UNIVERSITY OF ZIMBABWE

BOUNDS ON DISTANCE-BASED GRAPH PARAMETERS

Sheunesu Munyira

May 26, 2015

BOUNDS ON DISTANCE-BASED GRAPH PARAMETERS

by

Sheunesu Munyira

Submitted in fulfilment of the academic requirements for the degree of Doctor of Philosophy in the Faculty of Science, Department of Mathematics, University of Zimbabwe

Harare

November 2014

To

My Family and friends.

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 January 2012 to November 2014. 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.

S. Munyira

November 2014

Acknowledgments

I would like to thank my supervisors, Professor Simon Mukwembi and Professor A. G. R. Stewart for their kind help and guidance during the course of my research. It has been a pleasure working with them both.

Publications arising from this thesis

1 S. Mukwembi, S. Munyira, Degree distance and minimum degree. *Bulletin Australian Mathematical Society*, **87**(2013) 255-271.

2 P. Ali, S. Mukwembi, S. Munyira, Degree distance and vertex-connectivity. *Discrete Applied Mathematics*, **161**(2013) 2802-2811.

3 P. Ali, S. Mukwembi, S. Munyira, Degree distance and edge-connectivity. *Australasian Journal of Combinatorics,* **60**(1)(2014) 50-68.

4 S. Mukwembi, S. Munyira, Radius, diameter, size and vertex-connectivity. (submitted).

5 S. Mukwembi, S. Munyira, Radius, diameter and the leaf number. (submitted).

Abstract

In this thesis, we deal with bounds on distance measures, namely, degree distance, radius, diameter and the leaf number, in terms of other graph parameters, such as order and the three classical connectivity measures, minimum degree, vertex-connectivity and edge-connectivity.

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

Chapter 2 focuses on degree distance and minimum degree. Here, we give an asymptotically sharp upper bound on the degree distance in terms of order, minimum degree and diameter. As a corollary, we obtain the bound $D'(G) \leq \frac{n^4}{9(\delta+1)} + O(n^3)$ on the degree distance $D'(G)$ of a graph G of order n and minimum degree δ. This result apart from improving on a result of Dankelmann, Gutman, Mukwembi and Swart [10] for graphs of given order and minimum degree, completely settles a conjecture of Tomescu [57].

In Chapter 3, we deal with degree distance and vertex-connectivity. We give an asymptotically sharp upper bound on the degree distance in terms of order, vertex-connectivity, and diameter. As a corollary, we obtain the bound,
$D'(G) \leq \frac{n^4}{27\kappa} + O(n^3)$ on the degree distance in terms of order and vertex-connectivity. We give examples to show that this bound of a graph G, for fixed vertex-connectivity,

is asymptotically sharp.

Chapter 4 completes our study of degree distance, in relation to the three classical connectivity measures, by looking at degree distance and edge-connectivity. In this chapter, we give asymptotically tight upper bounds on degree distance in terms of order and edge-connectivity.

Chapter 5 is a chapter in which we use techniques introduced in Chapter 3 to solve new problems on the size of a graph. Here, we give an asymptotically sharp upper bound on size of a graph G, in terms of order, diameter and vertex-connectivity. The result is a strengthening of an old classical theorem of Ore [49] if vertex-connectivity is prescribed and constant. Using the same techniques, we obtained an asymptotically tight upper bound on the size of a graph in terms of order, radius and vertex-connectivity. The result is an improvement of Vizing's theorem [60] if vertex-connectivity is prescribed.

Finally, in Chapter 6, we discuss, radius, diameter and the leaf number. We give tight upper bounds on the maximum radius and diameter of a graph G in terms of minimum degree and the leaf number. We also give a tight lower bound on the radius in terms of order, and the leaf number. Equivalently, our result provides a lower bound on the leaf number of a graph in terms of minimum degree and diameter. Moreover, we prove a lower bound on the leaf number which essentially solves a conjecture of Linial reported in [17].

Contents

0.1 Index for notation

$G = (V, E)$	graph G with vertex set V and edge set E.
$\deg_G v$	degree of a vertex $v \in V$.
$d_G(u, v)$	distance between $u, v \in V$ in G.
$rad(G)$	radius of G.
$diam(G)$	diameter of G.
$diam(S)$	$\max_{x,y\in S} d_G(x, y)$, that is, diameter of $S \subset V$ in G.
$\mu(G)$	average distance of G
$ec_G(v)$	eccentricity of vertex $v \in V$.
$(N[v])\ N(v)$	(closed) 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.
$N_{\le i}(v)$	i-th neighbourhood of v, namely $\cup_{0\le j\le i} N_j$.
$N_{\ge i}(v)$	$\cup_{i\le j\le ex_G(v)} N_j(v)$.
$(N[S])\ N(S)$	(closed) neighbourhood of subset $S \subseteq V$.
$N_{\le i}(S)$	i-th neighbourhood of $S \subset V$, namely $\cup_{v\in S} N_{\le i}(v)$.
$E(V_1, V_2)$	$\{xy \in E(G) \mid x \in V_1, y \in V_2\},\ V_1, V_2 \subset V$.
$S_1 \backslash S_2$	$\{x \in S_1 \mid x \notin S_2\}$.
$\lambda(G)$	edge-connectivity of G.
$\kappa(G)$	vertex-connectivity of G.
$\lvert S \rvert$	cardinality of a set S.
$G[S]$	subgraph induced by S in G, $S \subseteq V$.
$G_1 \cup G_2$	union of graphs G_1 and G_2.
$G_1 + G_2 + \cdots + G_k$	sequential join of graphs $G_1, G_2, \cdots, G_k$.
$V_1 \uplus V_2$	disjoint union of sets V_1 and V_2.
$\mathbf{N}$	set of natural numbers.
$\mathbf{N}_0$	$\mathbf{N} \cup \{0\}$.
$\mathbf{Z}$	set of integers.

Chapter 1

Introduction and Preliminaries

1.1 Introduction

The purpose of this chapter is to define the most important terms that will be used in this thesis and to present motivation for our study as well as provide relevant background. 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 nonempty set V of elements called *vertices* and a (possibly empty) set E of 2-element subsets of V called *edges*. The number of elements in V is called the *order* and the number of elements in E is called the *size* of G. If G has only one vertex, then we say G is *trivial*; otherwise, G is *nontrivial*. Let $e = \{u, v\} \in E(G)$. Then we say u and v are *adjacent*, while e is *incident* with u and v. We also say that e *joins* u and v. Instead of writing $e = \{u, v\}$, we often write $e = uv$.

The *degree* $\deg v$ of a vertex v of G is the number of edges incident with v. A vertex of degree 1 is called an *end-vertex*. The *minimum degree* $\delta(G) = \delta$ of G is the minimum of the degrees of the vertices in G. The *open neighbourhood* $N_G(v)$ of a vertex $v \in V$ is the set of all vertices adjacent to v in G; while the *closed neighbourhood* $N_G[v]$ is the union of $\{v\}$ and its neighbourhood.

A *walk* W in a graph G is an alternating sequence

$$W : v_0, e_1, v_1, e_2, v_2, \cdots, v_{r-1}, e_r, v_r$$

of vertices and edges such that $e_i = v_{i-1}v_i$ for $i = 1, 2, \ldots, r$. Since the vertices that appear in a walk determine the edges in the walk, we can omit the edges in the description of a walk, and denote the walk W by $v_0v_1v_2 \cdots v_r$. 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 the walk are different, then the walk is called a *path*. A path $v_0v_1v_2 \cdots v_r$ that begins at vertex v_0 and ends at vertex v_r is called a $v_0 - v_r$ *path*. Let Q_1 and Q_2 be two $v_0 - v_r$ paths. Then Q_1 and Q_2 are *edge-disjoint* if Q_1 and Q_2 have no edges in common, whereas Q_1 and Q_2 are *internally disjoint* if $V(Q_1) \cap V(Q_2) = \{v_0, v_r\}$. A *closed walk* in G is a walk of the form $v_0v_1v_2 \cdots v_r$ where $v_0 = v_r$. If all the vertices except v_0 of a closed walk $v_0v_1v_2 \cdots v_r$ are different and $r \geq 3$, then the closed walk is called a *cycle* of *length* r or simply an r-*cycle*. We say G is *connected* if every pair of vertices is connected by a path. A *tree* is a connected graph with no cycles.

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

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

The *lollipop* $L_{n,d}$, also known as the *kite*, is obtained from a complete graph K_{n-d} and a path P_d, by joining one of the end vertices of P_d to all the vertices of K_{n-d}.

Let G_1 and G_2 be two vertex disjoint graphs. 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 $E(G_1) \cup E(G_2)$. 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 $E(G_1) \cup E(G_2) \cup \{uv \mid u \in V(G_1), v \in V(G_2)\}$. For $k \geq 3$ vertex disjoint graphs $G_1, G_2, \cdots, G_k$, the *sequential join* $G_1 + G_2 + \cdots + G_k$ is the graph

$$(G_1 + G_2) \cup (G_2 + G_3) \cup \cdots \cup (G_{k-1} + G_k).$$

1.3 Distance Concepts

All graphs considered here and in the sequel are connected and nontrivial, unless otherwise specified. Let G be a graph of order n with vertex set V. The *distance* $d_G(u, v) = d(u, v)$ between two vertices u, v of G is the length of a shortest $u - v$ path in G. The *diameter* $diam(G)$ of G is defined as the maximum value of $d_G(x, y)$ taken over all vertices x, y of G. The *eccentricity* $ex_G(u)$ of a vertex u of G is defined as the maximum distance between u and any other vertex in G. The *radius* $rad(G)$ of G is the minimum value of $ex_G(u)$ taken over all vertices u of G. Every vertex of G of minimum eccentricity is a *centre vertex* of G. We say that G is a *self-centred graph* if every vertex of G is a centre vertex.

The *average distance* $\mu(G)$ of G is defined as the average of the distances between all unordered pairs of vertices, that is,

$$\mu(G) = \binom{n}{2}^{-1} \sum_{\{u,v\} \subset V} d_G(u, v).$$

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 sometimes simply write N_i if v is understood. We denote the cardinality of N_i by k_i.

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

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

The *degree distance* $D'(G)$ of G is defined as

$$\sum_{\{u,v\} \subseteq V} (\deg\, u + \deg\, v) d(u, v),$$

where deg w is the degree of vertex w and $d(u, v)$ denotes the distance between u and v in G.

