \cup_{v \in S} N_G(v)$ and $N_G[S] = S \cup N_G(S)$. The closed k^{th}-neighbourhood of a vertex u of G is the set $\{x \in V : \ d_G(x,u) \leq k\}$ and is denoted by $N_G^k[u]$. We simply write $N_G[u]$ instead of $N_G^1[u]$. The closed neighbourhood, $N_G[S]$, of S is the set $\cup_{u \in S} N_G[u]$. Where there is no danger of confusion, we will drop the subscript G.

The *degree* $\deg_G(v)$ of a vertex v of G is the number of edges incident with v, i.e., $\deg_G(v) = |N(v)|$.

The *degree sequence* of a graph is the sequence of all vertex degrees of G. In other words, the degree sequence of G is a vector $(\deg_G(v_1); \deg_G(v_2); \ldots; \deg_G(v_n))$ with $\deg_G(v_1) \geq \deg_G(v_2) \geq \ldots \geq \deg_G(v_n)$ and $|V(G)| = n$. The *irregularity index* of a graph G is the number of distinct terms in its degree sequence.

The *minimum degree*, denoted by $\delta(G) = \delta$, of G is the smallest of the degrees of the vertices in G. We denote the maximum degree of G by Δ.

A *walk* W in a graph G is a sequence of vertices $v_0 v_1 v_2 \cdots v_r$ and edges such that $e_i = v_{i-1}v_i \in E(G)$ for $i = 1, 2, \ldots, r$. We call r the *length* of W and say that W begins at v_0 and ends at v_r. If all the vertices of W are different, then the walk is called a *path*. A path $v_0 v_1 v_2 \cdots v_r$ that begins at v_0 and ends at v_r is called a $v_0 - v_r$ *path*. Let P_1 and P_2 be two $v_0 - v_r$ paths. Then P_1 and P_2 are *edge-disjoint* if P_1 and P_2 have no edges in common, whereas P_1 and P_2 are *internally disjoint* if $V(P_1) \cap V(P_2) = \{v_0, v_r\}$. A *closed walk* in G is a walk of the form $v_0 v_1 v_2 \cdots v_r$ where $v_0 = v_r$. If all the vertices except v_0 of a closed walk $v_0 v_1 v_2 \cdots v_r$ are different and $r \geq 3$, then the closed walk is called a *cycle* of *length* r.

A graph G is said to be *connected* if every pair of distinct vertices of G are joined by a path.

The *distance*, $d_G(u, v)$, between two vertices u, v of G is the length of a shortest u-v path in G.

The *eccentricity*, $\mathrm{ec}_G(v)$, of a vertex $v \in V$ is the maximum distance between v and any other vertex in G.

Every vertex of G of minimum eccentricity is a *centre* vertex of G and the eccentricity of a centre vertex is called the *radius* of G, denoted by $\mathrm{rad}(G)$. G is a *self-centred graph* if every vertex of G is a centre vertex.

The *diameter*, $\mathrm{diam}(G)$, of G is defined as the maximum distance $d_G(u, v)$ over all pairs of vertices u and v in G, i.e., $\mathrm{diam}(G) = \max\limits_{u \in V} \mathrm{ec}_G(u)$.

The i^{th} *distance layer* $N_i(v)$ of a vertex $v \in V(G)$ is the set of vertices at distance i from v, that is, $N_i(v) = \{x \in V(G) \mid d_G(x, v) = i\}$. We simply write N_i if v is understood. We denote the cardinality of N_i by k_i.

A connected graph with no cycles is called a *tree*.

A graph G is *complete* if every pair of distinct vertices of G are adjacent in G.

A graph H is called a *subgraph* of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. If H is a subgraph of G, we write $H \leq G$. A *spanning subgraph* of G is a subgraph H of G with $V(H) = V(G)$. An *induced subgraph* denoted by $G[S]$ is a subgraph of G with vertex set S and any two vertices of S are adjacent in $G[S]$ if and only if they are adjacent in G.

A *bipartite* graph is a graph whose vertex set $V(G)$ can be partitioned into two non-empty subsets A and B such that each edge of G has one end in A and the other end in B.

A *complete bipartite* graph, denoted by $K_{p,q}$, is a bipartite graph G with bipartition A, B such that $A \cup B = V(G)$, $A \cap B = \emptyset$ with $|A| = p$, $|B| = q$ and every vertex in A is adjacent to every vertex in B.

The *vertex-connectivity* $\kappa = \kappa(G)$ of G is the minimum number of vertices whose deletion from G results in a trivial or disconnected graph. We say G is *k-vertex-connected* or simply *k-connected* if G is connected and $\kappa \geq k$.

The *edge-connectivity* $\lambda = \lambda(G)$ of G is the minimum number of edges whose deletion from G results in a trivial or disconnected graph. We say G is *k-edge-connected* if G is connected and $\lambda \geq k$.

Let G_1 and G_2 be two vertex disjoint graphs. The join $G_1 + G_2$ of G_1 and G_2 is the graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2) \cup \{uv | u \in V(G_1), v \in V(G_2)\}$. The union, $G_1 \cup G_2$, of G_1 and G_2 is the graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2)$. Also for $t \geq 3$ given vertex disjoint graphs $G_1, G_2, \ldots, G_t$, the sequential join, $G_1 + G_2 + G_3 + \ldots + G_t$, is the graph

$(G_1 + G_2) \cup (G_2 + \cup G_3) \cup \ldots \cup (G_{t-1} + G_t)$.

1.3 Distance Concepts and Topological indices

All graphs considered here are finite, simple, connected, undirected and non-trivial, unless otherwise specified. Throughout the study of graphs, distance concepts have played a central role. Investigations of distance concepts in graphs was enhanced by their wide applicability to facility location problems, network design in operations research and also prediction of properties of chemical compounds in chemistry.

The *Wiener index*, $W(G)$, of a graph G is defined as the sum of distances between all unordered pairs of vertices, that is,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v).$$

We may define the *Wiener index* also in a slightly different approach. First we define the *distance,* $d_G(v)$, of a vertex v as the sum of all distances between v and all other vertices of G. Thus,

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} d_G(v).$$

The distance between two edges of a connected graph G is, by definition, the distance between the corresponding vertices of the line graph of G. The *edge-Wiener index* of a connected graph G is defined as the sum of distances between all unordered pairs of edges of the graph G. That is,

$$W_e(G) = \sum_{\{f,g\} \subseteq E(G)} d_G(f, g).$$

We may also say that the *edge-Wiener index* of a graph G is equal to the Wiener index of the line graph of G.

The *Gutman index* of a connected graph G is defined as

$$\mathrm{Gut}(G) = \sum_{\{x,y\} \subseteq V(G)} \deg(x)\deg(y)d(x, y).$$

1.4 Literature Review

1.4.1 Motivation and Background

The purpose of this subsection is to give some motivation for our study and to provide background for relevant results. We give proofs of some of the results in the next subsection. For a given graph, the invariance, radius, diameter, Gutman index and the edge-Wiener index may be computed in polynomial time using for instance algorithms which determine the distance, $d(v)$ from a vertex v of the graph to every other vertex in the graph. Problems arise if the graph is not given. However if we are given some properties like order, minimum degree, irregularity index, maximum degree, vertex-connectivity, or edge-connectivity, say, then we may be interested in knowing upper bounds on parameters like radius and diameter in terms of some of the given properties of the graph.

The Diameter

The diameter is one of the most common of the classical distance parameters in graph theory, and much of the research on distances is in fact on the diameter. Apart from being an interesting graph-theoretical parameter, it plays a significant role in analysing communication networks, Chung [9]. In such networks, the time delay or signal degradation for sending a message from one point to another is often proportional to the distance between the two points. The diameter can be used to indicate the worst-case performance.

Let G be a connected graph of order n. Clearly, $1 \leq \mathrm{diam}(G) \leq n-1$. The diameter equals 1 or $n-1$ if and only if G is a complete graph or a path, respectively. If we consider the size and order of a graph, then we can give an upper bound on the diameter which is significantly stronger. Thus,

$$\mathrm{diam}(G) \leq n + \frac{1}{2} - \sqrt{2m - 2n + \frac{17}{4}}.$$

This result is an immediate consequence of the classical result by Ore [49] which characterises diameter-maximal graphs.

It is natural to ask if graphs with larger maximum degree or larger minimum degree can give stronger bounds. Bosak, Rosa and Snam [4] first proved that the diameter was at most $n+1-\Delta$. Upper bounds on the diameter in terms of order and minimum degree are far more interesting. They have been considered and rediscovered by several authors some of which are, Moon [41], Goldsmith, Manvel and Farber [27]. The most general result was proved by Erdős , Pach, Pollack and Tuza [24]. They proved that

Theorem 1.1 *[24] Let G be a connected graph of order n and minimum degree $\delta \geq 2$. Then*

$$\operatorname{diam}(G) \leq \left\lfloor \frac{3n}{\delta+1} \right\rfloor - 1.$$

Moreover the bound is tight apart from the exact value of the additive constant.

If G is triangle-free, then

$$\operatorname{diam}(G) \leq 4\left\lceil \frac{n-\delta-1}{2\delta} \right\rceil.$$

Moreover the bound is tight apart from the exact value of the additive constant.

If G is C_4-free and $\delta \geq 2$ is a fixed integer, then

$$\operatorname{diam}(G) \leq \frac{5n}{\delta^2 - 2[\frac{\delta}{2}] + 1}.$$

Furthermore, if δ is large, then this bound is almost tight.

Dankelmann, Dlamini and Swart [10, 11] used different methods to extend Theorem 1.1 to $K_{2,t}$-free graphs and to $K_{3,3}$-free graphs.

Particularly interesting is the fact that extremal graphs for the above bounds are close to being regular, i.e., with all vertices having the same degrees. A parameter of the degree sequence which gives an indication of how far or near a graph is from being regular, i.e., an indication of how unequal the vertex degrees of a given graph are, was seemingly discussed for the first time in the 105th conjecture of Graffiti according to which for every tree T, the irregularity of the degree sequence is not more than the irregularity of the transmission of distance. Precisely, the *irregularity index*, $t(G)$, of a graph G is the number of distinct terms in its degree sequence. Extremal graphs for the above bounds have irregularity index at most 2. In that spirit, the bound, in Theorem 1.1, was recently improved by Mukwembi [43] if the irregularity index, t, of the graph G is given:

$$\operatorname{diam}(G) \leq \frac{3(n-t)}{\delta+1} + O(1).$$

The Radius

The radius is (after the diameter) the second most important classical distance parameter in graph theory. It is a convenient measure of centrality in a model of a network. In terms of planning and organisation, central vertices are of particular interest in most networks. In such networks, decisions involving the optimal selection of a facility or two is only possible if central vertices are considered. For instance if a city council committee wishes to locate an emergency facility like a fire station, then the time or distance from the fire station to the furthest point in that city should be as short as possible. The radius is therefore a very good measure that indicates the furthest distance or the time in question from the central or emergency facility to a location furthest away.

Networks occur in different areas, for example in metabolic and gene regulation networks in each cell (see, [56]), transportation networks, food

webs in ecology, the organization of the internet and economic interactions. Structurally different classes of networks are identified by different useful parameters such as the irregularity index, minimum degree, maximum degree, vertex-connectivity and edge-connectivity just to mention but a few.

We begin by considering the relationship between the radius and the diameter. A useful and basic inequality which follows directly from the triangle inequality, the definition of the radius and diameter is that:

$$\mathrm{rad}(G) \leq \mathrm{diam}(G) \leq 2\mathrm{rad}(G).$$

Laskar and Shier [38] showed that, if a graph with no induced cycle of length greater than three, (chordal graph) has radius r and diameter d, then

$$\frac{d}{2} \leq r \leq \left\lfloor \frac{d}{2} \right\rfloor + 1.$$

We now bound the radius in terms of order and the maximum degree. It is folklore (see for instance [16]) that

$$\mathrm{rad}(G) \leq \frac{n - \Delta + 2}{2}.$$

Harant and Walther [31] proved the following upper bound on the radius.

Theorem 1.2 *[31] Let G be a 3-vertex-connected graph with n vertices. Then*

$$\mathrm{rad}(G) < \frac{n}{4} + O(\log n).$$

Egawa and Inoue [23] generalized the above result and obtained the following for all odd κ.

Theorem 1.3 *[23] Let κ be an odd integer, and let G be a κ-connected graph of order n. Then*

$$\text{rad}(G) \leq \frac{n + \kappa + 10}{\kappa + 1}.$$

This bound is best possible, up to an additive constant.

The upper bound on the radius in terms of order and minimum degree remained open for almost three decades. It was in 1989 when Erdös, Pach, Pollack and Tuza [24] proved the following result.

Theorem 1.4 *[24] Let G be a connected graph of order n and minimum degree $\delta \geq 2$. Then*

$$\text{rad}(G) \leq \frac{3(n-3)}{2(\delta+1)} + 5.$$

Moreover the bound is tight apart from the exact value of the additive constant.

If G is triangle-free, then

$$\text{rad}(G) \leq \frac{n-2}{\delta} + 12.$$

Moreover the bound is tight apart from the exact value of the additive constant.

If G is $C_4 - free$, then

$$\text{rad}(G) \leq \frac{5n}{2(\delta^2 - 2[\delta] + 1)}.$$

Furthermore, if δ is large, then this bound is almost tight.

These bounds on the radius for connected graphs have been rediscovered by several authors, for instance Dankelmann, Dlamini and Swart [10, 11, 19], using different techniques, proved the following slightly stronger bound:

$$\mathrm{rad}(G) \leq \frac{3n}{2(\delta+1)} + 1.$$

Results presented above in this subsection are known bounds on diameter in terms of order, size, minimum degree and irregularity index. We also presented known bounds on the radius in terms of order, maximum degree, vertex-connectivity, edge-connectivity and minimum degree. No bounds on these distance measures in terms of order and irregularity index seem to have been known to date. In chapters that follow, we prove upper bounds whose orders of magnitude are best possible, on the diameter in terms of order and the irregularity index of triangle-free graphs and C_4-free graphs. We also prove upper bounds on the radius in terms of order, minimum degree and the irregularity index. For the radius, we also consider the upper bounds for triangle-free graphs and C_4-free graphs.

The Gutman index and the edge-Wiener index

Graph indices have been studied for decades because of their extensive applications in chemistry. Several variants of the Wiener index have been proposed and studied. The Wiener index was used to describe molecular branching and cyclicity. It was also used to establish correlations with various physiochemical and thermodynamic parameters of chemical compounds. Among them are the boiling point, density, critical pressure, refractive indices, heats of isomerization and vaporization of various hydrocarbon species. The Wiener index found interesting applications in polymer chemistry, in studies of crystals and in drug design.

In this subsection we consider a variant of the well known and much studied Wiener index, a quantity put forward in [28] by Gutman and called there the Schultz index of the second kind, but for which the name Gutman index seems to be commonly used in [51]. The Gutman index has been studied for example in [2, 26, 25, 28]. Like Wiener's original index, Gutman index is also based on distances between vertices of graphs. We define the Gutman index of a connected graph G as

$$\mathrm{Gut}(G) = \sum_{\{x,y\} \subseteq V(G)} \deg(x)\deg(y)d(x,y).$$

Gutman in [28], presented that for acyclic structures, the Gutman index reflects exactly the same structural features as the Wiener index. The question, whether theoretical investigations on the Gutman index focusing on the more difficult polycyclic molecules can be done, was posed. Feng [25] studied the Gutman index for unicyclic graphs, and Feng and Liu in [26] considered bicyclic graphs in their research. Dankelmann, Gutman, Mukwembi and Swart in [18] showed that if G is a connected graph of order n, then

$$\mathrm{Gut}(G) \leq \frac{2^4 n^5}{5^5} + O(n^{\frac{9}{2}}).$$

Mukwembi in [43] improved this upper bound and presented the result

$$\mathrm{Gut}(G) \leq \frac{2^4 n^5}{5^5} + O(n^4),$$

which shows that $O(n^{\frac{9}{2}})$ can be replaced by $O(n^4)$.

Recall that the edge-Wiener index $W_e(G)$ of a connected graph G is equal to the sum of distances between all pairs of edges in G. This index was introduced by Iranmanesh, Gutman, Khormali and Mahmiani, in [32] and by Khalifeh, Yousefi-Azari, Ashrafi and Wagner in [34]. Azari and Iranmanesh in [3] studied the edge-Wiener index of the sum of graphs. Relations between the edge-Wiener index and other indices were studied in [8, 37, 48].

In this thesis, we provide upper bounds on the Gutman index in terms of order, minimum degree, $\delta \geq 2$, vertex-connectivity, $\kappa \geq 2$, and edge-connectivity, $\lambda \geq 2$. In particular, Chapter 2 is devoted to proving the following. Let G be a connected graph of order n and minimum degree δ, where δ is a constant. Then

$$\mathrm{Gut}(G) \leq \frac{2^4 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4).$$

Moreover, we demonstrate that apart from an additive constant, the given bound is best possible.

In Chapter 3, we prove that if $\kappa \geq 2$, and G is a $\kappa-$connected graph of order n with diameter d, then

$$\mathrm{Gut}(G) \leq \frac{1}{16} d(n-\kappa d)^4 + O(n^4).$$

Further, we also demonstrate that, apart from the additive constant, the value $\frac{1}{16} d(n-\kappa d)^4$ of the bound is best possible.

Chapter 4, is devoted to proving the following. Let G be a λ-edge-connected graph of order n. Then

$$\operatorname{Gut}(G) \leq \begin{cases} \dfrac{2^5 \cdot n^5}{3 \cdot 5^5} + O(n^4) & \text{if} \quad \lambda = 2, \\ \frac{2^3 \cdot n^5}{5^5} + O(n^4) & \text{if} \quad \lambda = 3, 4, \\ \frac{2^5 \cdot n^5}{5^6} + O(n^4) & \text{if} \quad \lambda = 5, 6, \\ \frac{2^4 \cdot n^5}{3 \cdot 5^5} + O(n^4) & \text{if} \quad \lambda = 7, \\ \frac{2^4 \cdot 3}{5^5(\lambda+1)} n^5 + O(n^4) & \text{if} \quad \lambda \geq 8. \end{cases}$$

Moreover, we demonstrate, in each case that apart from the additive constant, the given bound is best possible. Further, we include the upper bounds on the edge-Wiener index applying a relationship between the Gutman index and the edge-Wiener index.

Size of a graph

An upper bound on the size in terms of order and diameter was determined by Ore [49] as early as 1968 who showed that

$$m \leq \frac{1}{2}(n - d - 1)(n - d + 4) + d.$$

Several bounds on the size of a graph in terms of other graph parameters, for example, order and radius [15, 50, 54], order and degree set [52], and order and domination number [12] have been investigated. Several authors [50, 52] have presented simple and short proofs to Ore's theorem. Recently Mukwembi [45] reported on an asymptotically sharp upper bound on the size in terms of order, diameter and minimum degree. Mukwembi obtained the following result:

Theorem 1.5 *[45] Let G be a connected graph of order n, minimum degree δ, di-*

ameter d and size m. Then

$$\begin{aligned} m &\leq \frac{1}{2}\Big[n - \frac{1}{3}d(\delta+1)\Big]^2 + (2\delta+1)\Big(n - \frac{1}{6}d(\delta+2)\Big) \\ &= \frac{1}{2}\Big[n - \frac{1}{3}d(\delta+1)\Big]^2 + O(n), \end{aligned} \tag{1.1}$$

and the bound, for fixed δ, is asymptotically tight.

Again Mukwembi in [46] obtained an upper bound on the size in terms of order, radius and minimum degree. The following result was obtained

Theorem 1.6 *[46] Let G be a connected graph of order n, radius $r \geq 9$, minimum degree $\delta \geq 2$ and size m. Then*

$$m \leq \frac{1}{2}\Big[n - \frac{2r}{3}d(\delta+1)\Big]^2 + (\delta+1)\Big[13n - \frac{22r}{3}(\delta+1) + O(\delta^2)\Big].$$

Moreover this bound is asymptotically tight.

In [47], an asymptotically sharp upper bound on the size in terms of order, diameter and vertex-connectivity was presented.

Theorem 1.7 *[47] Let G be a κ-connected graph of order n, diameter d and size m. Then*

$$m \leq \frac{1}{2}(n - \kappa d)^2 + O(n),$$

and the bound, for fixed κ, is asymptotically tight.

In this thesis, we prove an upper bound on size of a triangle-free graph in terms of order, diameter and minimum degree. Further we provide upper bounds on the size in terms of order, diameter and edge-connectivity, $\lambda \geq 2$. In particular, Chapter 5 is devoted to proving upper bounds on size for connected graphs and triangle-free graphs. We prove the following. Let G be a connected triangle-free graph of order n, diameter d, minimum degree $\delta \geq 2$ and size m. Then

$$m \leq \frac{(n - \frac{\delta d}{2})^2}{4} + O(n).$$

Moreover, we demonstrate that apart from an additive constant, the given bound is best possible.

In Chapter 5 we also prove the following. Let G be a λ-edge-connected triangle-free graph of order n and diameter d. Then

$$m \leq \begin{cases} \frac{1}{4}\left(n - \frac{3d}{2}\right)^2 + O(n) & \text{if} \quad \lambda = 2, \\ \frac{1}{4}(n - 2d)^2 + O(n) & \text{if} \quad \lambda = 3, 4, \\ \frac{1}{4}(n - \frac{5d}{2})^2 + O(n) & \text{if} \quad \lambda = 5, 6, \\ \frac{1}{4}(n - 3d)^2 + O(n) & \text{if} \quad \lambda = 7, \\ \frac{(n - \frac{\lambda d}{2})^2}{4} + O(n) & \text{if} \quad \lambda \geq 8. \end{cases}$$

Moreover, we demonstrate in each case that apart from the additive constant, the given bound is best possible.