A subgraph H of G is said to be *distance preserving from* v in G if $d_H(v, u) = d_G(v, u)$ for all $u \in V(H)$ and H is *isometric* in G if $d_H(x, y) = d_G(x, y)$ for all $x, y \in V(H)$. For a positive integer k, a k*-packing* is a subset $A \subset V(G)$ with $d_G(a, b) > k$ for all $a, b \in A$.

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.

1.4.2 The degree distance

The degree distance, a Schultz-type molecular topological index and a variant of the well-known and much studied Wiener index, seems to have been considered first by Dobrynin and Kochetova [19] in 1994 and practically at the same time by Gutman

[31], who introduced it as a kind of a vertex-valency-weighted sum of the distances between all pairs of vertices in a graph. Gutman revealed that in the case of acyclic structures, the index is closely related to the Wiener index and reflects precisely the same structural features of a molecular graph as the Wiener index does.

However, somewhat before 1994, the degree distance was encountered in connection with certain chemical applications [41, 53]. After 1994, the degree distance was investigated by several authors, for instance, I. Tomescu [57], A. I. Tomescu [58], O. Bucicovschi and S. M. Cioabă [3], P. Dankelmann, I. Gutman, S. Mukwembi and H.C. Swart [10], and A. Ilić, D. Stevanović, L. Feng, G. Yu and P. Dankelmann [36]. Sharp upper and lower bounds on the degree distance for trees of given order were completely determined (see, for example a recent survey, [12]). For general graphs, Dobrynin and Kochetova [19] conjectured that the largest degree distance of all connected graphs of order n equals $\frac{n^4}{32} + O(n^3)$. This was refuted by Tomescu [57], who showed that graphs consisting of two cliques of order approximately $n/3$ joined by a path on approximately $n/3$ vertices, have degree distance $\frac{n^4}{27} + O(n^3)$. He then made the following attractive conjecture.

Conjecture 1.1 [57] *Let G be a connected graph of order n. Then*

$$D'(G) \leq \frac{n^4}{27} + O(n^3).$$

Nine years after the announcement of this conjecture, Bucicovschi and Cioabă [3] commented that Tomescu's conjecture "seems difficult at present time." In the following year, Dankelmann, Gutman, Mukwembi and Swart [10] considered this problem and though they came close to proving the conjecture, their proof was inadequate to meet the $O(n^3)$ error term. They proved the following bound.

Theorem 1.2 [10] *If G is a connected graph of order n, then*

$$D'(G) \leq \frac{n^4}{27} + O(n^{\frac{7}{2}}).$$

Recently the method developed in [10] was improved in [43] leading to a complete solution of Tomescu's conjecture.

Since the degree distance can be considered as a weighted version of the Wiener index, comparisons between the two indices are inevitable. For trees of given order, these two parameters actually determine each other: Klein, Mihalić, Plavšić, Trinajstić [37] and also Gutman [31] showed that, for every tree T of order n, $D'(T) = 4W(T) - n(n-1)$, where $W(G) = \sum_{\{u,v\} \subseteq V} d(u,v)$ is the Wiener index of G. Since its introduction in the late 1940's by the Chemist Harold Wiener in an attempt to analyze the chemical properties of paraffins (alkanes) [61], the mathematical properties of the Wiener index were studied by several authors. One of the oldest results on upper bounds of this quantity is that amongst all connected graphs of given order, the path has the maximum Wiener index. For graphs of given minimum degree, this result was improved independently by several authors, for instance, Kouider and Winkler [39], Dankelmann and Entringer [9], who proved the following bound.

Theorem 1.3 [9, 39] *Let G be a graph of order n and minimum degree δ. Then*

$$W(G) \leq \frac{n^3}{2(\delta+1)} + O(n^2),$$

and this bound is best possible.

In light of Theorem 1.3 and the fact that the degree distance can be considered as a weighted version of the Wiener index, it is natural to ask for a best upper bound on the degree distance of a connected graph of given order and minimum degree. In this thesis, we obtain an asymptotically sharp upper bound on the degree distance of a graph of given order and minimum degree. Our result, apart from being a strengthening of Theorem 1.2, and a theorem in [43], confirms and improves on Tomescu's conjecture, Conjecture 1.1, if minimum degree is prescribed. Our method is an improvement of the method initiated in [10].

We also give an asymptotically sharp upper bound on the degree distance in terms of order, vertex-connectivity, and diameter, and asymptotically sharp upper bounds on the degree distance and edge-connectivity.

The Diameter, Radius, Size and Leaf number

The diameter and radius, apart from being interesting graph theoretical parameters, play an important role in analysing communication networks (see for example, [4]). In such networks, the time delay or signal disgradation 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.

The radius is an important measure of centrality. The central vertices in a network are of particular interest because they can play the role of organizational hubs. In networks, decision problems involving the optimal selection of one or more sites to locate facilities centrally arise. The primary concern may be to choose a location such that the travel time/distance from the central facility to a location farthest away is as small as possible. The radius is a good measure that indicates the travel time from a central facility to a location farthest away, if the best location for the central facility is chosen.

Connectivity, on the other hand, is a key measure of network reliability; it is a criterion for gauging the ability of a network to withstand failure of components [2].

Several bounds on the size of a graph in terms of other graph parameters, for example, order and radius [15, 55, 60], order and degree set [59], and order and domination number [8] have been investigated. An upper bound on the size of a graph in terms of order and diameter was determined by Ore [49] as early as 1968. Several authors [55, 59] have presented simple and short proofs to Ore's theorem. Recently Mukwembi [46] reported on asymptotically sharp upper bounds on the size in terms of order, diameter and minimum degree, and in terms of order, radius and minimum degree [47]. Extremal graphs presented are graphs of connectivity 1. It is therefore natural to ask whether better bounds can be found when vertex-connecitvity is prescribed. In this thesis, we answer this question in the affirmative.

Several upper bounds on the radius and diameter in terms of other graph parameters, for example, order and minimum degree [24, 6, 7], order and size [49], order and inverse degree [14, 23, 44], order, minimum degree and irregularity index [45], independence number [26, 27, 25], order and vertex-connectivity [32, 33, 22, 34], order and edge-connectivity [13] have been investigated.

One graph parameter which, to date, has not been related to the radius and diameter is the leaf number. The *leaf number*, $L(G)$, of G is defined as the maximum number of leaf vertices contained in a spanning tree of G. (a leaf is an end vertex.) Apart from being an attractive graph parameter, the leaf number has many practical applications, for instance, in network design, and particularly in wireless ad hoc networks (see, for example [5, 16, 40, 52, 56]). As mentioned earlier on to date neither upper bounds on radius and diameter in terms of the leaf number nor lower bounds on the leaf number in terms of radius and diameter have been reported on. In this thesis, we contribute towards filling this gap.

We now turn to the leaf number as a parameter in its own right. Determining the leaf number of a graph is known to be NP-hard (see, for example [17] and references therein). It is therefore reasonable to ask for lower bounds on the leaf number in terms of other graph parameters. Lower bounds on the leaf number in terms of other parameters, for instance, order, independence number and maximum order of a bipartite graph [16], order and size [17] have been investigated. However, the first result on lower bounds seems to be a statement, without proof, by Storer [54] that every connected cubic graph G with n vertices has $L(G) \geq \frac{n}{4} + 2$. Linial (see, [17]) conjectured, more generally, that every connected graph G with n vertices and minimum degree δ satisfies

$$L(G) \geq \frac{\delta - 2}{\delta + 1} n + c_\delta,$$

where c_δ is a constant depending only on δ. Several authors have researched on this conjecture. Kleitman and West [39] introduced a heavy method, the dead leaves approach, with which they gave a proof of Linial's Conjecture for $\delta = 3$ with a best possible $c_\delta = 2$, and hence providing for the first time a rigorous proof to Storer's Theorem. Subsequently, Griggs and Wu [30], using the complicated dead leaves approach, settled Linial's Conjecture for $\delta = 4$ and 5. They proved the following two theorems.

Theorem 1.4 *If G is a connected simple graph with n vertices and minimum degree at least 4, then $L(G) \geq \frac{2}{5}n + \frac{8}{5}$.* □

Theorem 1.5 *If G is a connected simple graph with n vertices and minimum degree at least 5, then $L(G) \geq \frac{1}{2}n + 2$.* □

Linial's Conjecture is still open for the case when $\delta \geq 6$ whilst for δ sufficiently large the conjecture was disproved by Alon (see, for example [51]).

Further, in this thesis, using a technique developed by Dankelmann and Entringer [9], we prove a lower bound on the leaf number of a graph of given order and minimum degree. Our bound, for sufficiently large minimum degree, provides a very short, simple and unified proof to Theorems 1.4 and 1.5.

We conclude this chapter by summarizing the proof techniques that are important for this thesis.

Upper bounds on the diameter in terms of order and minimum degree have been considered and rediscovered by numerous authors, for example, [24, 28, 42]. The basic observation from which most of these bounds follow is simple. If we fix a shortest path between two vertices u and v at maximum distance and if we then consider the vertices on the path at distance $0, 3, 6, 9, \ldots$ on this path, then we obtain about $\frac{diam(G)}{3}$ vertices whose closed neighbourhoods are pairwise disjoint. Hence, approximately, $n > \frac{diam(G)}{3}(\delta + 1)$, and so the diameter is at most $\frac{3n}{\delta + 1} + O(1)$.

However, an important technique of proving upper bounds on the radius for connected graphs is to prove first that it holds for all trees, and then to make use of the fact that the radius of a connected graph is not greater than the radius of any of its spanning trees. This technique is less applicable for proving bounds on diameter because every connected graph has a spanning tree that preserves the radius, but not every connected graph has a spanning tree that preserves the diameter.

Finding bounds on the radius in terms of minimum degree is difficult. In [24] the authors proved that for a graph G of order n and minimum degree $\delta \geq 2$ the upper bound on the radius is $\frac{3(n-3)}{2(\delta + 1)} + 5$ and the bound is asymptotically sharp.

To prove this result, the technique is based on the observation that, given a centre vertex v, there exist vertices w_i at distance r or $r - 1$ from $v, i = 1, 2$, and shortest paths P_i from v to w_i with the following property: no vertex u_1 of P_1 shares a neighbour with vertex u_2 of P_2, unless u_1 or u_2 are very close to one of the vertices v, w_1 or w_2. Given P_1 and P_2, one can find approximately $2\frac{rad(G)}{3}$ vertices with disjoint neighbourhoods by choosing every third vertex on P_1 and P_2. This yields approximately $n \geq \frac{2}{3}rad(G)(\delta + 1)$, and the bound follows.

We use the methods above in proving parts of some of our results. However, the methods described above and the results are inadequate to capture the effect of vertex and edge- connectivity. In that case, we devise new techniques for handling the two connectivity measures.

In this thesis, the standard method we use for finding upper bounds on the degree distance $D'(G)$ of a graph G is by grouping vertices into pairs $\{a, b\}$ and then bounding the contribution of each pair a, b to the degree distance.

Chapter 2

Degree distance and minimum degree

2.1 Introduction

The goal of this chapter is to find asymptotically sharp upper bounds on the degree distance in terms of order and minimum degree. Due to the complexity of the problem, we will first establish upper bounds on the degree distance in terms of order, diameter and minimum degree. We will then deduce the results as corollaries. Further, we construct graphs to show that the bounds are asymptotically sharp. Our results, apart from improving on a result of Dankelmann et al [10], completely settle a conjecture of Tomescu [57].

The notation that we use is as follows. For a vertex v of G, we denote by $D(v)$ the total distance or the status of v. That is, $D(v) = \sum_{x\in V(G)} d(v,x)$. The quantity deg $vD(v)$ is denoted by $D'(v)$. We denote the open neighbourhood of v by $N(v)$, i.e., $N(v) = \{x \in V(G) \mid d(x,v) = 1\}$. The closed neighbourhood of v in G, i.e., $N(v)\cup\{v\}$, is denoted by $N[v]$. Here and in the sequel, we assume that the minimum degree δ is fixed.

The useful equation

$$D'(G) = \sum_{v \in V} D'(v)$$

was first observed by Tomescu [57].

2.2 Results

We begin by presenting a very simple, but handy, observation.

Fact 2.1 *Let G be a connected graph of order n, diameter d and minimum degree δ. If $v \in V(G)$, then $d \leq \frac{3}{\delta+1}(n - \deg v) + 6$.*

Proof of Fact 2.1: Assume that $v \in V(G)$ and let $P : v_0, v_1, \ldots, v_d$ be a diametric path of G. Let $S := \{v_{3i+1} \mid i = 0, 1, \ldots, \lfloor \frac{d-1}{3} \rfloor\}$. For each $x \in S$, choose any δ neighbours $x_1, x_2, \ldots, x_\delta$ of x and denote the set $\{x, x_1, x_2, \ldots, x_\delta\}$ by $M[x]$. Let $M = \cup_{x \in S} M[x]$. Then $|M| = (\delta + 1)(\lfloor \dfrac{d-1}{3} \rfloor + 1)$. Note that by the construction of S, $N[v] \cap M$ has at most $2\delta + 1$ vertices. Hence

$$n \geq |M| + |N[v]| - |M \cap N[v]| \geq (\delta+1)(\lfloor \frac{d-1}{3} \rfloor + 1) + \deg v + 1 - (2\delta+1) \geq (\delta+1)\frac{d}{3} + \deg v - 2\delta,$$

and rearranging the terms completes the proof. $\square$

Often, we will use the following simple and straightforward result or its variation.

Proposition 2.1 *Let G be a connected graph of order n, diameter d and fixed minimum degree δ. If $v \in V(G)$, then $D(v) \leq d(n - \frac{d}{6}(\delta + 1) - \deg v) + O(n)$.*

Proof: Denote the eccentricity of v by e. For all $i = 1, 2, \ldots, e$, let $N_i := \{x \in V(G) \mid d(v, x) = i\}$ and $|N_i| = k_i$. Note that if $x \in N_i$, $i = 2, 3, \ldots, e-1$, then $N[x] \subseteq N_{i-1} \cup N_i \cup N_{i+1}$ so that

$$k_{i-1} + k_i + k_{i+1} \geq \delta + 1.$$

Clearly,

$$D(v) = 1k_1 + 2k_2 + \cdots + ek_e. \tag{2.1}$$

We look at three cases separately.

Case 1: $e \equiv 0 \bmod 3$. Subject to

$$k_1 = \deg\, v,\ \ k_i \geq 1 \text{ for } i = 2, 3, \ldots, e,$$

and

$$k_2 + k_3 + k_4 \geq \delta + 1, \quad k_5 + k_6 + k_7 \geq \delta + 1, \ldots, k_{e-4} + k_{e-3} + k_{e-2} \geq \delta + 1,$$

(2.1) is maximized for

$$k_1 = \deg\, v,\ \ k_2 = 1 = k_3,\ \ k_4 = \delta - 1, k_5 = 1 = k_6,\ \ k_7 = \delta - 1, \ldots, k_{e-4} = 1 = k_{e-3},$$

$$k_{e-2} = \delta - 1,\ \ k_{e-1} = 1 \text{ and } k_e = n - \deg\, v - \frac{1}{3}(e-3)(\delta+1) - 1 - 1.$$

This gives

$$\begin{aligned} D(v) &\leq \deg\, v + 2 + 3 + 4(\delta - 1) + 5 + 6 + 7(\delta - 1) + \cdots \\ &\quad + (e-4) + (e-3) + (e-2)(\delta-1) + (e-1) + e\left(n - \deg\, v - \frac{1}{3}(e-3)(\delta+1) - 2\right) \\ &= e\left(n - \frac{e}{6}(\delta+1) - \deg\, v\right) + O(n). \end{aligned}$$

If $e = d - c$, where $c \in \{0, 1, \ldots, 5\}$, then

$$D(v) \leq (d-c)\left(n - \frac{d-c}{6}(\delta+1) - \deg\, v\right) + O(n) = d\left(n - \frac{d}{6}(\delta+1) - \deg\, v\right) + O(n),$$

as desired. So assume that $e \leq d - 6$. The function $f(e) = e\left(n - \frac{e}{6}(\delta+1) - \deg\, v\right)$ is increasing in e for all $e \leq \frac{3}{\delta+1}(n - \deg\, v)$. Note from Fact 2.1 that $d - 6 \leq \frac{3}{\delta+1}(n - \deg\, v)$. Hence $D(v) \leq f(d-6) = d\left(n - \frac{d}{6}(\delta+1) - \deg\, v\right) + O(n)$, and the proposition is proven for this case. This completes Case 1.

The other cases, i.e., $e \equiv 1 \bmod 3$ and $e \equiv 2 \bmod 3$, are treated similarly. $\square$

Theorem 2.1 *Let G be a connected graph of order n, diameter d and fixed minimum degree δ. Then*

$$D'(G) \leq \begin{cases} \frac{1}{4}dn\left(n - \frac{d}{3}(\delta+1)\right)^2 + O(n^3) & \text{if } d < \frac{3n}{2(\delta+1)}, \\ \\ \frac{1}{6}d^2(\delta+1)(n-\frac{d}{3}(\delta+1))^2 + O(n^3) & \text{if } d \geq \frac{3n}{2(\delta+1)}. \end{cases}$$

Moreover, this inequality is asymptotically tight.

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

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

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 $M[v]$. Let $M = \cup_{v \in S} M[v]$. Then $|M| = (\delta+1)(\lfloor \frac{d-1}{3} \rfloor + 1)$.

Claim 1

$$\sum_{u \in M} D'(u) \leq O(n^3).$$

Proof of Claim 1: Let $S_1 \subset S$ be the set $S_1 = \{v_j \in S : j \equiv 1 \bmod 6\}$. Let $S_2 = S - S_1$. Then for $u, v \in S_1$, $u \neq v$, we have $M[u] \cap M[v] = \emptyset$ and the neighbourhoods of $M[u]$ and $M[v]$ 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 $M[w_j] = \{w_j, u_1^j, u_2^j, \ldots, u_\delta^j\}$, where $u_1^j, u_2^j, \ldots, u_\delta^j$ are neighbours of w_j. Then

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

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

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

Summing, we get

$$(\delta+1)n \geq \sum_{x \in M[S_1]} \deg x + (\delta+1)|S_1|,$$

where $M[S_1] = \sum_{u \in S_1} M[u]$.

Similarly,

$$(\delta+1)n \geq \sum_{x \in M[S_2]} \deg x + (\delta+1)|S_2|.$$

Thus

$$\begin{aligned} 2(\delta+1)n &\geq \sum_{x \in M[S_1]} \deg x + \sum_{x \in M[S_2]} \deg x + (\delta+1)|S| \\ &= \sum_{x \in M[S_1]} \deg x + \sum_{x \in M[S_2]} \deg x + (\delta+1)\left(\lfloor \frac{d-1}{3} \rfloor + 1\right). \end{aligned}$$

Hence

$$\begin{aligned} \sum_{x \in M[S_1]} \deg x + \sum_{x \in M[S_2]} \deg x &\leq 2(\delta+1)n - (\delta+1)\left(\lfloor \frac{d-1}{3} \rfloor + 1\right) \\ &= (\delta+1)\left(2n - \lfloor \frac{d-1}{3} \rfloor - 1\right). \end{aligned}$$

Now for $u \in V(G)$, since $D(u) \leq (n-1)d \leq (n-1)^2$, it follows that

$$\begin{aligned} \sum_{v \in M} D'(v) &= \sum_{v \in M} \deg v D(v) \\ &= \sum_{v \in M[S_1]} \deg v D(v) + \sum_{v \in M[S_2]} \deg v D(v) \\ &\leq (n-1)^2 \left(\sum_{v \in M[S_1]} \deg v + \sum_{v \in M[S_2]} \deg v \right) \\ &\leq (n-1)^2(\delta+1)\left(2n - \lfloor \frac{d-1}{3} \rfloor - 1\right) \\ &= O(n^3), \end{aligned}$$

as required and so Claim 1 is proven.

Let $\mathcal{C}$ be a maximum set of disjoint pairs of vertices from $V - M$ which lie at a distance at least 3, i.e., if $\{a, b\} \in \mathcal{C}$, then $d(a, b) \geq 3$. If $\{a, b\} \in \mathcal{C}$, then we say a and b are partners. Finally, let K be the remaining vertices of G, i.e., $K = V - M - \{x : \quad x \in \{a,b\} \in \mathcal{C}\}$. Let $|K| = k$, and $|\mathcal{C}| = c$. Then

$$n = (\delta+1)\left(\lfloor\frac{d-1}{3}\rfloor + 1\right) + 2c + k. \tag{2.2}$$

Fact 2.2 *Let* $\{a,b\} \in \mathcal{C}$. *Then* $\deg a + \deg b \le n - \frac{d}{3}(\delta+1) + O(1)$.

Proof of Fact 2.2: Note that $N[a] \cap N[b] = \emptyset$, since $d(a,b) \ge 3$. Also, each of the two vertices can be adjacent to at most $2\delta + 1$ vertices on M. Thus,

$$\begin{aligned} n &\ge \deg a + 1 + \deg b + 1 + |M| - 2(2\delta+1) \\ &= \deg a + \deg b + (\delta+1)(\lfloor\frac{d-1}{3}\rfloor + 1) - 4\delta, \end{aligned}$$

and rearranging the terms completes the proof of Fact 2.2.