In this thesis attention is restricted to (un-weighted) graphs in which all edges have length one. For example weighted graphs are discussed in [5]. Note that graphs presented in this thesis generally consider a collection of n locations or nodes. These locations are interconnected for purposes of communicating data or messages. Instead of speaking of locations or nodes, we speak of vertices and interconnections are represented by edges. In addition, instead of speaking of the minimum number of interconnections, we speak of edge-connectivity while a minimum number of locations represents vertex-connectivity instead of speaking of port constraints, we refer to degree conditions.

1.4.2 Some Important Results

Theorem 1.8 *[55] Let G be a connected graph with minimum degree δ, vertex-connectivity κ and edge-connectivity λ. Then $\kappa \leq \lambda \leq \delta$.*

The proof can be found in many textbooks including [7]. □

For trees, we have a much stronger relationship stated in the following theorem which is due to Jordan, [33].

Theorem 1.9 *[33] Let T be a tree of order $n \geq 2$.*

(a) The centre of T consist of a single vertex or two adjacent vertices.

(b) If the centre of T consists of a single vertex then $\text{diam}(T) = 2\text{rad}(T)$, *and if the centre of T consists of two adjacent vertices then* $\text{diam}(T) = 2\text{rad}(T) - 1$.

Proof: The proof is by induction on the radius. We may easily verify the theorem for trees of radius 1 and 2. If $\text{rad}(T) \geq 3$, then consider the tree T_0 obtained from T by removing all end vertices. Since removing the end vertices reduces the radius by 1, the diameter by 2, and maintains the centre, the theorem follows. □

We present a very elementary, but handy, bound on the diameter due to Mukwembi, [42].

Theorem 1.10 *[42] Let G be a connected graph of order n. The diameter of G satisfies the inequality*

$$\text{diam}(G) \leq n - t + 1,$$

where t is the irregularity index of G. Moreover, this inequality is sharp.

Proof: Since every vertex can be adjacent to at most 3 vertices of a diametral path, then $\Delta \leq n - \text{diam}(G) + 1$. Clearly, $t \leq \Delta$. It follows that $t \leq n - \text{diam}(G) + 1$ from which the inequality is deduced. □

One quantity closely analogous to the Wiener index is the edge-Wiener index, $W_e(G)$ defined by Dankelmann, Gutman, Mukwembi and Swart, [18] as the sum of the distances (in the line graph) between all pairs of edges of G. It was shown in [18] that the Gutman index is connected to the edge-Wiener index by the following useful inequality. We therefore state the result without proof.

Theorem 1.11 *[18] Let G be a connected graph of order n. Then*

$$|W_e(G) - \frac{1}{4}\text{Gut}(G)| \leq \frac{n^4}{8}.$$

1.5 Conclusion

In the first chapter, we introduced the terminology, distance concepts, motivation and background to the study as well as some important results whose application is important in most of our proofs in the next chapters. In the following chapter, we prove an asymptotically sharp upper bound on the radius in terms of order, minimum degree and the irregularity index. Our bound is a strengthening of the bound by Erdös, Pach, Pollack and Tuza, [24]. We also give similar improved bounds on the diameter and radius for triangle-free and for C_4-free graphs. Further, we also give asymptotically sharp upper bounds on the radius and diameter when order, minimum, and maximum degree of the graph are given.

Chapter 2

Radius, diameter and the degree sequence of a graph

2.1 Introduction

The goal of this chapter is to find asymptotically sharp upper bounds on the radius and diameter of (i) a connected graph, (ii) a connected triangle-free graph, (iii) a connected C_4-free graph of given order, minimum degree, and given number of distinct terms in the degree sequence of the graph. We also give better bounds for graphs with a given order, minimum degree and maximum degree. Our results improve on old classical theorems by Erdös, Pach, Pollack and Tuza [24] on radius, diameter and minimum degree.

2.2 Definitions, notations and preliminaries

As mentioned in Chapter 1, in 1869, Jordan [33] showed that if T is a tree, then either $\text{diam}(T) = 2\text{rad}(T)$ or $\text{diam}(T) = 2\text{rad}(T) - 1$. In particular, we have the following fact.

Fact 2.1 *For every tree T,* $\text{rad}(T) \le \frac{1}{2}[\text{diam}(T) + 1]$.

A 2-packing of G is a subset $A \subseteq V$ with $d_G(u, v) > 2$ for all $u, v \in A$. A 4-packing is similarly defined. The k-th power of G, denoted by G^k, is the graph with vertex set $V(G)$, in which two distinct vertices u and v are adjacent if $d_G(u, v) \le k$. Recall that for an integer r, we denote the smallest integer greater than or equal to r by $\lceil r \rceil$.

Let v be a vertex of G. The i^{th} distance layer of v, $N_i(v)$, is the set of all vertices that are at distance i from v, i.e., $N_i(v) = \{x \in V(G) : \ d_G(v, x) = i\}$. Where there is no danger of confusion and if vertex v is understood, we simply write N_i instead of $N_i(v)$.

2.3 Results

We begin by presenting a result on an upper bound on the radius in terms of order, minimum degree and the irregularity index. The proof technique of this result is a refinement of the widely used method of spanning trees introduced by Dankelmann and Entringer [13].

Theorem 2.1 *Let G be a connected graph of order n, irregularity index t and minimum degree δ. Then*

$$\text{rad}(G) \le \frac{3(n - t)}{2(\delta + 1)} + O(1).$$

Moreover, this bound is asymptotically tight.

Proof: Since G has t vertices of distinct degrees, let $\{v_1, v_2, \ldots, v_t\}$ be a set of t vertices such that $\deg(v_1) < \deg(v_2) < \deg(v_3) < \cdots < \deg(v_t)$. Since $\deg(v_1) \geq \delta$, we have $\deg(v_t) \geq \delta + t - 1$. Hence $|N[v_t]| \geq \delta + t$. We find a maximal 2-packing A of G using the following procedure. Let $A = \{v_t\}$. If there exists a vertex x in G with $d(x, A) = 3$, add x to A. Add vertices x with $d(x, A) = 3$ to A until each of the vertices not in A are within distance 2 of A.

Fact 2.2 $|A| \leq \dfrac{n-t+1}{\delta+1}$.

Proof of Fact 2.2: First note that by our construction, for any two vertices $x, y \in A$, we have $N[x] \bigcap N[y] = \emptyset$. Since minimum degree is δ and $|N[v_t]| \geq \delta + t$, it follows that

$$\begin{aligned} n &\geq |\bigcup_{x \in A} N[x]| \\ &= |N[v_t]| + \sum_{x \in A - \{v_t\}} |N[x]| \\ &\geq \delta + t + (|A| - 1)(\delta + 1). \end{aligned}$$

Fact 2.2 is proven upon re-arranging the terms.

Let $T_1 \leq G$ be the forest with $V(T_1) = N[A]$, whose edge set consists of all edges incident with a vertex in A. By our construction of A, there exists $|A| - 1$ edges in G, each of them joining two neighbours of distinct elements of A whose addition to

T_1 gives a tree $T_2 \leq G$.

Every vertex x not in T_2 is adjacent to some vertex x' in T_2. Let T be a spanning tree of G with edge set $E(T_2) \cup \{xx' : x \in V(G) - V(T_2)\}$. We have by construction that $T^3[A]$ is connected and that $\text{diam}(T^3[A]) \leq |A| - 1$, and hence

$$d_T(x, y) \leq 3(|A| - 1) \text{ for all } x, y \in A. \tag{2.1}$$

Clearly, $\text{rad}(G) \leq \text{rad}(T)$. It follows from Fact 2.1 that

$$\text{rad}(G) \leq \frac{1}{2}[\text{diam}(T) + 1]. \tag{2.2}$$

We now bound $\text{diam}(T)$. Let u, v be arbitrary vertices in T. By our construction u and v are each within distance 2 of A. Let $u', v' \in A$ be such that $d_T(u, u') \leq 2$ and $d_T(v, v') \leq 2$.

Then, in conjunction with (2.1), we have

$$\begin{aligned} d_T(u, v) &\leq d_T(u, u') + d_T(u', v') + d_T(v', v) \\ &\leq 2 + d_T(u', v') + 2 \\ &\leq 2 + 3(|A| - 1) + 2 \\ &\leq 3(|A| - 1) + 4. \end{aligned}$$

By Fact 2.2, we get

$$\begin{aligned} d_T(u, v) &\leq 3\Big(\frac{n - t + 1}{\delta + 1} - 1\Big) + 4 \\ &= \frac{3(n - t)}{\delta + 1} + \frac{3}{\delta + 1} + 1, \end{aligned}$$

and so

$$\operatorname{diam}(T) \leq \frac{3(n-t)}{\delta+1} + \frac{3}{\delta+1} + 1.$$

This, in conjunction with (2.2), yields

$$\begin{aligned}\operatorname{rad}(G) &\leq \frac{1}{2}\Big[\frac{3(n-t)}{\delta+1} + \frac{3}{\delta+1} + 1 + 1\Big] \\ &= \frac{3(n-t)}{2(\delta+1)} + \frac{3}{2(\delta+1)} + 1,\end{aligned}$$

and the bound in the theorem is proven.

To see that the bound is asymptotically tight, let n, δ, t and k be positive integers for which $k = \frac{n-t-\delta+3}{\delta+1}$ and consider the graph $G_{n,\delta,t}$, $t \geq 2$, constructed as follows. Let $S_0, S_1, S_2, \ldots, S_{3k-1}, S_{3k}$ be mutually disjoint sets such that

$$|S_i| = \begin{cases} t-1 & \text{if} \quad i = 1, \\ \delta - 1 & \text{if} \quad i \equiv 0 (\text{mod } 3), \quad i \neq 0,\ 3k, \\ 1 & \text{if} \quad i \equiv 1 \text{ or } 2 (\text{mod } 3), \quad i \neq 1, \\ \delta & \text{if} \quad i = 0,\ 3k. \end{cases}$$

Define the following sets:

$$E_0 := \{uv \mid u, v \in S_0\},$$

$$E_{0,1} := \{uv \mid (u,v) \in S_0 \times S_1\}.$$

Write the elements of S_1 and S_2 as $S_1 = \{w_1, w_2, \ldots, w_{t-1}\}$, $S_2 = \{w\}$, respectively, and define

$$E_1 := \{w_i w_j \mid i + j \geq t,\ i \neq j\},$$

$$E_{1,2} := \{w_{t-1} w\},$$

$$E_{\geq 2} := \{uv \mid (u,v) \in S_i \times S_j, u \neq v, i,j \geq 2 \text{ and } |j-i| \leq 1\}.$$

Define the graph $G_{n,\delta,t}$ to be the graph with vertex set

$$V(G_{n,\delta,t}) = S_0 \cup S_1 \cup \cdots \cup S_{3k-1} \cup S_{3k},$$

and edge set

$$E(G_{n,\delta,t}) = E_0 \cup E_{0,1} \cup E_1 \cup E_{1,2} \cup E_{\geq 2}.$$

By inspection, $G_{n,\delta,t}$ has minimum degree δ, irregularity index t and $\mathrm{diam}(G_{n,\delta,t}) = 3k$. From $k = \frac{n-t-\delta+3}{\delta+1}$, we get

$$\mathrm{diam}(G_{n,\delta,t}) = \frac{3(n-t)}{\delta+1} + O(1).$$

Since $\mathrm{diam}(G_{n,\delta,t}) \leq 2\mathrm{rad}(G_{n,\delta,t})$, it follows that $\mathrm{rad}(G_{n,\delta,t}) \geq \dfrac{3(n-t)}{2(\delta+1)} + O(1)$, and so the bound is asymptotically tight, as desired. □

Consider the vertex v_t in the proof of Theorem 2.1. The lower bound

$$\deg(v_t) \geq \delta + t - 1$$

played a pivotal role in the proof of Theorem 2.1. It is not hard to show that in general $\delta + t - 1 \leq \Delta$, where Δ is the maximum degree of G. It is therefore natural to expect better bounds when the maximum degree of the graph is known. We prove this below.

Theorem 2.2 *Let G be a connected graph of order n, minimum degree δ and maximum degree Δ. Then*

$$\mathrm{rad}(G) \leq \frac{3(n-\Delta)}{2(\delta+1)} + O(1).$$

Moreover, this bound is asymptotically tight.

Proof: Let v be a vertex of maximum degree in G. We find a maximal 2-packing A of G using the following procedure. Let $A = \{v\}$. Add vertices x with $d(x, A) = 3$ to A until each of the vertices not in A are within distance 2 of A.

Fact 2.3 $|A| \leq \dfrac{n - \Delta + \delta}{\delta + 1}$.

Proof of Fact 2.3: First note that by our construction, for any two vertices $x, y \in A$, we have $N[x] \bigcap N[y] = \emptyset$. Since minimum degree is δ and $|N[v]| = \Delta + 1$, it follows that

$$\begin{aligned} n &\geq |\bigcup_{x \in A} N[x]| \\ &= |N[v]| + \sum_{x \in A - \{v\}} |N[x]| \\ &\geq \Delta + 1 + (|A| - 1)(\delta + 1). \end{aligned}$$

Fact 2.3 is proven upon re-arranging the terms. □

Let $T_1 \leq G$ be the forest with $V(T_1) = N[A]$, whose edge set consists of all edges incident with a vertex in A. By our construction of A, there exists $|A| - 1$ edges in G, each of them joining two neighbours of distinct elements of A whose addition to T_1 gives a tree $T_2 \leq G$.

Every vertex x not in T_2 is adjacent to some vertex x' in T_2. Let T be a spanning tree of G with edge set $E(T_2) \cup \{xx' : \ x \in V(G) - V(T_2)\}$. We have by construction that $T^3[A]$ is connected and that $\operatorname{diam}(T^3[A]) \leq |A| - 1$, and hence

$$d_T(x, y) \leq 3(|A| - 1) \text{ for all } x, y \in A. \tag{2.3}$$

Clearly, $\operatorname{rad}(G) \leq \operatorname{rad}(T)$. It follows from Fact 2.1 that

$$\operatorname{rad}(G) \leq \frac{1}{2}(\operatorname{diam}(T) + 1). \tag{2.4}$$

We now bound $\operatorname{diam}(T)$. Let u, v be arbitrary vertices in T. By our construction u and v are each within distance 2 of A. Let $u', v' \in A$ be such that $d_T(u, u') \leq 2$ and $d_T(v, v') \leq 2$.

Then, in conjunction with (2.3), we have

$$\begin{aligned} d_T(u, v) &\leq d_T(u, u') + d_T(u', v') + d_T(v', v) \\ &\leq 2 + 3(|A| - 1) + 2 \\ &= 3|A| + 1. \end{aligned}$$

By Fact 2.3, we get

$$\begin{aligned} d_T(u, v) &\leq 3\Big(\frac{n - \Delta + \delta}{\delta + 1}\Big) + 1 \\ &= \frac{3(n - \Delta)}{\delta + 1} + O(1), \end{aligned}$$

and so

$$\operatorname{diam}(T) \leq \frac{3(n - \Delta)}{\delta + 1} + O(1).$$

This, in conjunction with (2.4), yields

$$\begin{aligned} \operatorname{rad}(G) &\leq \frac{1}{2}\Big(\frac{3(n - \Delta)}{\delta + 1} + O(1) + 1\Big) \\ &= \frac{3(n - \Delta)}{2(\delta + 1)} + O(1), \end{aligned}$$

and the bound in the theorem is proven.

To see that the bound is asymptotically tight, let n, δ, Δ and k be positive integers for which $k = \frac{n-\Delta-2}{\delta+1} + 1$, $\delta \leq \Delta - 1$, and consider the graph $G_{n,\delta,\Delta}$ constructed as follows.

Let $S_0, S_1, S_2, \ldots, S_{3k-2}, S_{3k-1}$ be mutually disjoint sets such that

$$|S_i| = \begin{cases} \Delta - 1 & \text{if} \quad i = 1, \\ \delta - 1 & \text{if} \quad i \equiv 1 (\text{mod } 3), \quad i \neq 1, \\ 1 & \text{if} \quad i \equiv 0 \text{ or } 2 (\text{mod } 3), \quad i \neq 3k-1, \\ 2 & \text{if} \quad i = 3k-1. \end{cases}$$

Define graph $G_{n,\delta,\Delta}$ to be the graph with vertex set

$$V(G_{n,\delta,\Delta}) = S_0 \cup S_1 \cup \cdots \cup S_{3k-2} \cup S_{3k-1},$$

where vertices $u \in S_i$ and $v \in S_j$, $u \neq v$, are adjacent in $G_{n,\delta,\Delta}$ if $|i-j| \leq 1$. By inspection, $G_{n,\delta,\Delta}$ has minimum degree δ, maximum degree Δ and $\text{diam}(G_{n,\delta,\Delta}) = 3k-1$. From $k = \frac{n-\Delta-2}{\delta+1} + 1$, we get

$$\text{diam}(G_{n,\delta,\Delta}) \geq \frac{3(n-\Delta)}{\delta+1} + O(1).$$

Since $\text{diam}(G_{n,\delta,\Delta}) \leq 2\text{rad}(G_{n,\delta,\Delta})$, it follows that $\text{rad}(G_{n,\delta,\Delta}) \geq \dfrac{3(n-\Delta)}{2(\delta+1)} + O(1)$, and so the bound is asymptotically tight, as desired. $\square$

The following bound, which is attained by $G_{n,\delta,\Delta}$ constructed in Theorem 2.2, follows from Theorem 2.2 and the fact that $\text{diam}(G) \leq 2\text{rad}(G)$.

Corollary 2.3 *Let G be a connected graph of order n, minimum degree δ and maximum degree Δ. Then*

$$\mathrm{diam}(G) \leq \frac{3(n-\Delta)}{\delta+1} + O(1).$$

Moreover, this bound is asymptotically tight. $\square$

We now turn to triangle-free graphs. From now onwards, unless specified, z is a fixed centre vertex of G so that $\mathrm{rad}(G) = r = \mathrm{ec}(z)$. For each $i = 0, 1, \ldots, r$, let $N_i = \{v \in V(G) : \ d_G(v, z) = i\}$ be the i^{th} distance layer of z. We employ the notation $N_{\leq j} = \cup_{0 \leq i \leq j} N_i$ and $N_{\geq j} = \cup_{j \leq i \leq r} N_i$. Since $N_r \neq \emptyset$, from now onwards fix a vertex $z_r \in N_r$. Form a spanning tree T of G that is distance preserving from z, i.e., $d_T(z, x) = d_G(z, x)$ for all $x \in V(G)$. For a vertex $x, y \in V(G)$, denote by $T(x, y)$, the set of vertices on a path connecting x and y in T.

Definition 1 *Let $y \in V(G)$. We say y is* **related** *to z_r if there exist vertices $u, v \in V(G)$, where $u \in T(z, z_r) \cap N_{\geq 9}$ and $v \in T(z, y) \cap N_{\geq 9}$ such that $d_G(u, v) \leq 4$.*

The following important observation is an analogue of one due to Erdős et al. [24].

Lemma 2.4 *Let $rad(G) \geq 18$ and z, z_r as above. Then there exists a vertex in $N_{\geq r-9}$ which is not related to z_r.*

Proof: Suppose to the contrary that every vertex $y \in N_{\geq r-9}$ is related to z_r. Let z_9 be the vertex of $T(z, z_r)$ which belongs to N_9. We show that the eccentricity of z_9 is less than r. For any $x \in N_{\leq r-10}$, we have $d_G(z_9, x) \leq d_G(z_9, z) + d_G(z, x) \leq$

$9+r-10=r-1$. Since every vertex in $N_{\geq r-9}$ is related to z_r, for any $x \in N_{\geq r-9}$, there exists u, v, where $u \in T(z, z_r) \cap N_{\geq 9}$ and $v \in T(z, x) \cap N_{\geq 9}$ such that $d_G(u, v) \leq 4$. Since z_9 and u are on a z-z_r shortest path, we have, $d_G(z, u) = d_G(z, z_9)+d_G(z_9, u) = 9 + d_G(z_9, u)$. Thus, $d_G(z_9, u) = d_G(z, u) - 9$. It follows that

$$\begin{aligned} d_G(z_9, x) &\leq d_G(z_9, u) + d_G(u, v) + d_G(v, x) \\ &\leq d_G(z, u) - 9 + 4 + (r - d_G(z, v)) \\ &\leq r - 5 + d_G(z, u) - d_G(z, v) \\ &\leq r - 5 + d_G(u, v) \\ &\leq r - 1. \end{aligned}$$

Hence $\mathrm{ec}(z_9) \leq r - 1$, contradicting the fact that $\mathrm{rad}(G) = r$. □

Lemma 2.5 *Let G be a connected triangle-free graph with radius $r \geq 21$. Let z be a centre vertex of G and N_i be its i^{th} distance layer. Let k, l, where $9 \leq k \leq l \leq r-9$, be integers. Then*

$$(|N_k| + |N_{k+1}| + \cdots + |N_l|) \geq \left\lfloor \frac{l-k+1}{4} \right\rfloor 4\delta.$$

Proof: By Lemma 2.4, let $y \in N_{\geq r-9}$ be a fixed vertex that is not related to z_r. Hence for all $u \in T(z, z_r) \cap N_{\geq 9}$ and $v \in T(z, y) \cap N_{\geq 9}$ we have $d_G(u, v) \geq 5$. For $i \geq 9$, let N'_i denote the set of elements in N_i that are within a distance of 2 from $T(z, y) \cap N_{\geq 9}$. Similarly, let N''_i be the set of all elements in N_i that are within a distance of 2 from $T(z, z_r) \cap N_{\geq 9}$. By the un-relatedness of z_r and y, we have

$$(\cup_{i=9}^{r-9} N_i') \cap (\cup_{i=9}^{r} N_i'') = \emptyset. \tag{2.5}$$

Claim 1 *Let i, $10 \leq i \leq r-11$, be an integer. Then*

$$|N_{i-1}'| + |N_i'| + |N_{i+1}'| + |N_{i+2}'| \geq 2\delta, \tag{2.6}$$

and

$$|N_{i-1}''| + |N_i''| + |N_{i+1}''| + |N_{i+2}''| \geq 2\delta. \tag{2.7}$$

Proof of Claim 1: We prove (2.6); (2.7) is treated similarly. Consider the edge uv on T, where u and v is the only vertex in $N_i' \cap T(z, y)$ and $N_{i+1}' \cap T(z, y)$, respectively. Note that $N(u) \cup N(v) \subseteq N_{i-1}' \cup N_i' \cup N_{i+1}' \cup N_{i+2}'$. Since G is triangle-free, we have $N(u) \cap N(v) = \emptyset$. It follows that

$$\begin{aligned} |N_{i-1}'| + |N_i'| + |N_{i+1}'| + |N_{i+2}'| &= |N_{i-1}' \cup N_i' \cup N_{i+1}' \cup N_{i+2}'| \\ &\geq |N(u) \cup N(v)| \\ &= |N(u)| + |N(v)| \geq 2\delta, \end{aligned}$$

and the claim is proven.