Now consider two cases.

Case 1: $k \le 1$.

For $x \in K, \quad D(x) \le (n-1)^2$, so $D'(x) \le (n-1)^3$. Thus $\sum_{x\in K} D'(x) = O(n^3)$.

Claim 2 *If* $\{a,b\} \in \mathcal{C}$, *then* $D'(a) + D'(b) \le \frac{1}{2}dn\left(n - \frac{d}{3}(\delta+1)\right) + O(n^2)$.

Proof of Claim 2: By Proposition 2.1, $D(a) \le d\left(n - \frac{d}{6}(\delta+1) - \deg a\right) + O(n)$. It follows that $D'(a) \le \deg a\left(d\left(n - \frac{d}{6}(\delta+1) - \deg a\right)\right) + O(n^2)$.

Similarly, $D'(b) \le \deg b\left(d\left(n - \frac{d}{6}(\delta+1) - \deg b\right)\right) + O(n^2)$. Thus,

$$\begin{aligned} D'(a) + D'(b) &\le \deg a\left(d\left(n - \frac{d}{6}(\delta+1) - \deg a\right)\right) + \deg b\left(d\left(n - \frac{d}{6}(\delta+1) - \deg b\right)\right) + O(n^2) \\ &= d\left((\deg a + \deg b)\left(n - \frac{d}{6}(\delta+1)\right) - \left((\deg a)^2 + (\deg b)^2\right)\right) + O(n^2) \\ &\le d\left((\deg a + \deg b)\left(n - \frac{d}{6}(\delta+1)\right) - \frac{1}{2}(\deg a + \deg b)^2\right) + O(n^2). \end{aligned}$$

Denote $\deg a + \deg b$ by x and let $f(x) = d\left(x\left(n - \frac{d}{6}(\delta+1)\right) - \frac{1}{2}x^2\right)$. Then by Fact 2.2, $x \leq n - \dfrac{d}{3}(\delta+1) + O(1)$. A simple differentiation shows that f is increasing for all $x \leq n - \frac{d}{6}(\delta+1)$. Hence f attains its maximum for $x = n - \dfrac{d}{3}(\delta+1) + O(1)$, to give

$$\begin{aligned} D'(a) + D'(b) &\leq f\left(n - \frac{d}{3}(\delta+1) + O(1)\right) \\ &= \frac{1}{2}dn\left(n - \frac{d}{3}(\delta+1)\right) + O(n^2), \end{aligned}$$

and Claim 2 is proven.

From (2.2), we have $c = \frac{1}{2}\left(n - (\delta+1)\left(\lfloor\frac{d-1}{3}\rfloor + 1\right) - k\right)$. Since $k \leq 1$, we have $c = \frac{1}{2}\left(n - \frac{d}{3}(\delta+1)\right) + O(1)$. This, in conjunction with Claim 2, yields

$$\begin{aligned} \sum_{\{a,b\}\in\mathcal{C}} (D'(a) + D'(b)) &\leq c\left(\frac{1}{2}dn\left(n - \frac{d}{3}(\delta+1)\right) + O(n^2)\right) \\ &= \left(\frac{1}{2}\left(n - \frac{d}{3}(\delta+1)\right) + O(1)\right)\left(\frac{1}{2}dn\left(n - \frac{d}{3}(\delta+1)\right) + O(n^2)\right) \\ &= \frac{1}{4}dn\left(n - \frac{d}{3}(\delta+1)\right)^2 + O(n^3). \end{aligned}$$

Hence

$$\begin{aligned} D'(G) &= \sum_{\{a,b\}\in\mathcal{C}} (D'(a) + D'(b)) + \sum_{x\in K} D'(x) + \sum_{v\in M} D'(v) \\ &\leq \frac{1}{4}dn\left(n - \frac{d}{3}(\delta+1)\right)^2 + O(n^3) + O(n^3) + O(n^3). \end{aligned}$$

Note that, if $d \geq \dfrac{3n}{2(\delta+1)}$, then $\frac{1}{4}dn\left(n - \frac{d}{3}(\delta+1)\right)^2 \leq \frac{1}{6}d^2(\delta+1)\left(n - \frac{d}{3}(\delta+1)\right)^2$, and so the theorem is proved for Case 1.

Case 2: $k \geq 2$.

Now the pairs of vertices in $\mathcal{C}$ will be partitioned further. Fix a vertex $x \in K$. For each pair $\{a, b\} \in \mathcal{C}$, choose a vertex closer to x; if $d(a, x) = d(b, x)$, then arbitrarily choose one of the vertices. Let A be the set of all these vertices closer to x, and B be the set of partners of these vertices in A, so $|A| = |B| = c$. Furthermore, let $A_1(B_1)$ be the set of vertices $w \in A(B)$ whose partner is at a distance at most 9 from w. Let $c_1 = |A_1| = |B_1|$.

Claim 3 *For all* $u, v \in A \cup K$, $d(u, v) \leq 8$.

Proof of Claim 3: Since $\mathcal{C}$ is a maximum set of pairs of vertices of distance at least 3, any two vertices of K must be at a distance of at most 2. We show that $d(a, x) \leq 4$ for all $a \in A$. Suppose, to the contrary, that there exists a vertex $a \in A$ for which $d(a, x) \geq 5$. Let b be the partner of a. By definition of A, $d(x, b) \geq 5$. Now consider another vertex $x' \in K$, $x \neq x'$. Since $d(x, x') \leq 2$, we have

$$5 \leq d(b, x) \leq d(b, x') + d(x, x') \leq d(b, x') + 2$$

which implies $d(b, x') \geq 3$. This contradicts the maximality of $\mathcal{C}$ since $\{a, b\}$ will be replaced by $\{a, x\}$ and $\{b, x'\}$. Hence $d(a, x) \leq 4$, for each $a \in A$. Thus for $u, v \in A$, $d(u, v) \leq d(u, x) + d(x, v) \leq 8$.

Claim 4 *For all* $x \in K$,

$$D'(x) \leq d\left(n - \frac{d}{3}(\delta + 1) - c\right)\left(n - c - c_1 - k - \frac{d}{6}(\delta + 1)\right) + O(n^2).$$

Proof of Claim 4: By Claim 3, all $c + k$ vertices in $A \cup K$ lie within a distance of 8 from each vertex $x \in K$. This implies that all the c_1 vertices in B_1 lie within a distance of $9+8$ from x. Thus, as in Proposition 2.1,

$$\begin{aligned} D(x) &\leq 8(c+k)+17c_1+18+19+20(\delta-1)+21+22+23(\delta-1)+\cdots \\ &\quad + d\left(n-c-k-c_1-\frac{d}{3}(\delta+1)\right) \\ &= d\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right)+O(n). \end{aligned}$$

In order to find a bound on the degree of x, we use a counting argument. Note that x can have at most $2\delta+1$ neighbours in M. By definition of A and B, x cannot be adjacent to two vertices, w and z, where $w \in A$ is a partner of $z \in B$, since $d(w,z) \geq 3$. Thus, x is adjacent to at most c vertices in $A \cup B$. It follows that

$$\begin{aligned} n &\geq \deg x + |M| - (2\delta+1) + |A \cup B| - c \\ &= \deg x + (\delta+1)\left(\lfloor\frac{d-1}{3}\rfloor+1\right) - (2\delta+1) + c \\ &= \deg x + \frac{d}{3}(\delta+1) + c + O(1). \end{aligned}$$

Hence $\deg x \leq n - \frac{d}{3}(\delta+1) - c + O(1)$. Therefore,

$$\begin{aligned} D'(x) &= \deg x D(x) \\ &\leq d\left(n-\frac{d}{3}(\delta+1)-c\right)\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right)+O(n^2), \end{aligned}$$

and this proves Claim 4.

We now turn to finding an upper bound on the contribution of the pairs in $\mathcal{C}$ to the degree distance. We abuse notation and write $\{a,b\} \in A_1 \cup B_1$ if a and b are partners, i.e., $\{a,b\} \in \mathcal{C}$, with $a \in A_1$ and $b \in B_1$. Note that

$$\sum_{\{a,b\}\in\mathcal{C}} (D'(a)+D'(b)) = \sum_{\{a,b\}\in A_1\cup B_1} (D'(a)+D'(b)) + \sum_{\{a,b\}\in(A-A_1)\cup(B-B_1)} (D'(a)+D'(b)).$$

We first consider the set $A_1 \cup B_1$.

Claim 5 *Let $\{a,b\} \in \mathcal{C}$. If $d(a,b) \le 9$, i.e., if $\{a,b\} \in A_1 \cup B_1$, then*

$$D'(a) + D'(b) \le d\left(n - \frac{d}{3}(\delta+1)\right)\left(n - c - c_1 - k - \frac{d}{6}(\delta+1)\right) + O(n^2).$$

Proof of Claim 5: We first show that any two vertices in $A \cup K \cup B_1$ lie within a distance of 26 from each other. By Claim 3, any two vertices in $A \cup K$ lie within a distance of 8 from each other. Now assume that $b, v \in B_1$, and let a and u be the partners of b and v in A_1, respectively. Then $d(b,v) \le d(b,a) + d(a,u) + d(u,v) \le 9 + 8 + 9 = 26$. Thus any two vertices in B_1 are within a distance of 26 from each other. Now let $a \in A \cup K$ and $b \in B_1$, and let u be the partner of b in $A_1 \subseteq A$. Then $d(a,b) \le d(a,u) + d(u,b) \le 8 + 9 < 26$. Hence any two vertices in $A \cup K \cup B_1$ lie within a distance of 26 from each other.

Now let $w \in A_1 \cup B_1$. Since w is in $A \cup K \cup B_1$, all the $c + k + c_1 - 1$ vertices in $A \cup K \cup B_1$ lie within a distance of 26 from w. It follows, as in Proposition 2.1, that

$$\begin{aligned} D(w) &\le 26(c + k + c_1 - 1) + 27 + 28 + 29(\delta - 1) + 30 + 31 + 32(\delta - 1) + \cdots \\ &\quad + d\left(n - c - c_1 - k - \frac{d}{3}(\delta+1)\right) \\ &= d\left(n - c - c_1 - k - \frac{d}{6}(\delta+1)\right) + O(n). \end{aligned}$$

Thus, if $\{a,b\}$ is a pair in $A_1 \cup B_1$, then

$$\begin{aligned} D'(a) + D'(b) &\le \deg a\left(d\left(n - c - c_1 - k - \frac{d}{6}(\delta+1)\right) + O(n)\right) \\ &\quad + \deg b\left(d\left(n - c - c_1 - k - \frac{d}{6}(\delta+1)\right) + O(n)\right) \\ &= (\deg a + \deg b)\left(d\left(n - c - c_1 - k - \frac{d}{6}(\delta+1)\right) + O(n)\right). \end{aligned}$$

By Fact 2.2, $\deg a + \deg b \le n - \frac{d}{3}(\delta+1) + O(1)$. Therefore,

$$\begin{aligned} D'(a) + D'(b) &\le \left(n - \frac{d}{3}(\delta+1) + O(1)\right)\left(d\left(n - c - c_1 - k - \frac{d}{6}(\delta+1)\right) + O(n)\right) \\ &= d\left(n - \frac{d}{3}(\delta+1)\right)\left(n - c - c_1 - k - \frac{d}{6}(\delta+1)\right) + O(n^2), \end{aligned}$$

and Claim 5 is proven.

Now consider pairs $\{a,b\}$ of vertices in $\mathcal{C}$ which are not in $A_1 \cup B_1$.

Claim 6 *Let* $\{a,b\} \in \mathcal{C}$. *If* $d(a,b) \ge 10$, *i.e., if* $\{a,b\} \in (A - A_1) \cup (B - B_1)$, *then*

$$D'(a) + D'(b) \le d(c+k)\left(n - c - c_1 - k - \frac{d}{6}(\delta+1)\right) + cd\left(n - \frac{d}{6}(\delta+1) - c\right) + O(n^2).$$

Proof of Claim 6: We consider vertices from $A - A_1$ and from $B - B_1$ separately. Let $a \in A - A_1$. Then as in Claim 5, all the $c + k - 1$ vertices in $A \cup K$ lie at a distance of 8 from a and all the c_1 vertices in B_1 lie within a distance of $9 + 8 = 17$ from a. Thus, as in Proposition 2.1,

$$\begin{aligned} D(a) &\le 8(c+k-1) + 17c_1 + 18 + 19 + 20(\delta-1) + 21 + 22 + 23(\delta-1) + \cdots \\ &\quad + d\left(n - c - c_1 - k - \frac{d}{3}(\delta+1)\right) \\ &= d\left(n - c - c_1 - k - \frac{d}{6}(\delta+1)\right) + O(n). \end{aligned}$$

We now find a bound on the degree of a. By definition of $\mathcal{C}$, the vertex a cannot be adjacent to both w and u, where $w \in A$ is a partner of $u \in B$, since $d(w,u) \ge 3$. Hence a is adjacent to at most $c - 1$ vertices in $A \cup B$. Further, a is adjacent to at most $2\delta + 1$ vertices in M and has at most k neighbours in K. Thus,

$$\deg a \le c - 1 + 2\delta + 1 + k = c + 2\delta + k.$$

It follows that

$$\begin{aligned}
D'(a) &= (\deg a)D(a) \\
&\le (c+k+2\delta)\left(d\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right)+O(n^2)\right) \\
&= d(c+k)\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right)+O(n^2). \qquad (2.3)
\end{aligned}$$

Now let $b \in B - B_1$. By Proposition 2.1, we have

$$D(b) \le d\left(n-\frac{d}{6}(\delta+1)-\deg b\right)+O(n),$$

and so

$$D'(b) \le \deg b\left(d\left(n-\frac{d}{6}(\delta+1)-\deg b\right)\right)+O(n^2). \qquad (2.4)$$

We first maximize $\deg b\left(d\left(n-\frac{d}{6}(\delta+1)-\deg b\right)\right)$ with respect to $\deg b$. Let

$$f(x) := x\left(d\left(n-\frac{d}{6}(\delta+1)-x\right)\right),$$

where $x = \deg b$. A simple differentiation shows that f is increasing for $x \le \frac{1}{2}\left(n-\frac{d}{6}(\delta+1)\right)$. We find an upper bound on x, i.e., on $\deg b$. Note that as above, b can be adjacent to at most $c-1$ vertices in $A \cup B$, and has at most $2\delta+1$ neighbours in M. We show that b cannot be adjacent to any vertex in K. Suppose, to the contrary, that $y \in K$ and $d(b,y)=1$. Recall that a is the partner of b and $d(a,b) \ge 10$. By Claim 3, $d(a,y) \le 8$. Hence $10 \le d(a,b) \le d(b,y)+d(y,a) \le 1+8$, a contradiction. Thus, b cannot be adjacent to any vertex in K. We conclude that

$$\deg b \le c-1+2\delta+1 = c+2\delta.$$

We look at two cases separately. First assume that $\deg b = c + j$, where $j \in \{1, 2, \ldots, 2\delta\}$. Then

$$\begin{aligned} f(\deg b) &= f(c+j) \\ &= (c+j)\left(d\left(n - \frac{d}{6}(\delta+1) - (c+j)\right)\right) \\ &= cd\left(n - \frac{d}{6}(\delta+1) - c\right) + O(n^2). \qquad (2.5) \end{aligned}$$

Second, assume that $\deg b \leq c$. From (2.2), the fact that $k \geq 2$ and $\lfloor \frac{d-1}{3} \rfloor + 1 \geq \frac{d}{3}$, we have

$$c = \frac{1}{2}\left(n - (\delta+1)\left(\lfloor\frac{d-1}{3}\rfloor + 1\right) - k\right) \leq \frac{1}{2}\left(n - \frac{d}{3}(\delta+1) - 2\right).$$

Notice that

$$\frac{1}{2}\left(n - \frac{d}{3}(\delta+1) - 2\right) \leq \frac{1}{2}\left(n - \frac{d}{6}(\delta+1)\right),$$

and so f is increasing in $[1, c]$. Therefore,

$$f(\deg b) \leq f(c) = cd\left(n - \frac{d}{6}(\delta+1) - c\right),$$

for this case. Comparing this with (2.5), we get that

$$f(\deg b) \leq cd\left(n - \frac{d}{6}(\delta+1) - c\right) + O(n^2).$$

Thus, from (2.4), we have

$$D'(b) \leq cd\left(n - \frac{d}{6}(\delta+1) - c\right) + O(n^2).$$

Combining this with (2.3), we get

$$D'(a)+D'(b) \leq d(c+k)\left(n - c - c_1 - k - \frac{d}{6}(\delta+1)\right) + cd\left(n - \frac{d}{6}(\delta+1) - c\right) + O(n^2),$$

and Claim 6 is proven.

Using Claims 1, 4, 5, and 6 we bound $D'(G)$ as follows. Note that

$$\begin{aligned}
D'(G) &= \sum_{u\in M} D'(u) + \sum_{x\in K} D'(x) + \sum_{\{a,b\}\in\mathcal{C}} (D'(a)+D'(b)) \\
&\le dk\left(n-\frac{d}{3}(\delta+1)-c\right)\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right) \\
&+ c_1\left(d\left(n-\frac{d}{3}(\delta+1)\right)\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right)\right) \\
&+ (c-c_1)\left(d(c+k)\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right)+cd\left(n-\frac{d}{6}(\delta+1)-c\right)\right)+O(n^3) \\
&= dk\left(n-\frac{d}{3}(\delta+1)-c\right)\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right) \\
&+ c_1\left(d\left(n-\frac{d}{3}(\delta+1)\right)\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right)\right) \\
&+ d(c-c_1)\left((c+k)\left(n-c-k-\frac{d}{6}(\delta+1)\right)-c_1(c+k)+c\left(n-\frac{d}{6}(\delta+1)-c\right)\right)+O(n^3)
\end{aligned}$$

For easy calculation in maximizing this term, we note that $c-c_1\ge 0$, and that by (2.2), $n-c-k-\frac{d}{6}(\delta+1)\ge 0$. Hence the last term in the previous inequalities

$$d(c-c_1)\left((c+k)\left(n-c-k-\frac{d}{6}(\delta+1)\right)-c_1(c+k)+c\left(n-\frac{d}{6}(\delta+1)-c\right)\right)$$

is at most

$$d(c-c_1)\left((c+k+1)\left(n-c-k-\frac{d}{6}(\delta+1)\right)-c_1(c+k)+c\left(n-\frac{d}{6}(\delta+1)-c\right)\right).$$

It follows that

$$\begin{aligned} D'(G) \;\leq\; & dk\left(n-\frac{d}{3}(\delta+1)-c\right)\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right) \\ &+\; c_1\left(d\left(n-\frac{d}{3}(\delta+1)\right)\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right)\right) \\ &+\; d(c-c_1)\left((c+k+1)\left(n-c-k-\frac{d}{6}(\delta+1)\right)-c_1(c+k)\right. \\ &+\; \left.c\left(n-\frac{d}{6}(\delta+1)-c\right)\right)+O(n^3). \end{aligned}$$

Let $g(n,d,c,c_1)$ be the function

$$\begin{aligned} g(n,d,c,c_1) \;:=\; & dk\left(n-\frac{d}{3}(\delta+1)-c\right)\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right) \\ &+\; c_1\left(d\left(n-\frac{d}{3}(\delta+1)\right)\left(n-c-c_1-k-\frac{d}{6}(\delta+1)\right)\right) \\ &+\; d(c-c_1)\left((c+k+1)\left(n-c-k-\frac{d}{6}(\delta+1)\right)-c_1(c+k)\right. \\ &+\; \left.c\left(n-\frac{d}{6}(\delta+1)-c\right)\right). \end{aligned}$$