Now, if i, $10 \leq i \leq r-11$, is an integer, then

$$\begin{aligned} |N_{i-1}| + |N_i| + |N_{i+1}| + |N_{i+2}| &= |N_{i-1} \cup N_i \cup N_{i+1} \cup N_{i+2}| \\ &\geq \big| \big(N_{i-1}' \cup N_i' \cup N_{i+1}' \cup N_{i+2}'\big) \\ &\qquad \cup \big(N_{i-1}'' \cup N_i'' \cup N_{i+1}'' \cup N_{i+2}''\big) \big|. \end{aligned}$$

By (2.5),

$$\left(N'_{i-1} \cup N'_i \cup N'_{i+1} \cup N'_{i+2}\right) \cap \left(N''_{i-1} \cup N''_i \cup N''_{i+1} \cup N''_{i+2}\right) = \emptyset.$$

It follows that

$$\begin{aligned} |N_{i-1}| + |N_i| + |N_{i+1}| + |N_{i+2}| &\geq (|N'_{i-1}| + |N'_i| + |N'_{i+1}| + |N'_{i+2}|) \\ &\quad + (|N''_{i-1}| + |N''_i| + |N''_{i+1}| + |N''_{i+2}|). \end{aligned}$$

Therefore, by Claim 1, we have

$$|N_{i-1}| + |N_i| + |N_{i+1}| + |N_{i+2}| \geq 4\delta.$$

Applying this to the following sums, we get

$$\begin{aligned} |N_k| + |N_{k+1}| + \cdots + |N_l| &= (|N_k| + |N_{k+1}| + |N_{k+2}| + |N_{k+3}|) \\ &\quad + (|N_{k+4}| + |N_{k+5}| + |N_{k+6}| + |N_{k+7}|) + \cdots \\ &\geq \left\lfloor \frac{l-k+1}{4} \right\rfloor 4\delta, \end{aligned}$$

and the lemma is proven. □

Theorem 2.6 *Let G be a connected triangle-free graph of order n, minimum degree δ and maximum degree Δ. Then*

$$\text{rad}(G) \leq \frac{n - \Delta}{\delta} + O(1).$$

Moreover, this bound is asymptotically tight.

Proof: Denote the radius of G by r and assume the notation of z and N_i given above. If $r \leq 21$, then the theorem is trivially true, and so, from now onwards we assume that $r \geq 22$. Let v be a vertex in G of degree Δ. Let j be a fixed integer such that $v \in N_j$. Then $N[v] \subseteq N_{j-1} \cup N_j \cup N_{j+1}$, where $N_{-1} = \emptyset = N_{r+1}$, and so $\sum_{i=j-1}^{j+1} |N_i| \geq \Delta + 1$. We look at two cases:

Case A: $j \in \{11, 12, \ldots, r-11\}$. Then from Lemma 2.5, and the fact that $\sum_{i=j-1}^{j+1} |N_i| \geq \Delta + 1$, we get

$$\begin{aligned} n &= \sum_{i=0}^{r} |N_i| \\ &= \left(\sum_{i=0}^{8} |N_i|\right) + \left(\sum_{i=9}^{j-2} |N_i|\right) + \left(\sum_{i=j-1}^{j+1} |N_i|\right) + \left(\sum_{i=j+2}^{r-9} |N_i|\right) + \left(\sum_{i=r-8}^{r} |N_i|\right) \\ &\geq 9 + \left(\left\lfloor \frac{j-10}{4} \right\rfloor 4\delta\right) + (\Delta + 1) + \left(\left\lfloor \frac{r-j-10}{4} \right\rfloor 4\delta\right) + 9. \end{aligned}$$

The bound in the theorem follows upon re-arranging the terms.

Case B: $j \in \{0, 1, \ldots, 10\} \cup \{r-10, \ldots, r\}$. Then, as above,

$$n > \left(\sum_{i=j-1}^{j+1} |N_i|\right) + \left(\sum_{i=12}^{r-12} |N_i|\right) \geq (\Delta + 1) + \left(\left\lfloor \frac{r-21}{4} \right\rfloor 4\delta\right),$$

and again, the bound of the theorem follows upon re-arranging the terms.

To see that the bound is asymptotically tight, let n, δ, Δ and k, $k \geq 2$, be positive integers for which $k = \frac{n-\Delta+\delta-1}{2\delta}$, $2 \leq \delta \leq \Delta - 1$, and consider the graph $G_{n,\delta,\Delta}$ constructed as follows.

Let $S_1, S_2, \ldots, S_{4k-1}, S_{4k}$ be mutually disjoint sets such that

$$|S_i| = \begin{cases} 1 & \text{if} \quad i \equiv 0 \text{ or } 1 (\text{mod } 4), \\ \Delta - 1 & \text{if} \quad i = 2, \\ \delta & \text{if} \quad i = 4k-1, \\ \delta - 1 & \text{otherwise.} \end{cases}$$

Define graph $G_{n,\delta,\Delta}$ to be the graph with vertex set

$$V(G_{n,\delta,\Delta}) = S_1 \cup S_2 \cup \cdots \cup S_{4k-1} \cup S_{4k},$$

where vertices $u \in S_i$ and $v \in S_j$ are adjacent in $G_{n,\delta,\Delta}$ if $|i-j| = 1$. By inspection, $G_{n,\delta,\Delta}$ is triangle-free, has minimum degree δ, maximum degree Δ and $\text{rad}(G_{n,\delta,\Delta}) = 2k$. From $k = \frac{n-\Delta+\delta-1}{2\delta}$, we get

$$\text{rad}(G_{n,\delta,\Delta}) = \frac{n-\Delta}{\delta} + O(1),$$

as desired. □

From Theorem 2.6, we immediately obtain the following corollary.

Corollary 2.7 *Let G be a connected triangle-free graph of order n, minimum degree δ and maximum degree Δ. Then*

$$\text{diam}(G) \leq \frac{2(n-\Delta)}{\delta} + O(1).$$

Moreover, this bound is asymptotically tight. □

Next we show that if the irregularity index t is given, with $\Delta < \frac{3}{2}t$, then Theorem 2.6 and Corollary 2.7 can be improved.

Theorem 2.8 *Let G be a connected triangle-free graph of order n, irregularity index t, $t \geq 2$, and minimum degree δ. Then*

$$\mathrm{rad}(G) \leq \frac{n - \frac{3}{2}t}{\delta} + O(1).$$

Moreover, this bound is asymptotically tight.

Proof: Denote the radius of G by r and assume the notation of z and N_i given above. If $r \leq 22$, then the theorem is trivially true, and so, from now onwards we assume that $r > 22$. Let $\{v_1, v_2, \ldots, v_t\}$ be a set of t vertices such that $\deg(v_1) < \deg(v_2) < \cdots < \deg(v_t)$. Then $\deg(v_t) \geq \delta + t - 1$. Let

$$S = \{v_{\lceil \frac{t}{2} \rceil}, v_{\lceil \frac{t}{2} \rceil + 1}, \ldots, v_{t-1}\}.$$

Hence for every $x \in S$, $\deg(x) \geq \delta + \lceil \frac{t}{2} \rceil - 1$. Since $t \geq 2$, $S \neq \emptyset$. We now consider two cases.

CASE 1: *There exists a vertex $v \in S$ such that $d(v_t, v) \geq 3$.* Assume that $v_t \in N_i$ and $v \in N_j$, where $i, j \in \{0, 1, \ldots, r\}$. We assume that $i \leq j$; the case $j \leq i$ is treated analogously.

We look at two subcases separately.

SUBCASE 1: $|i - j| \leq 2$. Then since $N[v_t]$ and $N[v]$ are both contained in $\cup_{s=i-1}^{j+1} N_s$, and $N[v_t] \cap N[v] = \emptyset$, we have

$$\begin{aligned}
\sum_{s=i-1}^{j+1} |N_s| &\geq |N[v_t]| + |N[v]| \\
&\geq t + \delta - 1 + \left\lceil \frac{t}{2} \right\rceil + \delta - 1 \\
&\geq \frac{3}{2}t + 2\delta - 2.
\end{aligned}$$

Hence, if $11 \leq i \leq j \leq r - 11$, this, together with Lemma 2.5, gives

$$\begin{aligned}
n &= \sum_{s=0}^{r} |N_s| \\
&= \left(\sum_{s=0}^{8} |N_s|\right) + \left(\sum_{s=9}^{i-2} |N_s|\right) + \left(\sum_{s=i-1}^{j+1} |N_s|\right) + \left(\sum_{s=j+2}^{r-9} |N_s|\right) + \left(\sum_{s=r-8}^{r} |N_s|\right) \\
&\geq 9 + \left(\left\lfloor \frac{i-10}{4} \right\rfloor 4\delta\right) + \left(\frac{3}{2}t + 2\delta - 2\right) + \left(\left\lfloor \frac{r-j-10}{4} \right\rfloor 4\delta\right) + 9.
\end{aligned}$$

The bound in the theorem follows upon re-arranging the terms.

If either i or j is outside $\{11, 12, \ldots, r-11\}$, then the bound in the theorem is established as in Theorem 2.6, Case B.

Subcase 2: $|i - j| \geq 3$. Since $N[v_t] \subseteq N_{i-1} \cup N_i \cup N_{i+1}$, we have $\sum_{s=i-1}^{i+1} |N_s| \geq t + \delta - 1$. Similarly, since $N[v] \subseteq N_{j-1} \cup N_j \cup N_{j+1}$, we have $\sum_{s=j-1}^{j+1} |N_s| \geq \lceil \frac{t}{2} \rceil + \delta - 1$.

Assume that $11 \leq i < j \leq r - 11$. As in SUBCASE 1, we have

$$\begin{aligned}
n &= \sum_{s=0}^{r} |N_s| \\
&= \left(\sum_{s=0}^{8} |N_s|\right) + \left(\sum_{s=9}^{i-2} |N_s|\right) + \left(\sum_{s=i-1}^{i+1} |N_s|\right) + \left(\sum_{s=i+2}^{j-2} |N_s|\right) + \left(\sum_{s=j-1}^{j+1} |N_s|\right) + \\
&\quad \left(\sum_{s=j+2}^{r-9} |N_s|\right) + \left(\sum_{s=r-8}^{r} |N_s|\right) \\
&\geq 9 + \left(\left\lfloor \frac{i-10}{4} \right\rfloor 4\delta\right) + (t + \delta - 1) + \left(\left\lfloor \frac{j-i-3}{4} \right\rfloor 4\delta\right) + \left(\left\lceil \frac{t}{2} \right\rceil + \delta - 1\right) + \\
&\quad \left(\left\lfloor \frac{r-j-10}{4} \right\rfloor 4\delta\right) + 9.
\end{aligned}$$

The bound in the theorem follows upon re-arranging the terms. The case when either at least one of i or j is outside $\{11, 12, \ldots, r-11\}$ is treated similarly. This completes the proof for SUBCASE 2.

CASE 2: $d(v_t, x) \leq 2$ for every $x \in S$. Then $S \cup N[v_t] \subseteq N^2[v_t]$.

Claim 2 $|N^2[v_t]| \geq \frac{3}{2}t + \delta - 1$.

Proof of Claim 2: If v_t is adjacent to a vertex w of S, then since G is triangle-free,

$$\begin{aligned}
|N^2[v_t]| &\geq |N(v_t)| + |N(w)| \\
&\geq \delta + t - 1 + \delta + \left\lceil \frac{t}{2} \right\rceil - 1 \\
&= \frac{3}{2}t + 2\delta - 2 \geq \frac{3}{2}t + \delta - 1,
\end{aligned}$$

as claimed. If v_t is not adjacent to any vertex of S, then we have $N[v_t] \cap S = \emptyset$. Hence, from $S \cup N[v_t] \subseteq N^2[v_t]$, we get

$$\begin{aligned} |N^2[v_t]| &\geq |N[v_t]| + |S| \\ &\geq \delta + t + \left\lceil \frac{t}{2} \right\rceil - 1 \\ &\geq \frac{3}{2}t + \delta - 1, \end{aligned}$$

as desired. This completes the proof of Claim 2.

Let N_j be the distance layer containing v_t. Then, as before, using Lemma 2.5, Claim 2, and the equation

$$n = \sum_{s=0}^{j-3} |N_s| + \sum_{i=j-2}^{j+2} |N_s| + \sum_{s=j+3}^{r} |N_s|,$$

we get the bound in the theorem. We conclude from CASE 1 and 2 that

$$\mathrm{rad}(G) \leq \frac{n - \frac{3}{2}t}{\delta} + O(1),$$

and the bound in the theorem is proven. Finally, let us mention that, analogously to the construction done in Theorem 2.6, it is an easy exercise to construct a graph attaining the bound in the present theorem. □

Corollary 2.9 *Let G be a connected triangle-free graph of order n, irregularity index t, $t \geq 2$, and minimum degree δ. Then*

$$\mathrm{diam}(G) \leq \frac{2(n - \frac{3}{2}t)}{\delta} + O(1).$$

Moreover, this bound is asymptotically tight. □

We now turn our attention to C_4-free graphs.

Theorem 2.10 *Let G be a connected C_4-free graph of order n, minimum degree δ and maximum degree Δ. Then*

(i) $\mathrm{diam}(G) \leq \dfrac{5(n-\Delta(\delta-1)-1)}{\delta^2 - 2\lceil\frac{\delta}{2}\rceil + 1} + 8,$

(ii) $\mathrm{rad}(G) \leq \dfrac{5(n-\Delta(\delta-1)-1)}{2(\delta^2 - 2\lceil\frac{\delta}{2}\rceil + 1)} + \dfrac{9}{2}.$

Moreover these bounds are asymptotically tight.

Proof: Let v be a fixed vertex of G with degree Δ. Since G is C_4-free, each neighbour of v has at most one neighbour in $N(v)$ and no two neighbours of v have a common neighbour apart from v. It follows that

$$|N^2[v]| \geq \begin{cases} \Delta(\delta-1)+1, & \text{if} \quad \Delta \quad \text{is even,} \\ \Delta(\delta-1)+2, & \text{if} \quad \Delta \quad \text{is odd.} \end{cases}$$

Therefore, comparing the two lower bounds, we deduce that

$$|N^2[v]| \geq \Delta(\delta-1)+1. \tag{2.8}$$

Similarly, if w is in $V-\{v\}$, then $|N^2[w]| \geq \delta^2 - 2\lceil\frac{\delta}{2}\rceil + 1$.

We find a maximal 4-packing A of G using the following procedure. Let $A=\{v\}$. Add vertices x with $d(x,A)=5$ to A until each of the vertices not in A are within distance 4 of A. By our construction of A, for any two vertices $x, y \in A$, we have

$N^2[x] \bigcap N^2[y] = \emptyset$. Therefore,

$$\begin{aligned} n &\geq |\bigcup_{x \in A} N^2[x]| \\ &= |N^2[v]| + \sum_{x \in A - \{v\}} |N^2[x]| \\ &\geq (\Delta(\delta - 1) + 1) + (|A| - 1)\left(\delta^2 - 2\left\lceil \frac{\delta}{2} \right\rceil + 1\right). \end{aligned}$$

Hence, we have proved

Claim 3 $|A| \leq \dfrac{n - \Delta(\delta - 1) - 1}{\delta^2 - 2\lceil \frac{\delta}{2} \rceil + 1} + 1.$

For $x \in A$, let $T_1(x) \leq G$ be the tree with $V(T_1(x)) = N^2[x]$, which is distance preserving from x. Then $T_2 = \bigcup_{x \in A} T_1(x)$ is a subforest of G. By our construction of A, there exists $|A| - 1$ edges in G, each of them joining two components of T_2, whose addition to T_2 gives a tree $T_3 \leq G$.

Extend the tree T_3 to a spanning tree T of G with $d_T(x, A) = d_G(x, A)$ for each $x \in V(G)$. We have by construction that $T^5[A]$ is connected and that $\text{diam}(T^5[A]) \leq |A| - 1$, so

$$d_T(x, y) \leq 5(|A| - 1) \text{ for all } x, y \in A. \tag{2.9}$$

We now bound $\text{diam}(T)$. Let u, v be arbitrary vertices in T. By our construction u and v are each within distance 4 of A. Let $u', v' \in A$ be such that $d_T(u, u') \leq 4$ and $d_T(v, v') \leq 4$.

This, together with (2.9), gives

$$\begin{aligned} d_T(u,v) &\leq d_T(u,u') + d_T(u',v') + d_T(v',v) \leq 4 + d_T(u',v') + 4 \\ &\leq 4 + 5(|A|-1) + 4 \\ &= 5(|A|-1) + 8. \end{aligned}$$

It follows from Claim 3 that

$$d_T(u,v) \leq 5\Big(\frac{n-\Delta(\delta-1)-1}{\delta^2 - 2\lceil\frac{\delta}{2}\rceil + 1}\Big) + 8,$$

and so

$$\text{diam}(T) \leq 5\Big(\frac{n-\Delta(\delta-1)-1}{\delta^2 - 2\lceil\frac{\delta}{2}\rceil + 1}\Big) + 8.$$

Therefore,

$$\text{diam}(G) \leq 5\Big(\frac{n-\Delta(\delta-1)-1}{\delta^2 - 2\lceil\frac{\delta}{2}\rceil + 1}\Big) + 8, \tag{2.10}$$

and so the bound in (i) is proven. To establish the bound in (ii), observe from Fact 2.1 and (2.10) that $\text{rad}(T) \leq \frac{1}{2}(\text{diam}(T)+1) \leq \frac{5(n-\Delta(\delta-1)-1)}{2(\delta^2 - 2\lceil\frac{\delta}{2}\rceil + 1)} + \frac{9}{2}$.

Thus, $\text{rad}(G) \leq \text{rad}(T) \leq \frac{5(n-\Delta(\delta-1)-1)}{2(\delta^2 - 2\lceil\frac{\delta}{2}\rceil + 1)} + \frac{9}{2}$, and (ii) is proven. □

2.4 Conclusion

In this chapter, we proved an asymptotically sharp upper bound on the radius in terms of order, minimum degree and the irregularity index. Our bound is a strengthening of the bound by Erdös, Pach, Pollack and Tuza, [24]. We also gave similar improved bounds on the diameter and radius for triangle-free and for C_4-free graphs. Further, we also gave asymptotically sharp upper bounds on the radius and diameter when order, minimum, and maximum degree of the graph are given. In Chapter 3, we give asymptotically sharp upper bounds for the Gutman index in terms of order and minimum degree δ for every $\delta \geq 2$. Our method relies on the diameter of a graph.

Chapter 3

The Gutman index and minimum degree

3.1 Introduction

In Chapter 2, we improved the upper bound on the radius in terms of order, minimum degree and the irregularity index. We also gave similar improved bounds on the diameter and radius for triangle-free and for C_4-free graphs. In this chapter, we improve the bound of Mukwembi, [43], for $\delta \geq 3$, on the Gutman index and show that

$$\mathrm{Gut}(G) \leq \frac{2^4 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4),$$

where n is the order of the graph G and the minimum degree $\delta \geq 2$ is a constant. Moreover we show that our bound is asymptotically sharp for every $\delta \geq 2$.

3.2 Results

First we present the following lemma, which will be used in the proof of our main result.

Lemma 3.1 *Let G be a connected graph of order n, diameter d and minimum degree δ, where δ is a constant. Let v, v' be any vertices of G.*

(1) Then $\deg(v) \leq n - \frac{1}{3}d(\delta+1) + \delta$.

(2) If $d(v, v') \geq 3$, then $\deg(v) + \deg(v') \leq n - \frac{1}{3}d(\delta+1) + 4\delta$.

Proof: Let $P : v_0, v_1, \ldots, v_d$ be a diametric path of G. Let $S \subset V(P)$ be the set

$$S := \Big\{ v_{3i+1} : i = 0, 1, 2, \ldots, \Big\lfloor \frac{d-1}{3} \Big\rfloor \Big\}.$$

For each $u \in S$, choose any δ neighbours $u_1, u_2, \ldots, u_\delta$ of u and denote the set $\{u, u_1, u_2, \ldots, u_\delta\}$ by $P[u]$. Let $\mathbf{P} = \cup_{u \in S} P[u]$. Then

$$|\mathbf{P}| = (\delta+1)\Big(\Big\lfloor \frac{d-1}{3} \Big\rfloor + 1\Big).$$

Let v be any vertex of G. We denote by $N[v]$ the closed neighbourhood of v, which is the set that consists of v and its neighbours. Note that if $v \notin \mathbf{P}$, then v can be adjacent to at most one vertex in S and to neighbors of at most 2 vertices of S, hence v is adjacent to at most $2\delta + 1$ vertices in $\mathbf{P}$. If $v \in \mathbf{P}$, then it can be checked that v can be adjacent to at most 2δ vertices in $\mathbf{P}$. In both cases we obtain

$|\mathbf{P} \cap N[v]| \leq 2\delta + 1$ which implies

$$\begin{aligned} n &\geq |\mathbf{P}| + |N[v]| - |\mathbf{P} \cap N[v]| \\ &\geq (\delta+1)\Big(\Big\lfloor \frac{d-1}{3} \Big\rfloor + 1\Big) + (\deg(v)+1) - (2\delta+1) \\ &\geq (\delta+1)\frac{d}{3} + \deg(v) - 2\delta. \end{aligned}$$

Rearranging the terms, we obtain $\deg(v) \leq n - \frac{1}{3}d(\delta+1) + 2\delta$, which completes the proof of (1).

Now we prove the statement (2). If v, v' are any two vertices of G, such that $d(v, v') \geq 3$, then $N[v] \cap N[v'] = \emptyset$. It follows that

$$\begin{aligned} n &\geq |\mathbf{P}| + |N[v]| + |N[v']| - |\mathbf{P} \cap N[v]| - |\mathbf{P} \cap N[v']| \\ &\geq (\delta+1)\Big(\Big\lfloor \frac{d-1}{3} \Big\rfloor + 1\Big) + (\deg(v)+1) + (\deg(v')+1) - 2(2\delta+1) \\ &\geq (\delta+1)\frac{d}{3} + \deg(v) + \deg(v') - 4\delta, \end{aligned}$$

which implies $\deg(v) + \deg(v') \leq n - \frac{1}{3}d(\delta+1) + 4\delta$. □

Now we present our main result.

Theorem 3.2 *Let G be a connected graph of order n and minimum degree δ, where δ is a constant. Then*

$$\mathrm{Gut}(G) \leq \frac{2^4 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4),$$

and this bound is asymptotically sharp.

Proof: We denote the diameter of G (the largest distance between any two vertices in G) by d. Let $P : v_0, v_1, \ldots, v_d$ be a diametric path of G and let $S \subset V(P)$ be the set

$$S := \Big\{ v_{3i+1} : i = 0, 1, 2, \ldots, \Big\lfloor \frac{d-1}{3} \Big\rfloor \Big\}.$$

For each $v \in S$, choose any δ neighbours $u_1, u_2, \ldots, u_\delta$ of v and denote the set $\{v, u_1, u_2, \ldots, u_\delta\}$ by $P[v]$. Let $\mathbf{P} = \cup_{v \in S} P[v]$. Then

$$|\mathbf{P}| = (\delta + 1)\Big(\Big\lfloor \frac{d-1}{3} \Big\rfloor + 1 \Big). \tag{3.1}$$

Now let $\mathcal{V} = \{\{x, y\} : x, y \in V\}$. We partition $\mathcal{V}$ as follows:

$$\mathcal{V} = \mathcal{P} \cup \mathcal{A} \cup \mathcal{B},$$

where

$$\mathcal{P} := \{\{x, y\} \ : \ x \in \mathbf{P} \text{ and } y \in V(G)\}, \ \mathcal{A} := \{\{x, y\} \in \mathcal{V} - \mathcal{P} \ : \ d(x, y) \geq 3\}$$

and

$$\mathcal{B} := \{\{x, y\} \in \mathcal{V} - \mathcal{P} \ : \ d(x, y) \leq 2\}.$$

Setting $|\mathcal{A}| = a$, $|\mathcal{B}| = b$, we have $\binom{n}{2} = |\mathcal{P}| + a + b$, and so from (3.1), $a + b =$

$$\binom{n - |\mathbf{P}|}{2} = \frac{1}{2}\Big[n - (\delta + 1)\Big(\Big\lfloor \frac{d-1}{3} \Big\rfloor + 1 \Big) \Big] \Big[n - (\delta + 1)\Big(\Big\lfloor \frac{d-1}{3} \Big\rfloor + 1 \Big) - 1 \Big]. \tag{3.2}$$

Note that

$$\begin{aligned} \mathrm{Gut}(G) &= \sum_{\{x,y\} \in \mathcal{A}} \deg(x)\deg(y)d(x, y) + \sum_{\{x,y\} \in \mathcal{B}} \deg(x)\deg(y)d(x, y) \\ &+ \sum_{\{x,y\} \in \mathcal{P}} \deg(x)\deg(y)d(x, y). \end{aligned}$$

We bound each term separately.

Claim 4 *Assume the notation above. Then*

$$\sum_{\{x,y\}\in\mathcal{P}} \deg(x)\deg(y)d(x,y) \leq O(n^4).$$

Proof of Claim 4: We partition S as $S = S_1 \cup S_2$, where $S_1 = \{v_j \in S : j \equiv 1 \pmod 6\}$, and $S_2 = S - S_1$. It follows that $\mathbf{P} = (\cup_{v\in S_1} P[v]) \cup (\cup_{v\in S_2} P[v])$.

For each vertex x in $\mathbf{P}$, define the score $s(x)$ of x as

$$s(x) := \sum_{y\in V} \deg(x)\deg(y)d(x,y).$$

Then

$$\sum_{\{x,y\}\in\mathcal{P}} \deg(x)\deg(y)d(x,y) \leq \sum_{x\in\mathbf{P}} s(x) = \sum_{x\in(\cup_{v\in S_1} P[v])} s(x) + \sum_{x\in(\cup_{v\in S_2} P[v])} s(x).$$

We now consider $\cup_{v\in S_1} P[v]$. For each $u, v \in S_1$, $u \neq v$, we have $P[u] \cap P[v] = \emptyset$ and the neighbourhoods of $P[u]$ and $P[v]$ are also disjoint. Write the elements of S_1 as $S_1 = \{w_1, w_2, \ldots, w_{|S_1|}\}$. For each $w_j \in S_1$, let $P[w_j] = \{w_j, w_1^j, w_2^j, \ldots, w_\delta^j\}$, where $w_1^j, w_2^j, \ldots, w_\delta^j$ are neighbours of w_j. Then

$$n \geq (\deg(w_1)+1) + (\deg(w_2)+1) + \cdots + (\deg(w_{|S_1|})+1)$$

and for $t = 1, 2, \ldots, \delta$,

$$n \geq (\deg(w_t^1)+1) + (\deg(w_t^2)+1) + \cdots + (\deg(w_t^{|S_1|})+1).$$

Summing we get

$$(\delta+1)n \geq \sum_{x\in\left(\cup_{u\in S_1} P[u]\right)} \deg(x) + (\delta+1)|S_1|.$$

That is,

$$\sum_{x\in\left(\cup_{u\in S_1}P[u]\right)} \deg(x) \leq (\delta+1)n - (\delta+1)|S_1|. \tag{3.3}$$

Similarly,

$$\sum_{x\in\left(\cup_{u\in S_2}P[u]\right)} \deg(x) \leq (\delta+1)n - (\delta+1)|S_2|. \tag{3.4}$$

Now from Lemma 3.1, for every $x \in \mathbf{P}$, we have

$$\begin{aligned} s(x) &= \deg(x)\left(\sum_{y\in V}\deg(y)d(x,y)\right) \\ &\leq \deg(x)\left(\sum_{y\in V}\left(n-\frac{1}{3}d(\delta+1)+2\delta\right)d\right) \\ &\leq \deg(x)\left(dn\left(n-\frac{1}{3}d(\delta+1)+2\delta\right)\right). \end{aligned}$$

This, in conjunction with (3.3), (3.4) and the fact that δ is a constant, yields

$$\begin{aligned} &\sum_{\{x,y\}\in\mathcal{P}}\deg(x)\deg(y)d_G(x,y) \\ \leq\ & \sum_{x\in(\cup_{v\in S_1}P[v])}\left[\deg(x)\left[dn\left(n-\frac{1}{3}d(\delta+1)+2\delta\right)\right]\right] \\ +\ & \sum_{x\in(\cup_{v\in S_2}P[v])}\left[\deg(x)\left[dn\left(n-\frac{1}{3}d(\delta+1)+2\delta\right)\right]\right] \\ =\ & dn\left(n-\frac{1}{3}d(\delta+1)+2\delta\right)\left(\sum_{x\in(\cup_{v\in S_1}P[v])}\deg(x)+\sum_{x\in(\cup_{v\in S_2}P[v])}\deg(x)\right) \\ \leq\ & dn\left(n-\frac{1}{3}d(\delta+1)+2\delta\right)\left[(\delta+1)n-(\delta+1)|S_1|+(\delta+1)n-(\delta+1)|S_2|\right] \\ =\ & dn\left(n-\frac{1}{3}d(\delta+1)+2\delta\right)\left[2(\delta+1)n-(\delta+1)\left\lfloor\frac{d-1}{3}\right\rfloor\right] \\ =\ & O(n^4), \end{aligned}$$

as required and so Claim 4 is proven.

Now we bound those pairs of vertices, which are in $\mathcal{B}$.

Claim 5 *Assume the notation above. Then*

$$\sum_{\{x,y\}\in\mathcal{B}} \deg(x)\deg(y)d(x,y) \leq O(n^4).$$

Proof of Claim 5: Note that if $\{x,y\} \in \mathcal{B}$, then $d(x,y) \leq 2$. This, together with Lemma 3.1 and the fact that $b = O(n^2)$, gives

$$\begin{aligned}\sum_{\{x,y\}\in\mathcal{B}} \deg(x)\deg(y)d(x,y) &\leq \sum_{\{x,y\}\in\mathcal{B}} 2\Big(n - \frac{1}{3}d(\delta+1) + 2\delta\Big)^2 \\ &= 2b\Big(n - \frac{1}{3}d(\delta+1) + 2\delta\Big)^2 \\ &= O(n^4),\end{aligned}$$

as claimed.

Finally, we study pairs of vertices, which are in $\mathcal{A}$.

Claim 6 *Assume the notation above. Then*

$$\sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x,y) \leq \frac{1}{16}d\Big(n - \frac{1}{3}d(\delta+1)\Big)^4 + O(n^4).$$

Proof of Claim 6: Let $\{w,z\}$ be a pair in $\mathcal{A}$, such that $\deg(w)+\deg(z)$ is maximum. Let $\deg(w) + \deg(z) = s$. Since $\deg(w)\deg(z) \leq \frac{1}{4}(\deg(w) + \deg(z))^2$, we have

$$\deg(w)\deg(z) \leq \frac{1}{4}s^2. \tag{3.5}$$

Now we find an upper bound on a, the cardinality of $\mathcal{A}$. From (3.2) we have

$$a = \frac{1}{2}\Big[n-(\delta+1)\Big(\Big\lfloor\frac{d-1}{3}\Big\rfloor+1\Big)\Big]\Big[n-(\delta+1)\Big(\Big\lfloor\frac{d-1}{3}\Big\rfloor+1\Big)-1\Big]-b. \qquad (3.6)$$

Note that all pairs $\{x,y\}, x,y\in N[w]-\mathbf{P}$ and all pairs $\{x,y\}, x,y\in N[z]-\mathbf{P}$ (where $N[w]$ ($N[z]$) is the closed neighbourhood of w (of z)) are in $\mathcal{B}$. Since w (and z) can be adjacent to at most one vertex in S and to neighbours of at most 2 vertices of S, it follows that w (and z) is adjacent to at most $2\delta+1$ vertices in $\mathbf{P}$. Then we have

$$\begin{aligned} b &\geq \binom{\deg(w)-2\delta}{2}+\binom{\deg(z)-2\delta}{2} \\ &= \frac{1}{2}([\deg(w)]^2+[\deg(x)]^2)-\frac{4\delta+1}{2}(\deg(w)+\deg(z))+(4\delta^2+2\delta) \\ &\geq \frac{1}{4}s^2-\frac{4\delta+1}{2}s+(4\delta^2+2\delta). \end{aligned}$$

Hence from (3.6), we get

$$\begin{aligned} a &\leq \frac{1}{2}\Big[n-(\delta+1)\Big(\Big\lfloor\frac{d-1}{3}\Big\rfloor+1\Big)\Big]\Big[n-(\delta+1)\Big(\Big\lfloor\frac{d-1}{3}\Big\rfloor+1\Big)-1\Big] \\ &- \frac{1}{4}s^2+\frac{4\delta+1}{2}s-(4\delta^2+2\delta). \end{aligned}$$

From (3.5), we have

$$\begin{aligned} \sum_{\{x,y\}\in\mathcal{A}} & \deg(x)\deg(y)d(x,y) \leq \sum_{\{x,y\}\in\mathcal{A}}\frac{s^2d}{4} \\ \leq & \frac{s^2d}{4}\Bigg[\frac{1}{2}\Big[n-(\delta+1)\Big(\Big\lfloor\frac{d-1}{3}\Big\rfloor+1\Big)\Big]\Big[n-(\delta+1)\Big(\Big\lfloor\frac{d-1}{3}\Big\rfloor+1\Big)-1\Big] \\ - & \frac{1}{4}s^2+\frac{4\delta+1}{2}s-(4\delta^2+2\delta)\Bigg]. \end{aligned}$$

By Lemma 3.1, $s\leq n-\frac{1}{3}d(\delta+1)+4\delta$. Subject to this condition

$\frac{s^2d}{4}\Big[\frac{1}{2}\Big[n-(\delta+1)(\Big\lfloor\frac{d-1}{3}\Big\rfloor+1)\Big]\Big[n-(\delta+1)(\Big\lfloor\frac{d-1}{3}\Big\rfloor+1)-1\Big]-\frac{1}{4}s^2+\frac{4\delta+1}{2}s-(4\delta^2+2\delta)\Big]$

is maximized for $s = n - \frac{1}{3}d(\delta+1) + O(1)$ to give

$$\begin{aligned}
&\sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x,y) \\
&\leq \frac{d}{4}\Big(n-\frac{1}{3}d(\delta+1)\Big)^2\Big[\frac{1}{2}\Big(n-\frac{1}{3}d(\delta+1)\Big)^2-\frac{1}{4}\Big(n-\frac{1}{3}d(\delta+1)\Big)^2+O(n)\Big] \\
&= \frac{d}{16}\Big(n-\frac{1}{3}d(\delta+1)\Big)^4+O(n^4).
\end{aligned}$$

The proof of Claim 6 is complete.

Now we can complete the proof of the theorem. From Claims 4, 5 and 6, we get

$$\begin{aligned}
\mathrm{Gut}(G) &= \sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x,y) + \sum_{\{x,y\}\in\mathcal{B}} \deg(x)\deg(y)d(x,y) \\
&+ \sum_{\{x,y\}\in\mathcal{P}} \deg(x)\deg(y)d(x,y) \\
&\leq \frac{1}{16}d\Big(n-\frac{1}{3}d(\delta+1)\Big)^4+O(n^4)+O(n^4)+O(n^4) \\
&= \frac{1}{16}d\Big(n-\frac{1}{3}d(\delta+1)\Big)^4+O(n^4).
\end{aligned}$$

The term

$$\frac{1}{16}d\Big(n-\frac{1}{3}d(\delta+1)\Big)^4$$

is maximized, with respect to d, for $d = \frac{3n}{5(\delta+1)}$ to give

$$\mathrm{Gut}(G) \leq \frac{2^4\cdot 3}{5^5(\delta+1)}n^5+O(n^4),$$

as desired.

It remains to show that the bound is asymptotically sharp. We construct the graph

$G_{n,d,\delta}$ for $d \equiv 1 \pmod 3$. Let $V(G) = V_0 \cup V_1 \cup \ldots \cup V_d$, where

$$|V_i| = \begin{cases} \delta - 1 & \text{if} \quad i \equiv 2 \pmod 3, \\ \lceil \frac{1}{2}(n - \frac{1}{3}(d-1)(\delta+1)) \rceil & \text{if} \quad i = 0, \\ \lfloor \frac{1}{2}(n - \frac{1}{3}(d-1)(\delta+1)) \rfloor & \text{if} \quad i = d, \\ 1 & \text{otherwise.} \end{cases}$$

Let two distinct vertices $v \in V_i, v' \in V_j$ be adjacent if and only if $|j - i| \leq 1$, and let $d = \frac{3n}{5(\delta+1)}$ be an integer. Then the graph $G_{n, \frac{3n}{5(\delta+1)}, \delta}$ has order n, minimum degree δ and the Gutman index is $\frac{2^4 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4)$. □

Lemma 1.11 proved in [18] can be used to obtain a bound on the edge-Wiener index of a graph G.

Corollary 3.3 *Let G be a connected graph of order n. Then*

$$W_e(G) \leq \frac{2^2 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4)$$

and the bound is asymptotically sharp.

Proof: From Theorem 3.2 and Lemma 1.11, we obtain

$$W_e(G) \leq \frac{2^2 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4).$$

The graph $G_{n,d,\delta}$ is also the extremal graph on the edge-Wiener index

$$W_e(G_{n,d,\delta}) = \frac{2^2 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4),$$

therefore the bound is best possible. □

3.3 Conclusion

In this chapter, we improved the bound of Mukwembi, [43], for $\delta \geq 3$, and we precisely showed that

$$\text{Gut}(G) \leq \frac{2^4 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4),$$

where n is the order of the graph G and the minimum degree $\delta \geq 2$ is a constant. In [43], Mukwembi showed that for any graph of order n, the Gutman index of G, $\text{Gut}(G) \leq \frac{2^4}{5^5} n^5 + O(n^4)$. This bound is best possible only for graphs of vertex-connectivity $\kappa = 1$. In the next chapter, we show that $\text{Gut}(G) \leq \frac{2^4}{5^5 \kappa} n^5 + O(n^4)$ for graphs of order n and vertex-connectivity κ, where κ is a constant. Our bound is asymptotically sharp for every $\kappa \geq 1$ and it substantially generalizes the bound of Mukwembi, [43].

Chapter 4

The Gutman index and the edge-Wiener index of graphs with given vertex-connectivity

4.1 Introduction

In Chapter 3 we precisely showed that

$$\mathrm{Gut}(G) \le \frac{2^4 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4),$$

where n is the order of the graph G and the minimum degree $\delta \ge 2$ is a constant. The goal of this chapter is to find asymptotically sharp upper bounds on the Gutman index of graphs of given order and vertex-connectivity. We show that

$$\mathrm{Gut}(G) \le \frac{2^4}{5^5 \kappa} n^5 + O(n^4)$$

for connected graphs G of order n and vertex-connectivity $\kappa \ge 1$, where κ is a constant. Our bound is best possible for every $\kappa \ge 1$ and it substantially generalizes the bound in [43], and improves on the bound in [40]. We also obtain, as a corollary, a similar result for the edge-Wiener index of connected graphs of given order and vertex-connectivity.

4.2 Results

First we bound degrees of vertices of a graph G in terms of the order, diameter and vertex-connectivity of G. This result will be used in the proof of Theorem 4.2, which bounds the Gutman index of a graph.

Lemma 4.1 *Let G be a connected graph of order n, diameter d and vertex-connectivity κ, where κ is a constant. Let v, v' be any vertices of G.*

(i) Then $\deg(v) \leq n - \kappa d + 4\kappa - 3$.

(ii) If $d(v, v') \geq 3$, then $\deg(v) + \deg(v') \leq n - \kappa d + 7\kappa - 4$.

Proof: Let G be a connected graph of order n, diameter d and vertex-connectivity κ. Let v_0 be any vertex of G of eccentricity d and let N_i be the i-th neighbourhood of v_0, $i = 0, 1, 2, \ldots, d$.

Let $v \in V(G)$. Then $v \in N_i$ for some i. Note that $N(v) \subset N_{i-1} \cup N_i \cup N_{i+1}$, which implies that $\deg(v) \leq |N_{i-1}| + |N_i| + |N_{i+1}| - 1$. It is also easy to see that removal of all vertices in N_i, $i = 1, 2, \ldots, d-1$, disconnects G, thus $|N_i| \geq \kappa$ for

$i = 1, 2, \dots, d-1$. It follows that

$$\begin{aligned} n = |\cup_{j=0}^{d} N_j| &\geq |\cup_{j=0}^{i-2} N_j| + \deg(v) + |\{v\}| + |\cup_{j=i+2}^{d} N_j| \\ &\geq \deg(v) + 1 + \kappa(d-4) + 2, \end{aligned}$$

Rearranging the terms, we obtain $\deg(v) \leq n - \kappa d + 4\kappa - 3$, which completes the proof of (i).

Now we prove the statement (ii). Let $v, v' \in V(G)$ such that $d(v, v') \geq 3$. Then $N(v) \cap N(v') = \emptyset$. Since $|N_i| \geq \kappa$ for $i = 1, 2, \dots, d-1$ and $\deg(v) \leq |N_{i-1}| + |N_i| + |N_{i+1}| - 1$ (simiarly for v'), we obtain

$$n \geq (\deg(v) + 1) + (\deg(v') + 1) + (d-7)\kappa + 2.$$

Rearranging the terms, we get $\deg(v)+ \deg(v') \leq n - \kappa d + 7\kappa - 4$, which completes the proof of (ii). $\square$

In the following theorem we present an upper bound on the Gutman index of a graph G in terms of its order, diameter and vertex-connectivity.