We first maximize g subject to c_1, keeping the other variables fixed. It is easy to verify, using (2.2), that the derivative

$$\frac{dg}{dc_1} = -dk\left(n-\frac{d}{3}(\delta+1)\right)-dc\left(n-\frac{d}{3}(\delta+1)-2c+c_1\right)-d\left(c+\frac{d}{6}(\delta+1)\right)$$

is negative. Therefore, g is decreasing in c_1. Thus, in conjunction with (2.2), we have

$$\begin{aligned}
g(n,d,c,c_1) &\leq g(n,d,c,0)\\
&= dk\left(n-\frac{d}{3}(\delta+1)-c\right)\left(n-c-k-\frac{d}{6}(\delta+1)\right)\\
&\quad + dc\left((c+k+1)\left(n-c-k-\frac{d}{6}(\delta+1)\right)+c\left(n-\frac{d}{6}(\delta+1)-c\right)\right)\\
&= d\left(n-\frac{d}{3}(\delta+1)-2c\right)\left(n-\frac{d}{3}(\delta+1)-c\right)\left(n-c-\left(n-\frac{d}{3}(\delta+1)-2c\right)-\frac{d}{6}(\delta+1)\right)\\
&\quad + dc\left((c+\left(n-\frac{d}{3}(\delta+1)-2c\right)+1)\left(n-c-\left(n-\frac{d}{3}(\delta+1)-2c\right)-\frac{d}{6}(\delta+1)\right)\right)\\
&\quad + dc\left(c\left(n-\frac{d}{6}(\delta+1)-c\right)\right)+O(n^3)\\
&= d\left(n-\frac{d}{3}(\delta+1)-2c\right)\left(n-\frac{d}{3}(\delta+1)-c\right)\left(c+\frac{d}{6}(\delta+1)\right)\\
&\quad + dc\left(\left(n-\frac{d}{3}(\delta+1)-c+1\right)\left(c+\frac{d}{6}(\delta+1)\right)\right)\\
&\quad + dc\left(c\left(n-\frac{d}{6}(\delta+1)-c\right)\right)+O(n^3)\\
&= d\left(\left(n-\frac{d}{3}(\delta+1)-c\right)^2\left(c+\frac{d}{6}(\delta+1)\right)+c^2\left(n-\frac{d}{6}(\delta+1)-c\right)\right)+O(n^3).
\end{aligned}$$

A simple differentiation with respect to c shows that the function

$$\left(n-\frac{d}{3}(\delta+1)-c\right)^2\left(c+\frac{d}{6}(\delta+1)\right)+c^2\left(n-\frac{d}{6}(\delta+1)-c\right),$$

when $d \geq \dfrac{3n}{2(\delta+1)}$, is decreasing over the domain of c, and hence it is maximized at $c=0$. Thus,

$$\left(n-\frac{d}{3}(\delta+1)-c\right)^2\left(c+\frac{d}{6}(\delta+1)\right)+c^2\left(n-\frac{d}{6}(\delta+1)-c\right) \leq \left(n-\frac{d}{3}(\delta+1)\right)^2\frac{d}{6}(\delta+1).$$

Hence when $d \geq \dfrac{3n}{2(\delta+1)}$,

$$D'(G) \leq g(n,d,0) + O(n^3) = \frac{d^2}{6}(\delta+1)\left(n - \frac{d}{3}(\delta+1)\right)^2 + O(n^3),$$

as desired. If $d < \dfrac{3n}{2(\delta+1)}$, then

$$\left(n - \frac{d}{3}(\delta+1) - c\right)^2 \left(c + \frac{d}{6}(\delta+1)\right) + c^2 \left(n - \frac{d}{6}(\delta+1) - c\right)$$

attains its maximum for $c = \frac{1}{2}\left(n - \frac{d}{3}(\delta+1)\right)$ to give

$$\left(n - \frac{d}{3}(\delta+1) - c\right)^2 \left(c + \frac{d}{6}(\delta+1)\right) + c^2 \left(n - \frac{d}{6}(\delta+1) - c\right) \leq \frac{n}{4}\left(n - \frac{d}{3}(\delta+1)\right)^2.$$

Hence

$$g(n,d,c,c_1) \leq \frac{1}{4}dn\left(n - \frac{d}{3}(\delta+1)\right)^2 + O(n^3),$$

and so

$$D'(G) \leq g(n,d,c,c_1) + O(n^3) \leq \frac{1}{4}dn\left(n - \frac{d}{3}(\delta+1)\right)^2 + O(n^3),$$

and Case 2 of Theorem 2.1 is proven.

To see that the bound is asymptotically sharp, for $d \geq \dfrac{3n}{2(\delta+1)}$, the lollipop graph $L_{n,d,\delta}$, asymptotically meets the bound. For $d \leq \dfrac{3n}{2(\delta+1)}$, consider the graph $G_{n,d,\delta}$, $d \equiv 1 \bmod 3$, constructed as follows. First, let H be the graph with diameter $d-2$ obtained as follows: $V(H) = V_0 \cup V_1 \cup \cdots \cup V_{d-2}$, where

$$|V_i| = \begin{cases} 1 & \text{if } i \equiv 0 \text{ or } 2 \bmod 3, \\ \delta - 1 & \text{otherwise} \end{cases}$$

and two distinct vertices $v \in V_i, v' \in V_j$ are joined by an edge if and only if $|j-i| \leq 1$. Let the only vertex in V_0 be v_0 and the only vertex in V_{d-2} be v_{d-2}. Now let H_1

be the complete graph on $\lceil \frac{1}{2}(n - \frac{1}{3}(d-1)(\delta+1)) \rceil$ vertices and H_2 the complete graph on $\lfloor \frac{1}{2}(n - \frac{1}{3}(d-1)(\delta+1)) \rfloor$ vertices. The graph $G_{n,d,\delta}$ is obtained by joining the vertex v_0 in H to every vertex in H_1 and joining the vertex v_{d-2} in H to every vertex in H_2. Then $G_{n,d,\delta}$ has diameter d, minimum degree δ and degree distance at least $\frac{1}{4}dn\left(n - \frac{d}{3}(\delta+1)\right)^2$, as desired. □

Finally, the result below gives a strengthening of the bound in [10] and settles completely a conjecture of Tomescu [57].

Corollary 2.2 *Let G be a connected graph of order n and minimum degree δ. Then*

$$D'(G) \leq \frac{n^4}{9(\delta+1)} + O(n^3).$$

Moreover for a fixed δ, this inequality is asymptotically tight.

Proof: Let d be the diameter of G. By the theorem above, for $d \geq \dfrac{3n}{2(\delta+1)}$,

$$\frac{1}{6}d^2(\delta+1)(n - \frac{d}{3}(\delta+1))^2$$

reaches its maximum value for $d = \dfrac{3n}{2(\delta+1)}$, to give

$$D'(G) = \frac{3n^4}{32(\delta+1)} + O(n^3) \leq \frac{n^4}{9(\delta+1)} + O(n^3).$$

If $d < \dfrac{3n}{2(\delta+1)}$, then the term $\frac{1}{4}dn\left(n - \frac{d}{3}(\delta+1)\right)^2$ is maximized, with respect to d, for $d = \frac{n}{\delta+1}$, to give

$$\frac{1}{4}dn\left(n - \frac{d}{3}(\delta+1)\right)^2 \leq \frac{n^4}{9(\delta+1)}.$$

Hence $D'(G) \leq \frac{n^4}{9(\delta+1)} + O(n^3)$, as desired.

To see that the bound is asymptotically best possible consider the graph $G_{n,d,\delta}$ constructed above. Note that

$$D'(G_{n,\frac{n}{\delta+1},\delta}) > \frac{n^4}{9(\delta+1)},$$

as claimed. □

Chapter 3

Degree distance and vertex-connectivity

3.1 Introduction

In the previous chapter we improved the upper bound in Conjecture 1.1 for graphs with fixed minimum degree. Precisely, we proved the following bound.

Theorem 3.1 *[48] Let G be a connected graph of order n and minimum degree δ. Then*

$$D'(G) \leq \frac{n^4}{9(\delta+1)} + O(n^3).$$

The bound in Theorem 3.1 was shown to be asymptotically sharp for a fixed δ; the extremal graph being of vertex-connectivity 1. It is therefore natural to ask if the bound

$$D'(G) \leq \frac{n^4}{9(\kappa+1)} + O(n^3), \tag{3.1}$$

which follows from Theorem 3.1 by applying the inequality $\kappa \leq \delta$, can be improved.

In this chapter, we improve the bound, (3.1). Precisely, we prove that $D'(G) \leq \frac{n^4}{27\kappa} + O(n^3)$. We give examples to show that this bound, for a fixed κ, is asymptotically sharp.

Recall the useful equation

$$D'(G) = \sum_{v \in V} D'(v).$$

3.2 Results

Let G be a finite connected graph of order n and diameter d. From now on-wards $v_0 \in V(G)$ is a fixed vertex of eccentricity d and for each $i = 0, 1, 2, 3, \ldots, d$,

$$N_i := \{x \in V(G) | d_G(x, v_0) = i\}.$$

We begin by presenting a very simple, but important observation.

Fact 3.1 *Let G be a connected graph of order n, diameter d and vertex-connectivity κ. If $v \in V(G)$, then*

$$d \leq \frac{1}{\kappa}(n - \deg\ v) + O(1).$$

Proof of Fact 3.1: Let $v \in V(G)$. Then $v \in N_i$ for some i, and so $N(v) \subset N_{i-1} \cup N_i \cup N_{i+1}$. Thus, since $|N_i| \geq \kappa$ for all $i = 1, 2, \ldots, d-1$, we have

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

Hence, $d \leq \dfrac{1}{\kappa}(n - \deg\ v) + O(1)$, as required. □

We will need the following useful result.

Proposition 3.1 *Let G be a connected graph of order n, diameter d and vertex-connectivity κ. If $v \in V(G)$, then*

$$D(v) \leq d(n - \frac{\kappa}{2}d - \deg\ v) + O(n).$$

Proof: Let $v \in V(G)$ and let e be its eccentricity. Thus,

$$\begin{aligned} D(v) &\leq \deg v + \kappa(2+3+\ldots+e-1) + e(n-\kappa(e-2)-\deg v - 1) \\ &= \deg v + \kappa\left(\frac{e(e+1)}{2} - 2\right) + e(n - \kappa e - \deg v + 2\kappa - 1) \\ &= e\left(n - \frac{\kappa}{2}e - \deg v\right) + O(n). \end{aligned}$$

Now consider $f(x) := x(n - \frac{\kappa x}{2} - \deg v)$, where $x = e$. The function f is increasing on the interval $[1, \frac{1}{\kappa}(n - \deg v)]$. Using Fact 3.1 and $1 \leq e \leq d$, we consider two cases. First if $d \leq \frac{1}{\kappa}(n - \deg v)$, then $D(v) \leq f(d) + O(n) \leq d\left(n - \frac{\kappa d}{2} - \deg v\right) + O(n)$. Secondly if $d = \frac{1}{\kappa}(n - \deg v) + O(1)$, then $f \leq f\left(\frac{1}{\kappa}(n - \deg v)\right) = f(d - O(1))$. But

$$\begin{aligned} f(d - O(1)) &= (d - O(1))\left(n - \frac{\kappa}{2}(d - O(1)) - \deg v\right) + O(n) \\ &= d\left(n - \frac{\kappa}{2}d - \deg v\right) + O(n). \end{aligned}$$

Hence, in both cases $D(v) \leq d\left(n - \frac{\kappa d}{2} - \deg v\right) + O(n)$, as required. □

Proving an upper bound on degree distance in terms of order and vertex-connectivity is quite challenging. We will develop further the technique introduced in [10], which was refined in [43], to adequately capture the effect of vertex-connectivity on the degree distance. The diameter plays a crucial role and provides us with the following intermediate result.