Theorem 4.2 *Let G be a connected graph of order n, diameter d and vertex-connectivity κ, where κ is a constant. Then*

$$\mathrm{Gut}(G) \leq \frac{1}{16} d\Big(n - \kappa d\Big)^4 + O(n^4),$$

and the bound is asymptotically sharp.

Proof: Let v_0 be a vertex of G of eccentricity d and let N_i be the i-th neighbourhood of v_0, $i = 0, 1, 2, \dots, d$. Since $|N_i| \geq \kappa$ for all $i = 1, 2, \dots, d-1$, we can choose κ vertices $u_{i1}, u_{i2}, \ldots, u_{i\kappa}$ of N_i. Then for each $j = 1, 2, \ldots, \kappa$, let $P_j = \{u_{1j}, u_{2j}, u_{3j}, \ldots, u_{d-1j}\}$ and $P = \cup_{j=1}^{d-1} P_j$. We have

$$|P| = (d-1)\kappa \tag{4.1}$$

We partition the 2-subsets of $V(G)$, $\mathcal{V} = \{\{x, y\} : x, y \in V(G)\}$, as follows:

$$\mathcal{V} = \mathcal{P} \cup \mathcal{A} \cup \mathcal{B},$$

where

$$\mathcal{P} = \{\{x, y\} : x \in P \text{ and } y \in V(G)\},\ \mathcal{A} = \{\{x, y\} \in \mathcal{V} - \mathcal{P} : d(x, y) \geq 3\}$$

and

$$\mathcal{B} = \{\{x, y\} \in \mathcal{V} - \mathcal{P} : d(x, y) \leq 2\}.$$

We set $|\mathcal{A}| = a$, $|\mathcal{B}| = b$, which implies $\binom{n}{2} = |\mathcal{P}| + a + b$, and consequently from (4.1) we obtain

$$a + b = \binom{n - |P|}{2} = \frac{1}{2}\Big[n - (d-1)\kappa\Big]\Big[n - (d-1)\kappa - 1\Big]. \tag{4.2}$$

Note that

$$\begin{aligned} \mathrm{Gut}(G) &= \sum_{\{x,y\} \in \mathcal{A}} \deg(x)\deg(y)d(x, y) + \sum_{\{x,y\} \in \mathcal{B}} \deg(x)\deg(y)d(x, y) \\ &+ \sum_{\{x,y\} \in \mathcal{P}} \deg(x)\deg(y)d(x, y). \end{aligned}$$

We bound these three terms in the following claims.

Claim 7 *Assume the notation above. Then*

$$\sum_{\{x,y\} \in \mathcal{P}} \deg(x)\deg(y)d(x, y) \leq O(n^4).$$

Proof of Claim 7: For $j = 1, 2, \ldots \kappa$, let $P_j = U_{1j} \cup U_{2j} \cup U_{3j}$, where U_{1j}, U_{2j} and U_{3j} are defined as follows:

$$U_{1j} = \{u_{1j}, u_{4j}, u_{7j}, \ldots\},$$

$$U_{2j} = \{u_{2j}, u_{5j}, u_{8j}, \ldots\}.$$

$$U_{3j} = \{u_{3j}, u_{6j}, u_{9j}, \ldots\}.$$

Note that for any two different vertices x, y in the same set U_{ij}, $i = 1, 2, 3$, we have $N(x) \cap N(y) = \emptyset$, since $d(x, y) \geq 3$. Therefore $\sum_{x \in U_{ij}} \deg(x) < n$ for $i = 1, 2, 3$.

For each vertex x in P, we define the score $s(x)$ as

$$\begin{aligned} s(x) &= \sum_{y \in V(G)} \deg(x)\deg(y)d(x, y) \\ &= \deg(x)\Big(\sum_{y \in V(G)} \deg(y)d(x, y)\Big). \end{aligned}$$

Then from Lemma 4.1 we have

$$\begin{aligned} s(x) &\leq \deg(x)\Big(\sum_{y \in V(G)} (n - \kappa d + O(1))d(x, y)\Big) \\ &= \deg(x)(n - \kappa d + O(1))\Big(\sum_{y \in V(G)} d(x, y)\Big) \\ &< \deg(x)(n - \kappa d + O(1))(nd). \end{aligned}$$

Then for $j = 1, 2, \ldots \kappa$,

$$\begin{aligned}
\sum_{x \in P_j} s(x) &= \sum_{x \in U_{1j}} s(x) + \sum_{x \in U_{2j}} s(x) + \sum_{x \in U_{3j}} s(x) \\
&< \sum_{x \in U_{1j}} \deg(x)(n - \kappa d + O(1))(nd) + \sum_{x \in U_{2j}} \deg(x)(n - \kappa d + O(1))(nd) \\
&+ \sum_{x \in U_{3j}} \deg(x)(n - \kappa d + O(1))(nd) \\
&= (n - \kappa d + O(1))(nd)\Big(\sum_{x \in U_{1j}} \deg(x) + \sum_{x \in U_{2j}} \deg(x) + \sum_{x \in U_{3j}} \deg(x)\Big) \\
&< (n - \kappa d + O(1))(nd)(3n).
\end{aligned}$$

Hence

$$\begin{aligned}
\sum_{\{x,y\} \in \mathcal{P}} \quad & \deg(x)\deg(y)d(x,y) \le \sum_{x \in P} s(x) \\
= \quad & \sum_{x \in P_1} s(x) + \sum_{x \in P_2} s(x) + \ldots + \sum_{x \in P_\kappa} s(x) \\
< \quad & \kappa(n - \kappa d + O(1))(nd)(3n),
\end{aligned}$$

which implies Claim 7.

Now we study pairs of vertices, which are in $\mathcal{B}$.

Claim 8 *Assume the notation above. Then*

$$\sum_{\{x,y\} \in \mathcal{B}} \deg(x)\deg(y)d(x,y) \le O(n^4).$$

Proof of Claim 8: We know that if $\{x, y\} \in \mathcal{B}$, then $d(x, y) \leq 2$ and $b = O(n^2)$. Using these facts and Lemma 4.1, we obtain

$$\begin{aligned}\sum_{\{x,y\}\in\mathcal{B}} \deg(x)\deg(y)d(x, y) &\leq \sum_{\{x,y\}\in\mathcal{B}} 2(n - \kappa d + O(1))^2 \\ &= 2b(n - \kappa d + O(1))^2 \\ &\leq O(n^4),\end{aligned}$$

as claimed.

Finally, we bound those pairs of vertices, which are in $\mathcal{A}$.

Claim 9 *Assume the notation above. Then*

$$\sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x, y) \leq \frac{d}{16}\Big(n - \kappa d\Big)^4 + O(n^4).$$

Proof of Claim 9: Let $\{w, z\}$ be any pair in $\mathcal{A}$, such that deg(w)+deg(z) is maximum. Let $\deg(w) + \deg(z) = s$. Since $\deg(w)\deg(z) \leq \frac{1}{4}(\deg(w) + \deg(z))^2$, we get

$$\deg(w)\deg(z) \leq \frac{1}{4}s^2. \tag{4.3}$$

Now we find an upper bound on the cardinality of $\mathcal{A}$. From (4.2) it follows that

$$a = \frac{1}{2}\Big[n - (d - 1)\kappa\Big]\Big[n - (d - 1)\kappa - 1\Big] - b. \tag{4.4}$$

Note that all pairs $\{x, y\}, x, y \in N[w] - P$ and all pairs $\{x, y\}, x, y \in N[z] - P$ are in $\mathcal{B}$. Clearly, $w \in N_i$ for some $i = 0, 1, \ldots, d$, and consequently we have $N[w] \subseteq N_{i-1} \cup N_i \cup N_{i+1}$. Since $|N_i| \geq \kappa$ for any $i = 1, 2, \ldots, d - 1$, we obtain

$|N[w] \cap P| \leq 3\kappa$. Similarly, $|N[z] \cap P| \leq 3\kappa$, which implies

$$\begin{aligned} b &\geq \binom{\deg(w)+1-3\kappa}{2} + \binom{\deg(z)+1-3\kappa}{2} \\ &= \frac{1}{2}\Big[(\deg(w))^2 + (\deg(x))^2\Big] - \frac{6\kappa-1}{2}\Big(\deg(w)+\deg(z)\Big) + 9\kappa^2 - 3\kappa \\ &\geq \frac{1}{4}s^2 - \frac{6\kappa-1}{2}s + 9\kappa^2 - 3\kappa. \end{aligned}$$

Then from (4.4), we get

$$a \leq \frac{1}{2}\Big[n-(d-1)\kappa\Big]\Big[n-(d-1)\kappa-1\Big] - \frac{1}{4}s^2 + \frac{6\kappa-1}{2}s - 9\kappa^2 + 3\kappa,$$

and consequently from (4.3), we have

$$\sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x,y) \leq \sum_{\{x,y\}\in\mathcal{A}} \frac{s^2 d}{4} \leq$$

$$\frac{s^2 d}{4}\left[\frac{1}{2}\Big[n-(d-1)\kappa\Big]\Big[n-(d-1)\kappa-1\Big] - \frac{1}{4}s^2 + \frac{6\kappa-1}{2}s - 9\kappa^2 + 3\kappa\right]. \quad (4.5)$$

By Lemma 4.1, $s \leq n - \kappa d + 7\kappa - 4$. Subject to this condition, (4.5) is maximized for $s = n - \kappa d + O(1)$ to give

$$\begin{aligned} &\sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x,y) \\ &\leq \frac{d}{4}\Big((n-\kappa d)^2 + O(n)\Big)\Big[\frac{1}{2}\Big(n-\kappa d\Big)^2 - \frac{1}{4}\Big(n-\kappa d\Big)^2 + O(n)\Big] \\ &= \frac{d}{16}\Big(n-\kappa d\Big)^4 + O(n^4), \end{aligned}$$

which completes the proof of Claim 9.

Now we complete the proof of the theorem. From Claims 7, 8 and 9, we obtain

$$\begin{aligned}
\mathrm{Gut}(G) &= \sum_{\{x,y\}\in\mathcal{A}} \deg(x)\deg(y)d(x,y) + \sum_{\{x,y\}\in\mathcal{B}} \deg(x)\deg(y)d(x,y) \\
&+ \sum_{\{x,y\}\in\mathcal{P}} \deg(x)\deg(y)d(x,y) \\
&\le \frac{1}{16}d\Big(n-\kappa d\Big)^4 + O(n^4) + O(n^4) + O(n^4) \\
&= \frac{1}{16}d\Big(n-\kappa d\Big)^4 + O(n^4).
\end{aligned}$$

Finally we show that our bound is asymptotically sharp. We construct a graph $G_{n,d,\kappa}$ such that

$$\mathrm{Gut}(G_{n,d,\kappa}) = \frac{1}{16}d\Big(n-\kappa d\Big)^4 + O(n^4).$$

Let $G_{n,d,\kappa}$ be a graph join defined as follows:

$$G_{n,d,\kappa} = K_{\lceil \frac{1}{2}(n-\kappa(d-1))\rceil} + G_1 + G_2 + \cdots + G_{d-1} + K_{\lfloor \frac{1}{2}(n-\kappa(d-1))\rfloor},$$

where $G_1 = G_2 = \cdots = G_{d-1} = K_\kappa$. It can be checked that $G_{n,d,\kappa}$ has order n, diameter d, vertex-connectivity κ and $\mathrm{Gut}(G_{n,d,\kappa}) = \frac{1}{16}d(n-\kappa d)^4 + O(n^4)$. □

Now we present an upper bound on the Gutman index of a graph in terms of its order and vertex-connectivity.

Corollary 4.3 *Let G be a connected graph of order n and vertex-connectivity κ, where κ is a constant. Then*

$$\mathrm{Gut}(G) \le \frac{2^4}{5^5\kappa}n^5 + O(n^4),$$

and the bound is asymptotically sharp.

Proof: By Theorem 4.2, we have $\mathrm{Gut}(G) \le \frac{1}{16}d(n-\kappa d)^4 + O(n^4)$ for connected graphs G of order n, diameter d and vertex-connectivity κ. Since

$$\frac{1}{16}d\Big(n-\kappa d\Big)^4$$

is maximized, with respect to d, for $d = \frac{n}{5\kappa}$, we obtain $\mathrm{Gut}(G) \le \frac{2^4}{5^5\kappa}n^5 + O(n^4)$ for connected graphs G of order n and vertex-connectivity κ.

Consider the graph $G_{n,d,\kappa}$ described in the proof of Theorem 4.2. Let $\frac{n}{5\kappa}$ be an integer. Then the graph $G_{n,\frac{n}{5\kappa},\kappa}$ has the Gutman index $\frac{2^4}{5^5\kappa}n^5 + O(n^4)$. □

We can now use Lemma 1.11 to obtain a bound on the edge-Wiener index of a graph G.

Corollary 4.4 *Let G be a connected graph of order n and vertex-connectivity κ, where κ is a constant. Then*

$$W_e(G) \le \frac{2^2}{5^5\kappa}n^5 + O(n^4),$$

and the bound is asymptotically sharp.

Proof: From Theorem 4.2 and Lemma 1.11, we obtain $W_e(G) \le \frac{2^2}{5^5\kappa}n^5 + O(n^4)$. The graph $G_{n,\frac{n}{5\kappa},\kappa}$ is also the extremal graph on the edge-Wiener index ($W_e(G_{n,\frac{n}{5\kappa},\kappa}) = \frac{2^2}{5^5\kappa}n^5 + O(n^4)$), therefore the bound is best possible. □

4.3 Conclusion

In this chapter, we studied the Gutman index of graphs of given order and vertex-connectivity. We also obtained, as a corollary, a similar result for the edge-Wiener index of connected graphs of given order and vertex-connectivity. In Chapter 5, we give asymptotically sharp upper bounds on the Gutman index in terms of order and edge-connectivity. As a corollary, we obtain a similar result for the edge-Wiener index of graphs of given order and edge-connectivity.

Chapter 5

The Gutman index, the edge-Wiener index and the edge-connectivity of graphs

5.1 Introduction

This chapter is a continuation of the work that was started by Mazorodze, Mukwembi and Vetrík in [40] where upper bounds on the Gutman index of a graph in terms of order, diameter and minimum degree were given. Here we find, using ideas developed in the previous chapters, an asymptotically sharp upper bound on the Gutman index of graphs of given order n and edge-connectivity λ.

If $\lambda = 1$, then from Mukwembi in [43], we have $\mathrm{Gut}(G) \leq \frac{2^4}{5^5}n^5 + O(n^4)$, and the bound is asymptotically sharp, since the extremal graph given in [43] has edge-connectivity one.

It is well-known that $\lambda \leq \delta$ for any graph G, thus from Chapter 3, we obtain the inequality

$$\operatorname{Gut}(G) \leq \frac{2^4 \cdot 3}{5^5(\lambda+1)} n^5 + O(n^4). \tag{5.1}$$

We will show that this bound is best possible for $\lambda \geq 8$. The main challenge of this chapter is to obtain asymptotically sharp upper bounds on the Gutman index for graphs of given order and edge-connectivity λ, where $2 \leq \lambda \leq 7$. We prove that the bound (5.1) can be improved considerably for $2 \leq \lambda \leq 7$. We also obtain asymptotically sharp upper bounds on the edge-Wiener index of graphs of given order and edge-connectivity $\lambda \geq 2$.

5.2 Results

First we consider the Gutman index of graphs of edge-connectivity at least 8.

Theorem 5.1 *Let G be a graph of order n and edge-connectivity λ, where $\lambda \geq 8$ is a constant. Then*

$$\operatorname{Gut}(G) \leq \frac{2^4 \cdot 3}{5^5(\lambda+1)} n^5 + O(n^4)$$

and the bound is best possible.

Proof: The bound follows from Theorem 3.2 by applying the inequality $\lambda \leq \delta$. Thus it remains to show that the bound is best possible. We construct the graph G' of diameter $d = 3k+2$ where $k \geq 1$. Let $G' = G_0 + G_1 + G_2 + \cdots + G_{3k+1}$, where

$G_0 = K_{\lfloor \frac{1}{2}[n-k(\lambda+1)] \rfloor}$, $G_{3k+1} = K_{\lceil \frac{1}{2}[n-k(\lambda+1)] \rceil}$, and for $1 \le i \le 3k$

$$G_i = \begin{cases} K_{\frac{\lambda+1}{3}} & \text{if } \lambda \equiv 2 \pmod 3, \\ K_{\frac{\lambda}{3}+1} \quad \text{for } i = 0,1 \pmod 3 \quad \text{and } K_{\frac{\lambda}{3}} \quad \text{for } i = 2 \pmod 3 & \text{if } \lambda \equiv 0 \pmod 3, \\ K_{\frac{\lambda+2}{3}} \quad \text{for } i = 0,1 \pmod 3 \quad \text{and } K_{\frac{\lambda-1}{3}} \quad \text{for } i = 2 \pmod 3 & \text{if } \lambda \equiv 1 \pmod 3. \end{cases}$$

We have $|V(G_{j-2})|+|V(G_{j-1})|+|V(G_j)| = \lambda+1$ for $j = 3, 6, \ldots, 3k$, thus $|V(G_1)|+|V(G_2)|+\cdots+|V(G_{3k})| = k(\lambda+1)$. Since $|V(G_0)|+|V(G_{3k+1})| = n-k(\lambda+1)$, we have $|V(G')| = n$. Note that the edge-connectivity of G' is λ.

Let $\mathrm{Gut}(x,y) = \deg(x)\deg(y)d(x,y)$ where $x, y \in V(G')$. Clearly $\mathrm{Gut}(G) = \sum_{\{x,y\}\subseteq V(G')} \mathrm{Gut}(x,y)$. For any $x \in V(G_0)$ and $y \in V(G_{3k+1})$, we obtain

$$\begin{aligned} \mathrm{Gut}(x,y) &= \Big(\Big\lfloor \frac{1}{2}[n-k(\lambda+1)]\Big\rfloor + \Big\lceil \frac{\lambda+1}{3} \Big\rceil - 1\Big)\Big(\Big\lceil \frac{1}{2}[n-k(\lambda+1)]\Big\rceil + \Big\lfloor \frac{\lambda+1}{3} \Big\rfloor - 1\Big)(3k+2) \\ &= \frac{1}{4}[n-k(\lambda+1)]^2(3k+2) + O(nk). \end{aligned}$$

Then for $k = \frac{n}{5(\lambda+1)}$, we obtain

$$\begin{aligned} \sum_{x\in V(G_0), y\in V(G_{3k+1})} \mathrm{Gut}(x,y) &= \frac{1}{16}[n-k(\lambda+1)]^4(3k+2) + O(n^3k) \\ &= \frac{2^4\cdot 3}{5^5(\lambda+1)} n^5 + O(n^4). \end{aligned}$$

For $x \in H = V(G_1)\cup V(G_2)\cup\cdots\cup V(G_{3k})$ and $y \in V(G')$, we have $\mathrm{Gut}(x,y) = O(n^2)$ and consequently $\sum_{x\in H, y\in V(G')} \mathrm{Gut}(u,v) = O(n^4)$, which implies that $\mathrm{Gut}(G') = \frac{2^4\cdot 3}{5^5(\lambda+1)} n^5 + O(n^4)$. □

We present three lemmas, which will be used to prove our main results.

Lemma 5.2 *Let G be a graph of edge-connectivity λ and let v be any vertex of G. Then $|N_i(v)||N_{i+1}(v)| \ge \lambda$ for any $i = 0, 1, 2, \ldots, ec(v)-1$.*

Proof: For any vertex $v \in V(G)$ and $i = 0, 1, 2, \ldots, ec(v) - 1$, the number of edges between $N_i(v)$ and $N_{i+1}(v)$ is at most $|N_i(v)||N_{i+1}(v)|$. If $|N_i(v)||N_{i+1}(v)| < \lambda$, then we can disconnect G by removing less than λ edges which connect $N_i(v)$ and $N_{i+1}(v)$. $\square$

From the inequality $xy \le (\frac{x+y}{2})^2$, we obtain the following lemma.

Lemma 5.3 *Let x and y be positive integers.*

(a) If $xy \ge 2$, then $x + y \ge 3$.

(b) If $xy \ge 3$, then $x + y \ge 4$.

(c) If $xy \ge 4$, then $x + y \ge 4$.

(d) If $xy \ge 5$, then $x + y \ge 5$.

(e) If $xy \ge 6$, then $x + y \ge 5$.

(f) If $xy \ge 7$, then $x + y \ge 6$.

In the following lemma, we study the degrees of vertices in graphs of edge-connectivity 2.

Lemma 5.4 *Let G be a graph of order n, edge-connectivity 2 and diameter d. Let v, v' be any vertices of G.*

(i) Then $\deg(v) \le n - \frac{3}{2}d + O(1)$.

(ii) If $d(v, v') \ge 3$, then $\deg(v) + \deg(v') \le n - \frac{3}{2}d + O(1)$.

Proof: Let G be a graph of order n, edge-connectivity 2 and diameter d. Let v_0 be any vertex of G of eccentricity d. We denote the i-th neighbourhood of v_0 by N_i,

$i = 0, 1, 2, \ldots, d$.