Theorem 3.2 *Let G be a connected graph of order n, diameter $d \geq 2$ and fixed* *vertex-connectivity* κ. *Then*

$$D'(G) \le \begin{cases} \frac{1}{4}dn(n-\kappa d)^2 + O(n^3) & \text{if } d < \frac{n}{2\kappa}, \\ \\ \frac{1}{2}\kappa[d(n-\kappa d)]^2 + O(n^3) & \text{if } d \ge \frac{n}{2\kappa}. \end{cases}$$

Moreover, this inequality is asymptotically sharp.

Proof. Assume the notation for v_0 and N_i as above. Note that $|N_i| \ge \kappa$, for all $i = 1, 2, \ldots, d-1$. For each N_i, $i = 1, 2, \ldots, d-1$, choose any κ vertices and let this set be $\{u_{i1}, u_{i2}, \ldots, u_{i\kappa}\}$. For each $j = 1, 2, \ldots, \kappa$, let $P_j := \{u_{1j}, u_{2j}, u_{3j}, \ldots, u_{d-1j}\}$ and $N = \cup_{j=1}^{\kappa} P_j$.

Claim 7 *Let* N *be as above. Then*

$$\sum_{u \in N} D'(u) \le O(n^3).$$

Proof of Claim 7: Note that

$$\sum_{u \in N} D'(u) = \sum_{u \in P_1} D'(u) + \sum_{u \in P_2} D'(u) + \ldots + \sum_{u \in P_\kappa} D'(u).$$

For a fixed j, let $P_j = U_{0j} \cup U_{1j} \cup U_{2j}$, where U_{0j}, U_{1j} and U_{2j} are defined as follows:

$$U_{0j} = \{u_{3j}, u_{6j}, u_{9j}, \ldots\},$$

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

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

For each $x, y \in U_{ij}$ with $x \ne y$, $i = 0, 1, 2$, since $d(x, y) \ge 3$, we have $N(x) \cap N(y) = \emptyset$. It follows that $\sum_{x \in U_{ij}} \deg x \le n$ for $i = 0, 1, 2$. From Proposition 3.1,

$$\begin{aligned} D(x) &\le d(n - \frac{\kappa}{2}d - \deg x) + O(n) \\ &= O(n^2). \end{aligned}$$

Thus,

$$\begin{aligned}
\sum_{x\in P_j} D'(x) &= \sum_{x\in P_j} \deg\, xD(x) \\
&= \sum_{x\in U_{0j}} \deg\, xD(x) + \sum_{x\in U_{1j}} \deg\, xD(x) + \sum_{x\in U_{2j}} \deg\, xD(x) \\
&\leq O(n^2)\left(\sum_{x\in U_{0j}} \deg\, x + \sum_{x\in U_{1j}} \deg\, x + \sum_{x\in U_{2j}} \deg\, x\right) \\
&\leq O(n^2)(3n) \\
&= O(n^3).
\end{aligned}$$

Hence,

$$\begin{aligned}
\sum_{u\in N} D'(u) &= \sum_{u\in P_1} D'(u) + \sum_{u\in P_2} D'(u) + \ldots + \sum_{u\in P_\kappa} D'(u) \\
&\leq \kappa O(n^3) \\
&= O(n^3),
\end{aligned}$$

as required and Claim 7 is proven.

Let $\mathcal{C}$ be a maximum set of disjoint pairs of vertices from $V - N$ which lie at a distance at least 3, i.e., if $\{a, b\} \in \mathcal{C}$, then $d(a, b) \geq 3$. If $\{a, b\} \in \mathcal{C}$ we say that a and b are partners. Finally, let H be the remaining vertices of G, i.e., $H = V - N - \{x : x \in \{a, b\} \in \mathcal{C}\}$. Let $|H| = h$, and $|\mathcal{C}| = c$. Then

$$n = \kappa(d - 1) + 2c + h. \tag{3.2}$$

Fact 3.2 *Let* $\{a, b\} \in \mathcal{C}$. *Then* $\deg a + \deg b \leq n - \kappa d + O(1)$.

Proof of Fact 3.2: Note that since $d(a, b) \geq 3$, $N[a] \cap N[b] = \emptyset$. Also, each of the two vertices, a and b, can be adjacent to at most 3κ vertices in N. Thus,

$$\begin{aligned} n &\geq |N[a]| + |N[b]| + |N| \\ &\geq \deg a + 1 + \deg b + 1 + (d-1)\kappa - 6\kappa, \end{aligned}$$

and rearranging the terms completes the proof of Fact 3.2.

Now consider two cases.

Case 1: $h \leq 1$.

For $x \in H$, $D(x) \leq (n-1)d$, so $D'(x) \leq \deg x(n-1)d$. Thus $\sum_{x \in H} D'(x) \leq 1 \cdot \deg x(n-1)d = O(n^3)$.

Claim 8 *If $\{a, b\} \in \mathcal{C}$, then $D'(a) + D'(b) \leq \frac{1}{2}dn(n - \kappa d) + O(n^2)$.*

Proof of Claim 8: By Proposition 3.1, $D(a) \leq d\left(n - \frac{\kappa}{2}d - \deg a\right) + O(n)$. Hence,

$$D'(a) \leq \deg a \left(d\left(n - \frac{\kappa}{2}d - \deg a\right)\right) + O(n^2).$$

Similarly, $D'(b) \leq \deg b\left(d\left(n - \frac{\kappa}{2}d - \deg b\right)\right) + O(n^2)$. Thus,

$$\begin{aligned} D'(a) + D'(b) &\leq \deg a \left(d\left(n - \frac{\kappa}{2}d - \deg a\right)\right) + \deg b\left(d\left(n - \frac{\kappa}{2}d - \deg b\right)\right) + O(n^2) \\ &= d\left((\deg a + \deg b)\left(n - \frac{\kappa}{2}d\right) - \left((\deg a)^2 + (\deg b)^2\right)\right) + O(n^2) \\ &\leq d\left((\deg a + \deg b)\left(n - \frac{\kappa}{2}d\right) - \frac{1}{2}(\deg a + \deg b)^2\right) + O(n^2). \end{aligned}$$

Let $x = \deg a + \deg b$ and let $f(x) := d\left(x\left(n - \frac{\kappa}{2}d\right) - \frac{1}{2}x^2\right)$. Then by Fact 3.2, $x \leq n - \kappa d + O(1)$. A simple differentiation shows that f is increasing for all $x \leq n - \frac{\kappa}{2}d$. Hence f attains its maximum for $x = n - \kappa d + O(1)$. Thus,

$$\begin{aligned} D'(a) + D'(b) &\leq f\left(n - \kappa d + O(1)\right) \\ &= \frac{1}{2}dn\left(n - \kappa d\right) + O(n^2), \end{aligned}$$

and Claim 8 is proven.

From (3.2), we have $c = \frac{1}{2}(n - \kappa(d-1) - h)$. Hence, since $h \leq 1$, we have $c = \frac{1}{2}(n - \kappa d) + O(1)$. This, in conjunction with Claim 8, yields

$$\begin{aligned}
\sum_{\{a,b\}\in\mathcal{C}} (D'(a) + D'(b)) &\leq c\left(\frac{1}{2}dn\,(n-\kappa d) + O(n^2)\right) \\
&= \left(\frac{1}{2}(n-\kappa d) + O(1)\right)\left(\frac{1}{2}dn\,(n-\kappa d) + O(n^2)\right) \\
&= \frac{1}{4}dn\,(n-\kappa d)^2 + O(n^3).
\end{aligned}$$

Hence,

$$\begin{aligned}
D'(G) &= \sum_{\{a,b\}\in\mathcal{C}} (D'(a) + D'(b)) + \sum_{x\in H} D'(x) + \sum_{v\in N} D'(v) \\
&\leq \frac{1}{4}dn\,(n-\kappa d)^2 + O(n^3) + O(n^3) + O(n^3) \\
&= \frac{1}{4}dn\,(n-\kappa d)^2 + O(n^3).
\end{aligned}$$

Note that, when $d \geq \frac{n}{2\kappa}$, then $\frac{1}{4}dn\,(n-\kappa d)^2 + O(n^3) \leq \frac{1}{2}\kappa\,(d(n-\kappa d))^2 + O(n^3)$ and so the theorem is proved for Case 1.

Case 2: $h \geq 2$. Now the pairs of vertices in $\mathcal{C}$ will be partitioned further. Fix a vertex $z \in H$. For each pair $\{a,b\} \in \mathcal{C}$, choose a vertex closer to z; if $d(a,z) = d(b,z)$, arbitrarily choose one of the vertices. Let A be the set of all these vertices closer to z, and B be the set of partners of these vertices in A, so $|A| = |B| = c$. Furthermore, let $A_1(B_1)$ be the set of vertices $w \in A(B)$ whose partner is at a distance at most 9 from w. Let $c_1 = |A_1| = |B_1|$.

Claim 9 *For all $u, v \in A \cup H$, $d(u,v) \leq 8$.*

Proof of Claim 9: Since $\mathcal{C}$ is a maximum set of pairs of vertices of distance at least 3, any two vertices of H must be at a distance of at most 2. We show that

$d(a,z) \leq 4$ for all $a \in A$. Suppose, to the contrary, that there exists a vertex $a \in A$ for which $d(a,z) \geq 5$. Let b be the partner of a. By definition of A, $d(z,b) \geq 5$. Now consider another vertex $z' \in H$, $z \neq z'$. Since $d(z,z') \leq 2$ we have $5 \leq d(b,z) \leq d(b,z') + d(z,z') \leq d(b,z') + 2$ which implies $d(b,z') \geq 3$. This contradicts the maximality of $\mathcal{C}$ since $\{a,b\}$ will be replaced by $\{a,z\}$ and $\{b,z'\}$. Hence $d(a,z) \leq 4$, for each $a \in A$. Thus for $u,v \in A$, $d(u,v) \leq d(u,z) + d(z,v) \leq 8$.