Let $v \in V(G)$. Clearly $v \in N_i$ for some i and $N(v) \subset N_{i-1} \cup N_i \cup N_{i+1}$. Thus $\deg(v) \leq |N_{i-1}| + |N_i| + |N_{i+1}| - 1$. Since the edge-connectivity of G is 2, by Lemma 5.2 we have $|N_j||N_{j+1}| \geq 2$ for any $j = 0, 1, 2, \ldots, d-1$, and from Lemma 5.3 it follows that $|N_j| + |N_{j+1}| \geq 3$. It follows that $\sum_{j=0}^{i-2} |N_j| + \sum_{j=i+2}^{d} |N_j| \geq \frac{3}{2}(d-2) - 1$, and consequently

$$n = |\bigcup_{j=0}^{d} N_j| \geq \deg(v) + \frac{3}{2}(d-2) = \deg(v) + \frac{3}{2}d - O(1).$$

Hence $\deg(v) \leq n - \frac{3}{2}d + O(1)$. Note that the inequalities hold also if $v \in N_i$ where $i \in \{0, 1, d-1, d\}$.

Now we prove the statement (ii). Let $v, v' \in V(G)$ where $d(v, v') \geq 3$. We have $N(v) \cap N(v') = \emptyset$. Since $|N_j| + |N_{j+1}| \geq 3$ for any $j = 0, 1, 2, \ldots, d-1$, and $\deg(v) \leq |N_{i-1}| + |N_i| + |N_{i+1}| - 1$ (similarly for v'), we get

$$\begin{aligned} n &\geq (\deg(v) + 1) + (\deg(v') + 1) + \frac{3}{2}(d-5) - O(1) \\ &= (\deg(v)) + (\deg(v')) + \frac{3}{2}d - O(1). \end{aligned}$$

Rearranging the terms, we obtain $\deg(v) + \deg(v') \leq n - \frac{3}{2}d + O(1)$, which completes the proof of (ii). $\square$

In the following theorem we present an upper bound on the Gutman index of graphs G of given order, diameter and edge-connectivity 2.

Theorem 5.5 *Let G be a graph of order n, diameter d and edge-connectivity* 2. *Then*

$$\mathrm{Gut}(G) \leq \frac{d}{16}\left(n - \frac{3d}{2}\right)^4 + O(n^4),$$

and the bound is asymptotically sharp.

Proof: Let $v_0 \in V(G)$ be a vertex of eccentricity d. We denote the i-th neighbourhood of v_0 by N_i, $i = 0, 1, 2, \ldots, d$. Since $|N_i| + |N_{i+1}| \geq 3$ for every $i = 0, 1, 2, \ldots, d-1$, it is possible to choose three vertices u_{i1}, u_{i2}, u_{i3} from the set $N_{2i-2} \cup N_{2i-1}$ for each $i = 1, 2, \ldots, \lceil \frac{d}{2} \rceil$. Let $P_i = \{u_{i1}, u_{i2}, u_{i3}\}$ and let $P = \cup_{i=1}^{\lceil \frac{d}{2} \rceil} P_i$. Then

$$|P| = 3\left\lceil \frac{d}{2} \right\rceil. \tag{5.2}$$

Note that if d is even, then P does not contain vertices of N_d.

Let us partition the 2-subsets of $V(G)$, $Z = \{\{x, y\} : x, y \in V(G)\}$, as follows:

$$Z = C \cup A \cup B,$$

where

$$C = \{\{x, y\} : x \in P \text{ and } y \in V(G)\},$$

$$A = \{\{x, y\} \in Z - C : d(x, y) \geq 3\},$$

$$B = \{\{x, y\} \in Z - C : d(x, y) \leq 2\}.$$

Let $|A| = a$ and $|B| = b$. Then $\binom{n}{2} = |C| + a + b$ and from (5.2) we obtain

$$a + b = \binom{n - |P|}{2} = \frac{1}{2}\left(n - 3\left\lceil \frac{d}{2} \right\rceil\right)\left(n - 3\left\lceil \frac{d}{2} \right\rceil - 1\right). \tag{5.3}$$

We have

$$\begin{aligned}\mathrm{Gut}(G) &= \sum_{\{x,y\}\in A} \deg(x)\deg(y)d(x,y) + \sum_{\{x,y\}\in B} \deg(x)\deg(y)d(x,y) \\ &+ \sum_{\{x,y\}\in C} \deg(x)\deg(y)d(x,y).\end{aligned}$$

Let us bound these three terms in the following claims.

Claim 10 $\sum_{\{x,y\}\in C} \deg(x)\deg(y)d(x,y) \leq O(n^4)$.

Proof of Claim 10: Let $P = U_1 \cup U_2 \cup \cdots \cup U_6$ where

$$U_1 = \{u_{11}, u_{31}, u_{51}, \dots\},$$

$$U_2 = \{u_{12}, u_{32}, u_{52}, \dots\},$$

$$U_3 = \{u_{13}, u_{33}, u_{53}, \dots\},$$

$$U_4 = \{u_{21}, u_{41}, u_{61}, \dots\},$$

$$U_5 = \{u_{22}, u_{42}, u_{62}, \dots\},$$

$$U_6 = \{u_{23}, u_{43}, u_{63}, \dots\}.$$

For any two different vertices x, y in the same set U_i, $i = 1, 2, \dots, 6$, we have $N(x) \cap N(y) = \emptyset$, since $d(x,y) \geq 3$. Thus $\sum_{x\in U_i} \deg(x) < n$ for $i = 1, 2, \dots 6$.

Let us define the score $s(x)$ for each vertex $x \in P$ as

$$\begin{aligned}s(x) &= \sum_{y\in V(G)} \deg(x)\deg(y)d(x,y) \\ &= \deg(x) \sum_{y\in V(G)} \deg(y)d(x,y). \qquad (5.4)\end{aligned}$$

Then by Lemma 5.3,

$$\begin{aligned} s(x) &\leq \deg(x) \sum_{y \in V(G)} \Big(n - \frac{3}{2}d + O(1)\Big) d(x,y) \\ &= \deg(x)\Big(n - \frac{3}{2}d + O(1)\Big) \sum_{y \in V(G)} d(x,y) \\ &< \deg(x)\Big(n - \frac{3}{2}d + O(1)\Big) nd \end{aligned}$$

and

$$\begin{aligned} \sum_{x \in P} s(x) &= \sum_{x \in U_1} s(x) + \sum_{x \in U_2} s(x) + \cdots + \sum_{x \in U_6} s(x) \\ &< \sum_{x \in U_1} \deg(x)\Big(n - \frac{3}{2}d + O(1)\Big)nd + \cdots + \sum_{x \in U_3} \deg(x)\Big(n - \frac{3}{2}d + O(1)\Big)nd \\ &= \Big(\sum_{x \in U_1} \deg(x) + \sum_{x \in U_2} \deg(x) + \cdots + \sum_{x \in U_6} \deg(x)\Big)\Big(n - \frac{3}{2}d + O(1)\Big)nd \\ &< 6n\Big(n - \frac{3}{2}d + O(1)\Big)nd \leq O(n^4). \end{aligned}$$

Since $\sum_{\{x,y\} \in C} \deg(x)\deg(y)d(x,y) \leq \sum_{x \in P} s(x)$, the proof of Claim 10 is complete.

We bound those pairs of vertices, which are in B.

Claim 11 $\sum_{\{x,y\} \in B} \deg(x)\deg(y)d(x,y) \leq O(n^4)$.

Proof of Claim 11: Note that if $\{x,y\} \in B$, then $d(x,y) \le 2$ and $b = O(n^2)$. Using these facts and Lemma 5.3, we get

$$\begin{aligned}\sum_{\{x,y\}\in B} \deg(x)\deg(y)d(x,y) &\le \sum_{\{x,y\}\in B} 2\Big(n - \frac{3}{2}d + O(1)\Big)^2 \\ &= 2b\Big(n - \frac{3}{2}d + O(1)\Big)^2 \\ &\le O(n^4).\end{aligned}$$

Finally, we study the pairs of vertices, which are in A.

Claim 12 $\displaystyle\sum_{\{x,y\}\in A} \deg(x)\deg(y)d(x,y) \le \frac{d}{16}\Big(n - \frac{3d}{2}\Big)^4 + O(n^4).$

Proof of Claim 12: Let $\{w,z\}$ be any pair in A, where $\deg(w)+\deg(z)$ is maximum. Let $\deg(w) + \deg(z) = s$. Since $\deg(w)\deg(z) \le \frac{1}{4}(\deg(w) + \deg(z))^2$, we obtain

$$\deg(w)\deg(z) \le \frac{1}{4}s^2. \tag{5.5}$$

We find an upper bound on the cardinality of A. From (5.3) we have

$$a = \frac{1}{2}\Big(n - 3\Big\lceil\frac{d}{2}\Big\rceil\Big)\Big(n - 3\Big\lceil\frac{d}{2}\Big\rceil - 1\Big) - b. \tag{5.6}$$

Clearly, all pairs $\{x,y\}, x,y \in N[w] - P$ and all pairs $\{x,y\}, x,y \in N[z] - P$ are in B. Since $w \in N_i$ for some $i = 0,1,\ldots,d$, we have $N[w] \subseteq N_{i-1} \cup N_i \cup N_{i+1}$. Since $|N[w] \cap P| \le 6$ and $|N[z] \cap P| \le 6$, we obtain

$$\begin{aligned} b &\ge \binom{\deg(w)+1-6}{2} + \binom{\deg(z)+1-6}{2} \\ &= \frac{1}{2}[(\deg(w))^2 + (\deg(z))^2] - 11(\deg(w)+\deg(z)) + 30 \\ &\ge \frac{1}{4}s^2 - 11s + 30.\end{aligned}$$

Then by (5.6),

$$a \le \frac{1}{2}\Big(n - 3\Big\lceil\frac{d}{2}\Big\rceil\Big)\Big(n - 3\Big\lceil\frac{d}{2}\Big\rceil - 1\Big) - \frac{1}{4}s^2 + 11s - 30,$$

and by (5.5), we get

$$\begin{aligned}
&\sum_{\{x,y\}\in A} \deg(x)\deg(y)d(x,y) \le \sum_{\{x,y\}\in A} \frac{s^2 d}{4} = \frac{s^2 da}{4} \\
\le\ & \frac{s^2 d}{4}\Big[\frac{1}{2}\Big(n - 3\Big\lceil\frac{d}{2}\Big\rceil\Big)\Big(n - 3\Big\lceil\frac{d}{2}\Big\rceil - 1\Big) - \frac{1}{4}s^2 + 11s - 30\Big] \\
=\ & \frac{s^2 d}{4}\Big[\frac{1}{2}\Big(\Big(n - \frac{3d}{2}\Big)^2 + O(n)\Big) - \frac{1}{4}s^2 + O(n)\Big] \\
=\ & \frac{s^2 d}{4}\Big[\frac{1}{2}\Big(n - \frac{3d}{2}\Big)^2 - \frac{1}{4}s^2\Big] + O(n^4).
\end{aligned}$$

From Lemma 5.4, we have

$$s \le n - \frac{3d}{2} + O(1).$$

Subject to this condition, $\frac{s^2 d}{4}[\frac{1}{2}(n - \frac{3d}{2})^2 - \frac{1}{4}s^2]$ is maximized for $s = n - \frac{3d}{2} + O(1)$ and we obtain

$$\begin{aligned}
&\sum_{\{x,y\}\in A} \deg(x)\deg(y)d(x,y) \\
\le\ & \frac{d}{4}\Big[\Big(n - \frac{3d}{2}\Big)^2 + O(n)\Big]\Big[\frac{1}{2}\Big(n - \frac{3d}{2}\Big)^2 - \frac{1}{4}\Big(n - \frac{3d}{2}\Big)^2 + O(n)\Big] + O(n^4) \\
=\ & \frac{d}{16}\Big(n - \frac{3d}{2}\Big)^4 + O(n^4),
\end{aligned}$$

as claimed. □

Let us complete the proof of Theorem 5.5. From Claims 10, 11 and 12, we have

$$\begin{aligned}\mathrm{Gut}(G) &= \sum_{\{x,y\}\in A} \deg(x)\deg(y)d(x,y) + \sum_{\{x,y\}\in B} \deg(x)\deg(y)d(x,y)\\ &+ \sum_{\{x,y\}\in C} \deg(x)\deg(y)d(x,y)\\ &\le \frac{d}{16}\Big(n-\frac{3d}{2}\Big)^4 + O(n^4) + O(n^4) + O(n^4)\\ &= \frac{d}{16}\Big(n-\frac{3d}{2}\Big)^4 + O(n^4).\end{aligned}$$

It remains to show that the bound is asymptotically sharp. Let $G_{n,d,2}$ be a graph defined as follows:

$$G_{n,d} = K_{\lceil \frac{1}{2}(n-\lfloor\frac{3}{2}(d-1)\rfloor)\rceil} + G_1 + G_2 + \cdots + G_{d-1} + K_{\lfloor \frac{1}{2}(n-\lfloor\frac{3}{2}(d-1)\rfloor)\rfloor},$$

where

$$G_i = \begin{cases} K_1 & \text{if} \quad i \text{ is odd,}\\ K_2 & \text{if} \quad i \text{ is even,}\end{cases}$$

$i = 1, 2, 3, \ldots, d-1$. Since $|V(G_1) \cup V(G_2) \cup \cdots \cup V(G_{d-1})| = \lfloor \frac{3}{2}(d-1)\rfloor$ and $|V(K_{\lceil \frac{1}{2}(n-\lfloor\frac{3}{2}(d-1)\rfloor)\rceil})| + |V(K_{\lfloor \frac{1}{2}(n-\lfloor\frac{3}{2}(d-1)\rfloor)\rfloor})| = n - \lfloor\frac{3}{2}(d-1)\rfloor$, the order of $G_{n,d,2}$ is n. It can be checked that $G_{n,d,2}$ has diameter d, edge-connectivity 2 and $\mathrm{Gut}(G_{n,d,2}) = \frac{d}{16}(n-\frac{3d}{2})^4 + O(n^4)$. □

Let us present an upper bound on the Gutman index of graphs of given order and edge-connectivity 2.

Corollary 5.6 *Let G be a graph of order n and edge-connectivity 2. Then*

$$\mathrm{Gut}(G) \le \frac{2^5}{3\cdot 5^5} n^5 + O(n^4)$$

and the bound is asymptotically sharp.

Proof: By Theorem 5.5, $\mathrm{Gut}(G) \le \frac{d}{16}(n - \frac{3d}{2})^4 + O(n^4)$ for graphs G of order n, diameter d and edge-connectivity 2. Since

$$\frac{d}{16}\left(n - \frac{3d}{2}\right)^4$$

is maximized, with respect to d, for $d = \frac{2n}{15}$, we get $\mathrm{Gut}(G) \le \frac{2^5}{3 \cdot 5^5} n^5 + O(n^4)$ for graphs G of order n and edge-connectivity 2.

Consider the graph $G_{n,d,2}$ described in the proof of Theorem 5.5. Let $\frac{2n}{15}$ be an integer. Then the Gutman index of the graph $G_{n,\frac{2n}{15},2}$ is $\frac{2^5}{3 \cdot 5^5} n^5 + O(n^4)$. □

Now we study graphs of edge-connectivity λ for $3 \le \lambda \le 7$.

Lemma 5.7 *Let G be a graph of order n, edge-connectivity λ and diameter d. Let v, v' be any vertices of G such that $d(v, v') \ge 3$.*

(a) If $\lambda = 3$ or 4, then $\deg(v) \le n - 2d + O(1)$ and $\deg(v) + \deg(v') \le n - 2d + O(1)$.

(b) If $\lambda = 5$ or 6, then $\deg(v)$ and $\deg(v) + \deg(v')$ are at most $n - \frac{5}{2}d + O(1)$.

(c) If $\lambda = 7$, then $\deg(v)$ and $\deg(v) + \deg(v')$ are at most $n - 3d + O(1)$.

Proof: The proof is similar to the proof of Lemma 5.4.

(a) If $\lambda = 3$ or 4, then from Lemmas 5.2 and 5.3 we have $|N_j| + |N_{j+1}| \ge 4$ for any $j = 0, 1, 2, \dots, d-1$. Then $\sum_{j=0}^{i-2} |N_j| + \sum_{j=i+2}^{d} |N_j| \ge 2d - O(1)$, which implies that $n \ge \deg(v) + 2d - O(1)$. Similarly we obtain $n \ge \deg(v) + \deg(v') + 2d - O(1)$.

(b) If $\lambda = 5$ or 6, then by Lemmas 5.2 and 5.3 we get $|N_j| + |N_{j+1}| \ge 5$ for any $j = 0, 1, 2, \dots, d-1$. Thus $\sum_{j=0}^{i-2} |N_j| + \sum_{j=i+2}^{d} |N_j| \ge \frac{5}{2}d - O(1)$ and $n \ge$

$\deg(v) + \frac{5}{2}d - O(1)$. Similarly $n \geq \deg(v) + \deg(v') + \frac{5}{2}d - O(1)$.

(c) If $\lambda = 7$, then $|N_j| + |N_{j+1}| \geq 6$ for any $j = 0, 1, 2, \ldots, d-1$, which can be used to obtain the inequalities $n \geq \deg(v) + 3d - O(1)$ and

$n \geq \deg(v) + \deg(v') + 3d - O(1)$. □

We are now ready to give an upper bound on the Gutman index of graphs of given order, diameter and edge-connectivity λ, where $3 \leq \lambda \leq 7$.

Theorem 5.8 *Let G be a graph of order n, diameter d and edge-connectivity λ.*

(a) If $\lambda = 3$ or 4, then $\mathrm{Gut}(G) \leq \frac{d}{16}(n-2d)^4 + O(n^4)$.

(b) If $\lambda = 5$ or 6, then $\mathrm{Gut}(G) \leq \frac{d}{16}(n-\frac{5}{2}d)^4 + O(n^4)$.

(c) If $\lambda = 7$, then $\mathrm{Gut}(G) \leq \frac{d}{16}(n-3d)^4 + O(n^4)$.

The bounds are asymptotically sharp.

The proof of Theorem 5.8 is similar to the proof of Theorem 5.5. We present the main differences between the proof of part (a) of Theorem 5.8 and the proof of Theorem 5.5.

If $\lambda = 3$ or 4, then $|N_i| + |N_{i+1}| \geq 4$ for every $i = 0, 1, 2, \ldots, d-1$. We define $P_i = \{u_{i1}, u_{i2}, u_{i3}, u_{i4}\}$ where $u_{i1}, u_{i2}, u_{i3}, u_{i4} \in N_{2i-2} \cup N_{2i-1}$ for each $i = 1, 2, \ldots, \lceil \frac{d}{2} \rceil$

and $P = \cup_{i=1}^{\lceil \frac{d}{2} \rceil} P_i$. Then $|P| = 4\lceil \frac{d}{2} \rceil$. Let $P = U_1 \cup U_2 \cup \cdots \cup U_8$ where

$$U_1 = \{u_{11}, u_{31}, u_{51}, \dots\},$$

$$U_2 = \{u_{12}, u_{32}, u_{52}, \dots\},$$

$$U_3 = \{u_{13}, u_{33}, u_{53}, \dots\},$$

$$U_4 = \{u_{14}, u_{34}, u_{54}, \dots\},$$

$$U_5 = \{u_{21}, u_{41}, u_{61}, \dots\},$$

$$U_6 = \{u_{22}, u_{42}, u_{62}, \dots\},$$

$$U_7 = \{u_{23}, u_{43}, u_{63}, \dots\},$$

$$U_8 = \{u_{24}, u_{44}, u_{64}, \dots\}.$$

The rest of the proof of (a) can be easily obtained by following the proof of Theorem 5.5 and using Lemma 5.7 instead of Lemma 5.4.

For $\lambda = 3, 4, 5, 6, 7$ we construct the graph $G_{n,d,\lambda}$, such that $\mathrm{Gut}(G_{n,d,\lambda})$ is equal to the bound presented in Theorem 5.8.

Let $G_{n,d,\lambda} = G_0 + G_1 + G_2 + \cdots + G_d$.

For $\lambda = 3$ let $G_1 = K_1$, $G_2 = K_3$, $G_i = K_2$ for $i = 3, 4, \dots, d-1$, $G_0 = K_{\lceil \frac{1}{2}(n-2(d-1)) \rceil}$ and $G_d = K_{\lfloor \frac{1}{2}(n-2(d-1)) \rfloor}$.

For $\lambda = 4$ let $G_i = K_2$ for $i = 1, 2, \dots, d-1$, $G_0 = K_{\lceil \frac{1}{2}(n-2(d-1)) \rceil}$ and $G_d = K_{\lfloor \frac{1}{2}(n-2(d-1)) \rfloor}$.

For $\lambda = 5$ let $G_1 = K_1$, $G_2 = K_5$,

$$G_i = \begin{cases} K_2 & \text{if} \quad i \text{ is odd}, \\ K_3 & \text{if} \quad i \text{ is even}, \end{cases}$$

$i = 3, 4, \ldots, d-1$, $G_0 = K_{\lceil \frac{1}{2}(n - \lfloor \frac{5}{2}(d-1) \rfloor - 1) \rceil}$ and $G_d = K_{\lfloor \frac{1}{2}(n - \lfloor \frac{5}{2}(d-1) \rfloor - 1) \rfloor}$.

For $\lambda = 6$ let

$$G_i = \begin{cases} K_2 & \text{if} \quad i \text{ is odd}, \\ K_3 & \text{if} \quad i \text{ is even}, \end{cases}$$

$i = 1, 2, \ldots, d-1$, $G_0 = K_{\lceil \frac{1}{2}(n - \lfloor \frac{5}{2}(d-1) \rfloor) \rceil}$ and $G_d = K_{\lfloor \frac{1}{2}(n - \lfloor \frac{5}{2}(d-1) \rfloor) \rfloor}$.

For $\lambda = 7$ let $G_1 = K_1$, $G_2 = K_7$, $G_i = K_3$ for $i = 3, 4, \ldots, d-1$, $G_0 = K_{\lceil \frac{1}{2}(n-3d+1) \rceil}$ and $G_d = K_{\lfloor \frac{1}{2}(n-3d+1) \rfloor}$.

It can be checked that the graphs $G_{n,d,\lambda}$ have order n, diameter d, edge-connectivity λ and $\mathrm{Gut}(G_{n,d,\lambda})$ is equal to the bound given in Theorem 5.8. □

From Theorem 5.8 we obtain the following corollary.

Corollary 5.9 *Let G be a graph of order n and edge-connectivity λ.*

(a) If $\lambda = 3$ or 4, then $\mathrm{Gut}(G) \leq \frac{2^3}{5^5} n^5 + O(n^4)$.

(b) If $\lambda = 5$ or 6, then $\mathrm{Gut}(G) \leq \frac{2^5}{5^6} n^5 + O(n^4)$.

(c) If $\lambda = 7$, then $\mathrm{Gut}(G) \leq \frac{2^4}{3 \cdot 5^5} n^5 + O(n^4)$.

The bounds are asymptotically sharp.

Proof: (a) If $\lambda = 3$ or 4, then by Theorem 5.8 we have

$$\mathrm{Gut}(G) \leq \frac{d}{16}(n-2d)^4 + O(n^4)$$

for graphs G of order n and diameter d. Since $\frac{d}{16}(n-2d)^4$ is maximized for $d=\frac{n}{10}$, we obtain $\mathrm{Gut}(G)\leq \frac{2^3}{5^5}n^5+O(n^4)$ for graphs G of order n.

Let $\frac{n}{10}$ be an integer. Then the graphs $G_{n,\frac{n}{10},\lambda}$ described above for $\lambda=3$ and 4 have the Gutman index $\frac{2^3}{5^5}n^5+O(n^4)$.

(b) Let $\lambda=5$ or 6. Then $\frac{d}{16}(n-\frac{5}{2}d)^4$ is maximized for $d=\frac{2n}{25}$ and we obtain the bound $\mathrm{Gut}(G)\leq \frac{2^5}{5^6}n^5+O(n^4)$.

If $\frac{2n}{25}$ is an integer, then the graphs $G_{n,\frac{2n}{25},\lambda}$ described above for $\lambda=5$ and 6 have the Gutman index $\frac{2^5}{5^6}n^5+O(n^4)$.

(c) Let $\lambda=7$. Then $\frac{d}{16}(n-3d)^4$ is maximized for $d=\frac{n}{15}$ and we obtain the bound $\mathrm{Gut}(G)\leq \frac{2^4}{3\cdot 5^5}n^5+O(n^4)$.

If $\frac{n}{15}$ is an integer, then the graph $G_{n,\frac{n}{15},7}$ described above for $\lambda=7$ has the Gutman index $\frac{2^4}{3\cdot 5^5}n^5+O(n^4)$. □

We use Lemma 1.11 to get bounds on the edge-Wiener index of graphs of given order and edge-connectivity.

Corollary 5.10 *Let G be a graph of order n and edge-connectivity λ.*

(a) If $\lambda=2$, then $W_e(G)\leq \frac{2^3}{3\cdot 5^5}n^5+O(n^4)$.

(b) If $\lambda=3$ or 4, then $W_e(G)\leq \frac{2}{5^5}n^5+O(n^4)$.

(c) If $\lambda=5$ or 6, then $W_e(G)\leq \frac{2^3}{5^6}n^5+O(n^4)$.

(d) If $\lambda=7$, then $W_e(G)\leq \frac{2^2}{3\cdot 5^5}n^5+O(n^4)$.

(e) If $\lambda\geq 8$ is a constant, then $W_e(G)\leq \frac{2^2\cdot 3}{5^5(\lambda+1)}n^5+O(n^4)$.

The bounds are asymptotically sharp.

Proof: From Corollary 5.6 and Lemma 1.11 we obtain the bound

$$W_e(G) \leq \frac{2^3}{3 \cdot 5^5} n^5 + O(n^4)$$

for $\lambda = 2$. From Corollary 5.9 and Lemma 1.11 we have the results (b), (c) and (d). From Theorem 5.1 and Lemma 1.11 we get $W_e(G) \leq \frac{2^2 \cdot 3}{5^5(\lambda+1)} n^5 + O(n^4)$. The graphs which have the largest Gutman index in terms of the order and the edge-connectivity $\lambda \geq 2$ also achieve also the bounds given in this corollary, thus the bounds on $W_e(G)$ are best possible. □

5.3 Conclusion

In this chapter we gave asymptotically sharp upper bounds on the Gutman index in terms of order and edge-connectivity. As a corollary, we obtain a similar result for the edge-Wiener index of graphs of given order and edge-connectivity. In Chapter 6, we will give asymptotically sharp upper bounds on the size of a connected triangle-free graph in terms of order, diameter and minimum degree. We also give a sharp upper bound on the size of a connected graph in terms of order, diameter and edge-connectivity. Lastly we give an upper bound on the size of a connected triangle-free graph in terms of edge-connectivity, order and diameter.

Chapter 6

Size, order, diameter and edge-connectivity

6.1 Introduction

In this chapter, we bound the size (the number of edges) of a graph in terms of other parameters of the graph, namely order, diameter and edge-connectivity. This forms a very important family of problems in the extremal graph theory. We considerably extend known results in this area by presenting a number of upper bounds on the size of general graphs and triangle-free graphs. We also give an upper bound on the size of triangle-free graphs of given order, diameter and minimum degree. All bounds presented in this chapter are asymptotically sharp.

Recall that Mukwembi in [45], obtained the following result:

Theorem 6.1 *[45] Let G be a connected graph of order n, minimum degree δ, di-*

ameter d and size m. Then

$$\begin{aligned} m &\leq \frac{1}{2}\Big[n - \frac{1}{3}d(\delta+1)\Big]^2 + (2\delta+1)\Big(n - \frac{1}{6}d(\delta+2)\Big) \\ &= \frac{1}{2}\Big[n - \frac{1}{3}d(\delta+1)\Big]^2 + O(n), \end{aligned} \tag{6.1}$$

and the bound, for fixed δ, is asymptotically tight.

Hence, it becomes natural to ask if an asymptotically sharp upper bound on the size of a graph G can be obtained in terms of order, diameter and the third classical connectivity measure, edge-connectivity.

6.2 Results

First we give an upper bound on the number of edges in any graph G in terms of order, diameter and edge-connectivity of G.

Theorem 6.2 *Let G be a graph of order n, size m, diameter d and edge-connectivity λ, where $\lambda \geq 8$ is a constant. Then*

$$m \leq \frac{1}{2}\Big[n - \frac{d}{3}(\lambda+1)\Big]^2 + O(n)$$

and the bound is asymptotically sharp.

Proof: It is well-known that $\lambda \leq \delta$ for any graph, thus the bound presented in Theorem 6.2 follows from (6.1).

Let us show that the bound is asymptotically sharp. We construct the graph G' of diameter $d = 3k + 1$ where $k \geq 1$. Let $G' = G_0 + G_1 + G_2 + \cdots + G_{3k+1}$, where $G_0 = K_\lambda$, for $1 \leq i \leq 3k$

$$G_i = \begin{cases} K_{\frac{\lambda+1}{3}} & \text{if } \lambda \equiv 2 \pmod 3, \\ K_{\frac{\lambda}{3}} \quad \text{for } i = 0, 1 \pmod 3 \quad \text{and } K_{\frac{\lambda}{3}+1} \quad \text{for } i = 2 \pmod 3 & \text{if } \lambda \equiv 0 \pmod 3, \\ K_{\frac{\lambda+2}{3}} \quad \text{for } i = 0, 1 \pmod 3 \quad \text{and } K_{\frac{\lambda-1}{3}} \quad \text{for } i = 2 \pmod 3 & \text{if } \lambda \equiv 1 \pmod 3, \end{cases}$$

and $G_{3k+1} = K_{n-k(\lambda+1)-\lambda}$. We have $|V(G_{j-2})| + |V(G_{j-1})| + |V(G_j)| = \lambda + 1$ for $j = 3, 6, \ldots, 3k$, thus $|V(G_1)| + |V(G_2)| + \cdots + |V(G_{3k})| = k(\lambda + 1)$. Since $|V(G_0)| = \lambda$ and $|V(G_{3k+1})| = n - k(\lambda + 1) - \lambda$, we have $|V(G')| = n$. Note that the edge-connectivity of G' is λ. Since λ is a constant, we have $|E(G')| = |E(G_{3k+1})| + O(n) = \frac{1}{2}[n - k(\lambda + 1)]^2 + O(n) = \frac{1}{2}[n - \frac{d}{3}(\lambda + 1)]^2 + O(n)$. □

The following lemma will be used in the study of graphs with edge-connectivity λ where $2 \leq \lambda \leq 7$.

Lemma 6.3 *Let G be a graph of edge-connectivity λ and let v be any vertex of G. Then $|N_i(v)||N_{i+1}(v)| \geq \lambda$ for any $i = 0, 1, 2, \ldots, ec(v) - 1$.*

Proof: For any vertex $v \in V(G)$ and $i = 0, 1, 2, \ldots, ec(v) - 1$, the number of edges between $N_i(v)$ and $N_{i+1}(v)$ is at most $|N_i(v)||N_{i+1}(v)|$. If $|N_i(v)||N_{i+1}(v)| < \lambda$, then we can disconnect G by removing less than λ edges which connect $N_i(v)$ and $N_{i+1}(v)$. □

For graphs of edge-connectivity smaller than 8 we can get bounds better than the result given in Theorem 6.2.

Theorem 6.4 *Let G be a graph of order n, size m, diameter d and edge-connectivity 2. Then*

$$m \leq \frac{1}{2}\Big(n - \frac{3d}{2}\Big)^2 + O(n)$$

and the bound is asymptotically sharp.

Proof: Let $v_0 \in V(G)$ be a vertex of eccentricity d. We denote the i-th neighbourhood of v_0 by N_i, $i = 0, 1, 2, \ldots, d$. Since the edge-connectivity of G is 2, by Lemma 6.3 we have $|N_j||N_{j+1}| \geq 2$ for any $j = 0, 1, 2, \ldots, d-1$, and from Lemma 5.3 it follows that $|N_j| + |N_{j+1}| \geq 3$. Then it is possible to choose three vertices u_{i1}, u_{i2}, u_{i3} from the set $N_{2i-2} \cup N_{2i-1}$ for each $i = 1, 2, \ldots, \lceil \frac{d}{2} \rceil$. Let $P_i = \{u_{i1}, u_{i2}, u_{i3}\}$ and let $P = \cup_{i=1}^{\lceil \frac{d}{2} \rceil} P_i$. Then

$$|P| = 3\Big\lceil \frac{d}{2} \Big\rceil. \tag{6.2}$$

Note that if d is even, then P does not contain vertices of N_d. Let

$$P = U_1 \cup U_2 \cup \cdots \cup U_6$$

where

$$\begin{aligned} U_1 &= \{u_{11}, u_{31}, u_{51}, \ldots\}, & U_4 &= \{u_{21}, u_{41}, u_{61}, \ldots\}, \\ U_2 &= \{u_{12}, u_{32}, u_{52}, \ldots\}, & U_5 &= \{u_{22}, u_{42}, u_{62}, \ldots\}, \\ U_3 &= \{u_{13}, u_{33}, u_{53}, \ldots\}, & U_6 &= \{u_{23}, u_{43}, u_{63}, \ldots\}. \end{aligned}$$

For any two different vertices x, y in the same set U_i, $i = 1, 2, \ldots, 6$, we have $N(x) \cap N(y) = \emptyset$, since $d(x, y) \geq 3$. Thus $\sum_{x \in U_i} \deg(x) < n$ for $i = 1, 2, \ldots, 6$. Thus

$$\sum_{x \in P} \deg(x) = \sum_{x \in U_1} \deg(x) + \sum_{x \in U_2} \deg(x) + \cdots + \sum_{x \in U_6} \deg(x) < 6n. \tag{6.3}$$

Let $Q = V(G) \setminus P$. From (6.2) we have

$$|Q| = n - 3\left\lceil \frac{d}{2} \right\rceil. \tag{6.4}$$

Note that each vertex $x \in Q$ is adjacent to at most 6 vertices in P, therefore $\deg(x) \leq n - 3\lceil \frac{d}{2} \rceil - 1 + 6$. Then

$$\begin{aligned} \sum_{x \in Q} \deg(x) &\leq \sum_{x \in Q} \Big(n - 3\Big\lceil \frac{d}{2} \Big\rceil + O(1)\Big) = \Big(n - 3\Big\lceil \frac{d}{2} \Big\rceil\Big)\Big(n - 3\Big\lceil \frac{d}{2} \Big\rceil + O(1)\Big) \\ &= \Big(n - \frac{3d}{2}\Big)^2 + O(n). \end{aligned} \tag{6.5}$$

From (6.3) and (6.5) we obtain

$$\sum_{x \in V(G)} \deg(x) = \sum_{x \in P} \deg(x) + \sum_{x \in Q} \deg(x) \leq \Big(n - \frac{3d}{2}\Big)^2 + O(n).$$

By the Handshaking lemma, we have $m = \frac{1}{2} \sum_{x \in V(G)} \deg(x)$, hence

$$m \leq \frac{1}{2}(n - \frac{3d}{2})^2 + O(n).$$

It remains to show that the bound is asymptotically sharp. Let $G_{n,d,2}$ be a graph defined as follows:

$$G_{n,d,2} = G_0 + G_1 + \cdots + G_{d-1} + K_{n - \lfloor \frac{3}{2}d \rfloor},$$

where

$$G_i = \begin{cases} K_1 & \text{if } i \text{ is even,} \\ K_2 & \text{if } i \text{ is odd,} \end{cases}$$

$i = 0, 1, \ldots, d-1$. Since $|V(G_0) \cup V(G_1) \cup \cdots \cup V(G_{d-1})| = \lfloor \frac{3d}{2} \rfloor$, the order of $G_{n,d,2}$ is n. It can be checked that $G_{n,d,2}$ has diameter d and edge-connectivity 2. For the number of edges in $G_{n,d,2}$ we have $|E(G_{n,d,2})| = |E(K_{n-\lfloor \frac{3}{2}d \rfloor})| + O(n) = \frac{1}{2}(n - \frac{3d}{2})^2 + O(n)$.

□

The following theorem yields upper bounds on the number of edges in any graph of given order, diameter and edge-connectivity λ, where $3 \leq \lambda \leq 7$.

Theorem 6.5 *Let G be a graph of order n, size m, diameter d and edge-connectivity λ.*

(a) If $\lambda = 3$ or 4, then $m \leq \frac{1}{2}(n-2d)^2 + O(n)$.

(b) If $\lambda = 5$ or 6, then $m \leq \frac{1}{2}(n-\frac{5d}{2})^2 + O(n)$.

(c) If $\lambda = 7$, then $m \leq \frac{1}{2}(n-3d)^2 + O(n)$.

The bounds are asymptotically sharp.

The proof of Theorem 6.5 is similar to the proof of Theorem 6.4. We present the main differences between the proof of part (a) of Theorem 6.5 and the proof of Theorem 6.4.

If $\lambda = 3$ or 4, then $|N_i| + |N_{i+1}| \geq 4$ for every $j = 0, 1, 2, \ldots, d-1$. We define $P_i = \{u_{i1}, u_{i2}, u_{i3}, u_{i4}\}$ where $u_{i1}, u_{i2}, u_{i3}, u_{i4} \in N_{2i-2} \cup N_{2i-1}$ for each $i = 1, 2, \ldots, \lceil \frac{d}{2} \rceil$ and $P = \cup_{i=1}^{\lceil \frac{d}{2} \rceil} P_i$. Then $|P| = 4\lceil \frac{d}{2} \rceil$. Let $P = U_1 \cup U_2 \cup \cdots \cup U_8$ where

$$\begin{aligned} U_1 &= \{u_{11}, u_{31}, u_{51}, \ldots\}, & U_5 &= \{u_{21}, u_{41}, u_{61}, \ldots\}, \\ U_2 &= \{u_{12}, u_{32}, u_{52}, \ldots\}, & U_6 &= \{u_{22}, u_{42}, u_{62}, \ldots\}, \\ U_3 &= \{u_{13}, u_{33}, u_{53}, \ldots\}, & U_7 &= \{u_{23}, u_{43}, u_{63}, \ldots\}, \\ U_4 &= \{u_{14}, u_{34}, u_{54}, \ldots\}, & U_8 &= \{u_{24}, u_{44}, u_{64}, \ldots\}. \end{aligned}$$

Then $\sum_{x \in P} \deg(x) < 8n$, $|Q| = n - 4\lceil \frac{d}{2} \rceil$ and $\sum_{x \in Q} \deg(x) \leq (n - 2d)^2 + O(n)$. Thus $m = \frac{1}{2} \sum_{x \in V(G)} \deg(x) \leq (n - 2d)^2 + O(n)$.

For $\lambda = 3, 4, 5, 6, 7$ we construct the graph $G_{n,d,\lambda}$, such that the size, m, is equal to the bound presented in Theorem 6.5. Let $G_{n,d,\lambda} = G_0 + G_1 + G_2 + \cdots + G_d$.

For $\lambda = 3$ let $G_i = K_2$ for $i = 0, 1, \ldots, d-1$ and $G_d = K_{n-2d}$.

For $\lambda = 4$ let $G_0 = K_3$, $G_i = K_2$ for $i = 1, 2, \ldots, d-1$, and $G_d = K_{n-2d-1}$.

For $\lambda = 5$ let $G_0 = K_3$,

$$G_i = \begin{cases} K_3 & \text{if } i \text{ is odd,} \\ K_2 & \text{if } i \text{ is even,} \end{cases}$$

where $i = 1, 2, \ldots, d-1$, and $G_d = K_{n - \lfloor \frac{5d}{2} \rfloor - 1}$. Note that

$$|V(G_0) \cup V(G_1) \cup \cdots \cup V(G_{d-1})| = \lfloor \frac{5d}{2} \rfloor + 1.$$

For $\lambda = 6$ let $G_0 = K_4$,

$$G_i = \begin{cases} K_3 & \text{if } i \text{ is odd,} \\ K_2 & \text{if } i \text{ is even,} \end{cases}$$

where $i = 1, 2, \ldots, d-1$, and $G_d = K_{n - \lfloor \frac{5d}{2} \rfloor - 2}$.

For $\lambda = 7$ let $G_0 = K_5$, $G_i = K_3$ for $i = 1, 2, \ldots, d-1$, and $G_d = K_{n-3d-2}$. Note that $|V(G_1) \cup V(G_2) \cup \cdots \cup V(G_d)| = 3d + 2$.

It can be checked that the graphs $G_{n,d,\lambda}$ have order n, diameter d, edge-connectivity λ and the number of edges of $G_{n,d,\lambda}$ is equal to the bound given in Theorem 6.5. $\square$

In the rest of this chapter we study triangle-free graphs. In our proofs we use

Mantel's theorem, which says that for any triangle-free graph of order n and size m, we have

$$m \leq \left\lfloor \frac{n^2}{4} \right\rfloor. \tag{6.6}$$

Let us present an upper bound on the number of edges in a triangle-free graph G in terms of order, diameter and minimum degree of G.

Theorem 6.6 *Let G be a connected triangle-free graph of order n, size m, diameter d and minimum degree δ, where $\delta \geq 2$ is a constant. Then*

$$m \leq \frac{1}{4}\Big(n - \frac{\delta d}{2}\Big)^2 + O(n).$$

Moreover, the bound is asymptotically sharp.

Proof: Let $P : v_0, v_1, \ldots, v_d$ be a diametric path of G. Let $A \subset V(P)$ be the set

$$A = \{v_i \mid i \equiv 1 \text{ or } 2 \pmod 4, 1 \leq i \leq d\}.$$

For each vertex $v_i \in A$ let $M(v_i)$ be a set containing any δ neighbours of v_i and let $S = \cup_{v_i \in A} M(v_i)$. Since G is triangle-free, $M(v_i) \cap M(v_j) = \emptyset$ for any $v_i, v_j \in A$. Since A contains about $\frac{d}{2}$ vertices, we can write $|A| = \frac{d}{2} + O(1)$ and then

$$|S| = \delta |A| = \frac{\delta d}{2} + O(1). \tag{6.7}$$

We show that $\sum_{u \in S} \deg(u) = O(n)$. Let us partition A as $A = A_1 \cup A_2 \cup A_3 \cup A_4$, where

$$\begin{aligned} A_1 &= \{v_i \mid i \equiv 1 \pmod 8, 1 \le i \le d\}, \\ A_2 &= \{v_i \mid i \equiv 2 \pmod 8, 2 \le i \le d\}, \\ A_3 &= \{v_i \mid i \equiv 5 \pmod 8, 5 \le i \le d\}, \\ A_4 &= \{v_i \mid i \equiv 6 \pmod 8, 6 \le i \le d\}. \end{aligned}$$

We can write $A_1 = \{w_1, w_2, \ldots, w_{|A_1|}\}$. For each $w_j \in A_1$, $j = 1, 2, \ldots, |A_1|$ let $M(w_j) = \{u_1^j, u_2^j, \ldots, u_\delta^j\}$ be a set of δ neighbours of w_j. Since $d_G(w, w') \ge 8$ for any $w, w' \in A_1$, for $s = 1, 2, \ldots, \delta$ we have

$$n \ge \deg(u_s^1) + \deg(u_s^2) + \cdots + \deg(u_s^{|A_1|}),$$

and consequently

$$\delta n \ge \sum_{u \in (\cup_{w \in A_1} M(w))} \deg(u).$$

Similarly it can be shown that $\delta n \ge \sum_{u \in (\cup_{w \in A_i} M(w))} \deg(u)$ for $i = 2, 3, 4$. Thus

$$\sum_{u \in S} \deg(u) \le 4\delta n = O(n). \tag{6.8}$$

Let $Q = V(G) \setminus S$. Then from (6.7) we have $|Q| = n - \frac{\delta d}{2} + O(1)$. Note that $m = |E(G[S]) \cup E(G[Q]) \cup E(S, Q)|$ and by (6.8),

$$|E(G[S]) \cup E(S, Q)| < \sum_{u \in S} \deg(u) = O(n). \tag{6.9}$$

Since $G[Q]$ is triangle-free, by (6.6) we obtain

$$|E(G[Q])| \leq \frac{|Q|^2}{4} = \frac{1}{4}\Big(n - \frac{\delta d}{2}\Big)^2 + O(n). \tag{6.10}$$

From (6.9) and (6.10) it follows that $m \leq \frac{1}{4}(n - \frac{\delta d}{2})^2 + O(n)$.

We show that the bound is asymptotically sharp. Let $G' = G_0 + G_1 + \cdots + G_{2k+1}$, where

$$G_i = \begin{cases} \overline{K}_1 & \text{if } i \equiv 0 \text{ or } 3 \pmod 4,\ 0 \leq i \leq 2k-1, \\ \overline{K}_{\delta-1} & \text{if } i \equiv 1 \text{ or } 2 \pmod 4,\ 2 \leq i \leq 2k-1, \\ \overline{K}_{\delta} & \text{if } i = 1, \\ \overline{K}_{\lceil \frac{1}{2}(n-\delta k-1)\rceil} & \text{if } i = 2k, \\ \overline{K}_{\lfloor \frac{1}{2}(n-\delta k-1)\rfloor} & \text{if } i = 2k+1. \end{cases}$$

Note that $|V(G_0) \cup V(G_1)| = \delta + 1$ and $|V(G_i) \cup V(G_{i+1})| = \delta$ for $i = 2, 4, \ldots, 2k-2$, which means that $|V(G_0) \cup V(G_1) \cup \cdots \cup V(G_{2k-1})| = \delta k + 1$. Since $|V(\overline{K}_{\lceil \frac{1}{2}(n-\delta k-1)\rceil})| + |V(\overline{K}_{\lfloor \frac{1}{2}(n-\delta k-1)\rfloor})| = n - \delta k - 1$, the order of G' is n. It is easy to see that G' is a triangle-free graph of diameter $d = 2k+1$ and minimum degree δ. Since δ is a constant, we have $|E(G_0 + G_1 + \cdots + G_{2k})| = O(n)$ and hence the number of edges in G' is $|E(G')| = |E(G_{2k} + G_{2k+1})| + O(n) = \frac{1}{4}(n - \delta k)^2 + O(n) = \frac{1}{4}(n - \frac{\delta d}{2})^2 + O(n)$.

□

We obtain similar results for triangle-free graphs of given edge-connectivity.

Theorem 6.7 *Let G be a triangle-free graph of order n, size m, diameter d and edge-connectivity λ, where $\lambda = 4$ or $\lambda \geq 6$ is a constant. Then*

$$m \leq \frac{1}{4}\Big(n - \frac{\lambda d}{2}\Big)^2 + O(n)$$

and the bound is asymptotically sharp.

Proof: The bound follows from Theorem 6.6 by applying the inequality $\lambda \le \delta$. Let us show that the bound is best possible. We construct the graph G' of diameter $d = 2k$. Let $G' = G_0 + G_1 + G_2 + \cdots + G_{2k}$, where $G_0 = \overline{K}_{\lfloor \frac{\lambda}{2} \rfloor}$, $G_1 = \overline{K}_\lambda$,

$$G_i = \begin{cases} \overline{K}_{\lfloor \frac{\lambda}{2} \rfloor} & \text{if } i \equiv 0 \text{ or } 1 \pmod 4, \\ \overline{K}_{\lceil \frac{\lambda}{2} \rceil} & \text{if } i \equiv 2 \text{ or } 3 \pmod 4) \end{cases}$$

for $2 \le i \le 2k-2$, $G_{2k-1} = \overline{K}_{\lceil \frac{1}{2}(n-\lambda k) \rceil}$ and $G_{2k} = \overline{K}_{\lfloor \frac{1}{2}(n-\lambda k) \rfloor}$. Then we obtain $|V(G_1)| = \lambda$, $|V(G_0) \cup V(G_2)| = \lambda$ and $|V(G_i) \cup V(G_{i+1})| = \lambda$ for $i = 3, 5, \ldots, 2k-3$, thus $|V(G_0) \cup V(G_1) \cup \cdots \cup V(G_{2k-2})| = \lambda k$. Clearly $|V(\overline{K}_{\lceil \frac{1}{2}(n-\lambda k) \rceil})| + |V(\overline{K}_{\lfloor \frac{1}{2}(n-\lambda k) \rfloor})| = n - \lambda k$, so $V(G') = n$. The graph G' is a triangle-free graph of diameter $d = 2k+1$ and edge-connectivity λ. Since λ is a constant, the number of edges in G' is

$$\begin{aligned} |E(G_{2k-1} + G_{2k})| + O(n) &= \frac{1}{4}(n - \lambda k)^2 + O(n) \\ &= \frac{1}{4}(n - \frac{\lambda d}{2})^2 + O(n). \quad \square \end{aligned}$$

The bound given in the previous theorem holds also for $\lambda = 2, 3$ and 5, but for these values we can improve the bound presented in Theorem 6.7.

Theorem 6.8 *Let G be a triangle-free graph of order n, size m, diameter d and edge-connectivity* 2*. Then*

$$m \le \frac{1}{4}\Big(n - \frac{3d}{2}\Big)^2 + O(n)$$

and the bound is asymptotically sharp.

Proof: Let $v_0 \in V(G)$ be a vertex of eccentricity d. We denote the i-th neighbourhood of v_0 by N_i, $i = 0, 1, 2, \ldots, d$. From Lemmas 5.3 and 6.3 it follows that $|N_j| + |N_{j+1}| \geq 3$ for $j = 0, 1, 2, \ldots, d-1$. Let $P_i = \{u_{i1}, u_{i2}, u_{i3}\}$, where $u_{i1}, u_{i2}, u_{i3} \in N_{2i-2} \cup N_{2i-1}$ for each $i = 1, 2, \ldots, \lceil \frac{d}{2} \rceil$, and let $P = \cup_{i=1}^{\lceil \frac{d}{2} \rceil} P_i$. From the proof of Theorem 6.4 we know that $\sum_{x \in P} \deg(x) = O(n)$.

Let $Q = V(G) \setminus P$. Since $|P| = 3\lceil \frac{d}{2} \rceil$, we have $|Q| = n - 3\lceil \frac{d}{2} \rceil$. Note that

$$m = |E(G[P])| + |E(P,Q)| + |E(G[Q])| \text{ and } |E(G[P])| + |E(P,Q)| < \sum_{x \in P} \deg(x).$$

Since by (6.6), $|E(G[Q])| \leq \lfloor \frac{1}{4}(n - 3\lceil \frac{d}{2} \rceil)^2 \rfloor = \frac{1}{4}(n - \frac{3d}{2})^2 + O(n)$, we obtain $m \leq \frac{1}{4}(n - \frac{3d}{2})^2 + O(n)$, as desired.

It remains to show that the bound is asymptotically sharp.

Let $G_{n,d,2} = G_0 + G_1 + \cdots + G_d$, where

$$G_i = \begin{cases} \overline{K}_1 & \text{if } i \text{ is even,} \\ \overline{K}_2 & \text{if } i \text{ is odd,} \end{cases}$$

$i = 0, 1, \ldots, d-2$, $G_{d-1} = \overline{K}_{\lceil \frac{1}{2}(n - \lfloor \frac{3}{2}(d-1) \rfloor) \rceil}$ and $G_d = \overline{K}_{\lfloor \frac{1}{2}(n - \lfloor \frac{3}{2}(d-1) \rfloor) \rfloor}$ It is easy to see that $|V(G_0) \cup V(G_1) \cup \cdots \cup V(G_{d-2})| = \lfloor \frac{3}{2}(d-1) \rfloor$ and $|V(\overline{K}_{\lceil \frac{1}{2}(n - \lfloor \frac{3}{2}(d-1) \rfloor) \rceil})| + |V(\overline{K}_{\lfloor \frac{1}{2}(n - \lfloor \frac{3}{2}(d-1) \rfloor) \rfloor})| = n - \lfloor \frac{3}{2}(d-1) \rfloor$, thus the order of $G_{n,d,2}$ is n. The graph $G_{n,d,2}$ is a triangle-free graph of diameter d, edge-connectivity 2 and $|E(G_{n,d,2})| = |E(G_{d-1} + G_d)| + O(n) = \frac{1}{4}(n - \frac{3d}{2})^2 + O(n)$. □

Theorem 6.9 *Let G be a triangle-free graph of order n, size m, diameter d and* *edge-connectivity* 3. *Then*

$$m \le \frac{1}{4}(n-2d)^2 + O(n)$$

and the bound are asymptotically sharp.

The proof of Theorem 6.9 is similar to the proof of Theorem 6.8. Let us construct the graph $G_{n,d,3} = G_0 + G_1 + G_2 + \cdots + G_d$, where $G_0 = \overline{K}_1$, $G_1 = \overline{K}_3$, $G_i = \overline{K}_2$ for $i = 2, 3, \ldots, d-2$, $G_{d-1} = \overline{K}_{\lceil \frac{1}{2}(n-2(d-1)) \rceil}$ and $G_d = \overline{K}_{\lfloor \frac{1}{2}(n-2(d-1)) \rfloor}$. Since $G_{n,d,3}$ is a traingle-free graph of diameter d, edge-connectivity 3 and $|E(G_{n,d,3})| = \frac{1}{4}(n-2d)^2 + O(n)$, the bound $m \le \frac{1}{4}(n-2d)^2 + O(n)$ is asymptotically sharp.

One might have an impression that the bound stated in Theorem 6.7 is an asymptotically sharp bound also if the edge-connectivity is 5. But let us note that the graph G' described in the proof of Theorem 6.7 cannot be used for $\lambda = 5$. For $i \equiv 0 \pmod 4$, $4 \le i \le 2k-4$ the number of edges between G_i and G_{i+1} is $(\lfloor \frac{\lambda}{2} \rfloor)^2$, which is at least λ for any $\lambda \ge 6$ or $\lambda = 4$, but not for $\lambda = 5$.

We use additional arguments to improve the bound given in Theorem 6.7 for triangle-free graphs of edge-connectivity 5.

Theorem 6.10 *Let G be a triangle-free graph of order n, size m, diameter d and edge-connectivity* 5. *Then*

$$m \le \frac{1}{4}\left(n - \frac{8d}{3}\right)^2 + O(n)$$

and the bound is asymptotically sharp.

Proof: Let $v_0 \in V(G)$ be a vertex of eccentricity d and denote the i-th neighbourhood of v_0 by N_i, $i = 0, 1, 2, \ldots, d$. From Lemmas 5.3 and 6.3 we have $|N_{j-1}| + |N_j| \geq 5$ and $|N_j| + |N_{j+1}| \geq 5$ for $j = 1, 2, \ldots, d-1$. To prove the theorem, we need the following claim.

Claim 13 $|N_{j-1}| + |N_j| + |N_{j+1}| \geq 8$ *for* $j = 1, 2, \ldots, d-1$.

Proof of Claim 13: We distinguish two cases:

Case 1: There are two vertices u and v in N_j, which are adjacent in G.

Then u and v do not have a common neighbour (because G is a triangle-free graph). Since $\lambda \leq \delta$ for any graph, the vertex u is adjacent to at least 4 vertices other than v and the vertex v is adjacent to at least 4 vertices other than u. It follows that $|N_{j-1}| + |N_j| + |N_{j+1}| \geq 10$.

Case 2: No two vertices u, v of N_j are adjacent in G.

Since $\lambda \leq \delta$, any vertex in N_i is adjacent to at least 5 vertices and all of them must be in $N_{j-1} \cup N_{j+1}$. Thus $|N_{j-1}| + |N_{j+1}| \geq 5$. If $|N_j| \geq 3$, then $|N_{j-1}| + |N_j| + |N_{j+1}| \geq 8$. If $|N_j| \leq 2$, then from the inequalities $|N_{j-1}| + |N_j| \geq 5$ and $|N_j| + |N_{j+1}| \geq 5$ we have $|N_{j-1}| + 2|N_j| + |N_{j+1}| \geq 10$ and consequently $|N_{j-1}| + |N_j| + |N_{j+1}| \geq 10 - |N_j| \geq 8$. The proof of Claim 13 is complete.

Let $P_i = \{u_{i1}, u_{i2}, \ldots, u_{i8}\}$, where $u_{i1}, u_{i2}, \ldots, u_{i8}$ are any 8 vertices in $N_{3i-3} \cup N_{3i-2} \cup N_{3i-1}$ for each $i = 1, 2, \ldots, \lceil \frac{d-1}{3} \rceil$, and let $P = \cup_{i=1}^{\lceil \frac{d-1}{3} \rceil} P_i$. Then $|P| = 8\lceil \frac{d-1}{3} \rceil$. Let

$P = U_1 \cup U_2 \cup \cdots \cup U_{16}$ where

$$U_1 = \{u_{11}, u_{31}, u_{51}, \dots\},\ U_2 = \{u_{12}, u_{32}, u_{52}, \dots\}, \dots,\ U_8 = \{u_{18}, u_{38}, u_{58}, \dots\},$$
$$U_9 = \{u_{21}, u_{41}, u_{61}, \dots\}, U_{10} = \{u_{22}, u_{42}, u_{62}, \dots\}, \dots, U_{16} = \{u_{28}, u_{48}, u_{68}, \dots\}.$$

For any two different vertices x, y in the same set U_i, $i = 1, 2, \dots, 16$, we have $d(x, y) \geq 4$, thus $N(x) \cap N(y) = \emptyset$. This implies that $\sum_{x \in U_i} \deg(x) < n$ for $i = 1, 2, \dots, 16$, and $\sum_{x \in P} \deg(x) < 16n = O(n)$.

Let $Q = V(G) \setminus P$. We have $|Q| = n - 8\lceil \frac{d-1}{3} \rceil$. Note that $|E(G[P])| + |E(P, Q)| < \sum_{x \in P} \deg(x)$ and by (6.6), $|E(G[Q])|$ is at most $\lfloor \frac{1}{4}(n - 8\lceil \frac{d-1}{3} \rceil)^2 \rfloor$, thus $m = |E(G[P])| + |E(P, Q)| + |E(G[Q])| \leq \frac{1}{4}(n - \frac{8d}{3})^2 + O(n)$.

We show that the bound is best possible. Let $G_{n,d,5} = G_0 + G_1 + \cdots + G_d$, where $G_1 = \overline{K}_5$,

$$G_i = \begin{cases} \overline{K}_2 & \text{if } i \equiv 0 \pmod 3,\ 0 \leq i \leq d-2, \\ \overline{K}_3 & \text{if } i \equiv 1 \text{ or } 2 \pmod 3,\ 2 \leq i \leq d-2, \end{cases}$$

$G_{d-1} = \overline{K}_{\lceil \frac{1}{2}(n - \lfloor \frac{8}{3}(d-1) \rfloor - 2) \rceil}$ and $G_d = \overline{K}_{\lfloor \frac{1}{2}(n - \lfloor \frac{8}{3}(d-1) \rfloor - 2) \rfloor}$. It can be checked that $|V(G_0) \cup V(G_1) \cup \cdots \cup V(G_{d-2})| = \lfloor \frac{8}{3}(d-1) \rfloor + 2$ and $|V(\overline{K}_{\lceil \frac{1}{2}(n - \lfloor \frac{8}{3}(d-1) \rfloor - 2) \rceil})| + |V(\overline{K}_{\lfloor \frac{1}{2}(n - \lfloor \frac{8}{3}(d-1) \rfloor - 2) \rfloor})| = n - \lfloor \frac{8}{3}(d-1) \rfloor - 2$, thus $|V(G_{n,d,5})| = n$. The graph $G_{n,d,5}$ is a triangle-free graph of diameter d, edge-connectivity 5 and $|E(G_{n,d,2})| = |E(G_{d-1} + G_d)| + O(n) = \frac{1}{4}(n - \frac{8d}{3})^2 + O(n)$. □

6.3 Conclusion

We studied an important topic in the extremal graph theory: bounds on the size of a graph in terms of other parameters of the graph. Let us summarize results obtained in this chapter. We proved that for any graph G of order n, size m, diameter d and edge-connectivity λ,

$$m \leq \begin{cases} \frac{1}{2}\left(n - \frac{3d}{2}\right)^2 + O(n) & \text{if } \lambda = 2, \\ \frac{1}{2}\left(n - 2d\right)^2 + O(n) & \text{if } \lambda = 3 \text{ or } 4, \\ \frac{1}{2}\left(n - \frac{5d}{2}\right)^2 + O(n) & \text{if } \lambda = 5 \text{ or } 6, \\ \frac{1}{2}\left(n - 3d\right)^2 + O(n) & \text{if } \lambda = 7, \\ \frac{1}{2}\left[n - \frac{d}{3}(\lambda+1)\right]^2 + O(n) & \text{if } \lambda \geq 8 \text{ is a constant.} \end{cases}$$

For any triangle-free graph G of order n, size m, diameter d and edge-connectivity λ, we have

$$m \leq \begin{cases} \frac{1}{4}\left(n - \frac{3d}{2}\right)^2 + O(n) & \text{if } \lambda = 2, \\ \frac{1}{4}(n - 2d)^2 + O(n) & \text{if } \lambda = 3, \\ \frac{1}{4}\left(n - \frac{8d}{3}\right)^2 + O(n) & \text{if } \lambda = 5, \\ \frac{1}{4}\left(n - \frac{\lambda d}{2}\right)^2 + O(n) & \text{if } \lambda = 4 \text{ or if } \lambda \geq 6 \text{ is a constant.} \end{cases}$$

We also showed that for connected triangle-free graphs G of order n, size m, diameter d and minimum degree δ, where $\delta \geq 2$ is a constant.

$$m \leq \frac{1}{4}\left(n - \frac{\delta d}{2}\right)^2 + O(n).$$

All bounds presented in this chapter are asymptotically sharp. These bounds considerably extend known results in the area.

Chapter 7

Conclusion

In this thesis we have completely solved the problem of determining upper bounds on four distances measures, namely, radius, diameter, the Gutman index and the edge-Wiener index, in terms of other graph parameters, namely, order, irregularity index and the three classical connectivity measures, minimum degree, vertex-connectivity and edge-connectivity.

In Chapter 2 focused on the radius, diameter and the degree sequence of a graph. We gave asymptotically sharp upper bounds on the radius and diameter of (i) a connected graph, (ii) a connected triangle-free graph, (iii) a connected C_4-free graph of given order, minimum degree, and given number of distinct terms in the degree sequence of the graph. We also gave better bounds for graphs with a given order, minimum degree and maximum degree. Our results improved on old classical theorems by Erdös, Pach, Pollack and Tuza [24] on radius, diameter and minimum degree.

In Chapter 3, we showed that for finite connected graphs of order n and minimum degree δ, where δ is a constant, $\mathrm{Gut}(G) \leq \frac{2^4 \cdot 3}{5^5(\delta+1)} n^5 + O(n^4)$. Our bound is asymptotically sharp for every $\delta \geq 2$ and it extended results of Dankelmann, Gutman, Mukwembi and Swart [18] and Mukwembi [43], whose bound is sharp only for graphs of minimum degree 2.

In Chapter 4, we showed that $\mathrm{Gut}(G) \leq \frac{2^4}{5^5 \kappa} n^5 + O(n^4)$ for graphs of order n and vertex-connectivity κ, where κ is a constant. Our bound is asymptotically sharp for every $\kappa \geq 1$ and it substantially generalized the bound of Mukwembi [43]. As a corollary, we obtained a similar result for the edge-Wiener index of graphs of given order and vertex-connectivity.

Chapter 5 completed our study on the Gutman index $\mathrm{Gut}(G)$ and on the edge-Wiener index $W_e(G)$ of graphs G of given order n and edge-connectivity λ. We showed that the bound $\mathrm{Gut}(G) \leq \frac{2^4 \cdot 3}{5^5(\lambda+1)} n^5 + O(n^4)$ is asymptotically sharp for $\lambda \geq 8$. We improved this result considerably for $\lambda \leq 7$ by presenting asymptotically sharp upper bounds on $\mathrm{Gut}(G)$ and $W_e(G)$ for $2 \leq \lambda \leq 7$.

In Chapter 6, we gave asymptotically sharp upper bounds on the size, m of (i) a connected graph in terms of order, diameter and edge-connectivity, (ii) a connected triangle-free graph in terms of order, diameter and minimum degree, (iii) a connected triangle-free graph in terms of edge-connectivity, order and diameter. The result was a strengthening of an old classical theorem of Ore [49] if edge-connectivity was prescribed and constant.

The following are some interesting problems for further investigation.

Problem 1 *Finding the upper bound on the Gutman index of triangle-free or* C_4-*free graphs in terms of order* n, *diameter* d *and minimum degree* δ.

Problem 2 *Finding the upper bound on the Gutman index of triangle-free or* C_4-*free graphs in terms of order* n, *diameter* d *and vertex-connectivity* κ.

Problem 3 *Finding the upper bound on the Gutman index of triangle-free or* C_4-*free graphs in terms of order* n, *diameter* d *and and edge-connectivity* λ.

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