Claim 10 *For all $x \in H$,*

$$D'(x) \leq d\,(n - \kappa d - c)\left(n - c - c_1 - h - \frac{\kappa}{2}d\right) + O(n^2).$$

Proof of Claim 10: By Claim 9, all $c+h$ vertices in $A \cup H$ lie within a distance of 8 from each vertex $x \in H$. This implies that all the c_1 vertices in B_1 lie within a distance of $9+8$ from x. Thus, as in Proposition 3.1,

$$\begin{aligned} D(x) &\leq 8(c+h) + 17c_1 + \kappa(18+19+20+\cdots+d-1) + \ d\,(n-c-h-c_1-\kappa(d-18)) \\ &= d\left(n - c - c_1 - h - \frac{\kappa}{2}d\right) + O(n^2). \end{aligned}$$

In order to find a bound on the degree of x, we use a counting argument. Note that x can have at most 3κ neighbours in N. By definition of A and B, x cannot be adjacent to two vertices, w and t, where $w \in A$ is a partner of $t \in B$, since $d(w,t) \geq 3$. Thus, x is adjacent to at most c vertices in $A \cup B$. It follows that

$$\begin{aligned} n &\geq \deg x + 1 + |N| - 3\kappa + c \\ &= \deg x + 1 + \kappa(d-1) - 3\kappa + c \\ &= \deg x + \kappa d + c + O(1). \end{aligned}$$

Hence $\deg x \leq n - \kappa d - c + O(1)$. Therefore,

$$\begin{aligned} D'(x) &= \deg x D(x) \\ &\leq d\,(n-\kappa d - c)\left(n - c - c_1 - h - \frac{\kappa}{2}d\right) + O(n^2), \end{aligned}$$

and this proves Claim 10.

We now turn to finding an upper bound on the contribution of the pairs in $\mathcal{C}$ to the degree distance. We abuse notation and write $\{a,b\} \in A_1 \cup B_1$ if a and b are partners, i.e., $\{a,b\} \in \mathcal{C}$, with $a \in A_1$ and $b \in B_1$. Note that

$$\sum_{\{a,b\}\in\mathcal{C}} (D'(a)+D'(b)) = \sum_{\{a,b\}\in A_1\cup B_1} (D'(a)+D'(b)) + \sum_{\{a,b\}\in(A-A_1)\cup(B-B_1)} (D'(a)+D'(b)).$$

We first consider the set $A_1 \cup B_1$.

Claim 11 *Let $\{a,b\} \in \mathcal{C}$. If $d(a,b) \le 9$, i.e., if $\{a,b\} \in A_1 \cup B_1$, then*

$$D'(a) + D'(b) \le d\,(n - \kappa d)\left(n - c - c_1 - h - \frac{\kappa}{2}d\right) + O(n^2).$$

Proof of Claim 11: We first show that any two vertices in $A \cup H \cup B_1$ lie within a distance of 26 from each other. By Claim 9, any two vertices in $A \cup H$ lie within a distance of 8 from each other. Now assume that $b, v \in B_1$, and let a and u be the partners of b and v in A_1, respectively. Then $d(b,v) \le d(b,a) + d(a,u) + d(u,v) \le 9 + 8 + 9 = 26$. Thus any two vertices in B_1 are within a distance of 26 from each other. Now let $a \in A \cup H$ and $b \in B_1$, and let u be the partner of b in $A_1 \subseteq A$. Then $d(a,b) \le d(a,u) + d(u,b) \le 8 + 9 < 26$. Hence any two vertices in $A \cup H \cup B_1$ lie within a distance of 26 from each other.

Now let $w \in A_1 \cup B_1$. Since w is in $A \cup H \cup B_1$, all the $c + h + c_1 - 1$ vertices in $A \cup H \cup B_1$ lie within a distance of 26 from w. It follows, as in Proposition 3.1, that

$$\begin{aligned} D(w) &\le 26(c + h + c_1 - 1) + \kappa(27 + 28 + \cdots + d - 1) \\ &\quad + d\,(n - c - c_1 - h - \kappa(d - 27)) \\ &= d\left(n - c - c_1 - h - \frac{\kappa}{2}d\right) + O(n). \end{aligned}$$

Thus, if $\{a,b\}$ is a pair in $A_1 \cup B_1$, then

$$\begin{aligned} D'(a)+D'(b) &\leq \deg a \left(d\left(n-c-c_1-h-\frac{\kappa}{2}d\right)+O(n)\right) \\ &+ \deg b \left(d\left(n-c-c_1-h-\frac{\kappa}{2}d\right)+O(n)\right) \\ &= (\deg a+\deg b)\left(d\left(n-c-c_1-h-\frac{\kappa}{2}d\right)+O(n)\right). \end{aligned}$$

By Fact 3.2, $\deg a + \deg b \leq n - \kappa d + O(1)$. Therefore,

$$\begin{aligned} D'(a)+D'(b) &\leq (n-\kappa d+O(1))\left(d\left(n-c-c_1-h-\frac{\kappa}{2}d\right)+O(n)\right) \\ &= d\,(n-\kappa d)\left(n-c-c_1-h-\frac{\kappa}{2}d\right)+O(n^2), \end{aligned}$$

and Claim 11 is proven.

Now consider pairs $\{a,b\}$ of vertices in $\mathcal{C}$ which are not in $A_1 \cup B_1$.

Claim 12 *Let $\{a,b\} \in \mathcal{C}$. If $d(a,b) \geq 10$, i.e., if $\{a,b\} \in (A-A_1)\cup(B-B_1)$, then*

$$D'(a)+D'(b) \leq d(c+h)\left(n-c-c_1-h-\frac{\kappa}{2}d\right)+cd\left(n-\frac{\kappa}{2}d-c\right)+O(n^2).$$

Proof of Claim 12: We consider vertices from $A - A_1$ and from $B - B_1$ separately. Let $a \in A - A_1$. Then as in Claim 11, all the $c+h-1$ vertices in $A \cup H$ lie at a distance of 8 from a and all the c_1 vertices in B_1 lie within a distance of $9+8=17$ from a. Thus, as in Proposition 3.1,

$$\begin{aligned} D(a) &\leq 8(c+h-1)+17c_1+\kappa(18+19+\cdots+d-1) \\ &+ d\,(n-c-c_1-h-\kappa(d-18)) \\ &= d\left(n-c-c_1-h-\frac{\kappa}{2}d\right)+O(n). \end{aligned}$$

We now find a bound on the degree of a. By definition of $\mathcal{C}$, a cannot be adjacent to both w and u, where $w \in A$ is a partner of $u \in B$, since $d(w,u) \geq 3$. Hence a

is adjacent to at most $c-1$ vertices in $A \cup B$. Further, a is adjacent to at most 3κ vertices in N and has at most h neighbours in H. Thus,

$$\deg a \leq c - 1 + 3\kappa + h = c + h + 3\kappa - 1.$$

It follows that

$$\begin{aligned} D'(a) &= \deg a D(a) \\ &\leq (c+h+3\kappa-1)\left(d\left(n-c-c_1-h-\frac{\kappa}{2}d\right)+O(n^2)\right) \\ &= d(c+h)\left(n-c-c_1-h-\frac{\kappa}{2}d\right)+O(n^2). \end{aligned} \tag{3.3}$$

Now let $b \in B - B_1$. By Proposition 3.1, we have

$$D(b) \leq d\left(n - \frac{\kappa}{2}d - \deg b\right) + O(n),$$

and so

$$D'(b) \leq \deg b\left(d\left(n - \frac{\kappa}{2}d - \deg b\right)\right) + O(n^2). \tag{3.4}$$

We first maximize $\deg b\left(d\left(n - \frac{\kappa}{2}d - \deg b\right)\right)$ with respect to $\deg b$. Let

$$f(x) := x\left(d\left(n - \frac{\kappa}{2}d - x\right)\right),$$

where $x = \deg b$. A simple differentiation shows that f is increasing for $x \leq \frac{1}{2}\left(n - \frac{\kappa}{2}d\right)$. We find an upper bound on x, i.e., on $\deg b$. Note that as above, b can be adjacent to at most $c-1$ vertices in $A \cup B$, and has at most 3κ neighbours in N. We show that b cannot be adjacent to any vertex in H. Suppose to the contrary that $s \in H$ and $d(b,s) = 1$. Recall that a is the partner of b and $d(a,b) \geq 10$. By Claim 9, $d(a,s) \leq 8$. Hence $10 \leq d(a,b) \leq d(b,s) + d(s,a) \leq 1 + 8$, a contradiction. Thus, b cannot be adjacent to any vertex in H. We conclude that

$$\deg b \leq c - 1 + 3\kappa = c + 3\kappa - 1.$$

We look at two cases separately. First assume that $\deg b = c + j$, where $j \in \{1, \ldots, 3\kappa - 1\}$. Then

$$\begin{aligned} f(\deg b) &= f(c+j) \\ &= (c+j)\left(d\left(n - \frac{\kappa}{2}d - (c+j)\right)\right) \\ &= cd\left(n - \frac{\kappa}{2}d - c\right) + O(n^2). \end{aligned} \tag{3.5}$$

Second, assume that $\deg b \leq c$. From (3.2) and the fact that $d \geq 2$, we have

$$c = \frac{1}{2}(n - \kappa d - h) + \frac{\kappa}{2} \leq \frac{1}{2}\left(n - \frac{\kappa}{2}d\right),$$

and so f is increasing in $[1, c]$. Therefore,

$$f(\deg b) \leq f(c) = cd\left(n - \frac{\kappa}{2}d - c\right),$$

for this case. Comparing this with (3.5), we get that

$$f(\deg b) \leq cd\left(n - \frac{\kappa}{2}d - c\right) + O(n^2).$$

Thus, from (3.4), we have

$$D'(b) \leq cd\left(n - \frac{\kappa}{2}d - c\right) + O(n^2).$$

Combining this with (3.3), we get

$$D'(a) + D'(b) \leq d(c+h)\left(n - c - c_1 - h - \frac{\kappa}{2}d\right) + cd\left(n - \frac{\kappa}{2}d - c\right) + O(n^2),$$

and Claim 12 is proven.

Using Claims 7, 10, 11, and 12 we have

$$\begin{aligned}
D'(G) &= \sum_{u\in N} D'(u) + \sum_{x\in H} D'(x) + \sum_{\{a,b\}\in \mathcal{C}} (D'(a)+D'(b)) \\
&\le dh\,(n-\kappa d - c)\left(n-c-c_1-h-\frac{\kappa}{2}d\right) \\
&\quad + c_1\left(d\,(n-\kappa d)\left(n-c-c_1-h-\frac{\kappa}{2}d\right)\right) \\
&\quad + (c-c_1)\left(d(c+h)\left(n-c-c_1-h-\frac{\kappa}{2}d\right) + cd\left(n-\frac{\kappa}{2}d-c\right)\right) + O(n^3) \\
&= dh\,(n-\kappa d - c)\left(n-c-c_1-h-\frac{\kappa}{2}d\right) \\
&\quad + c_1\left(d\,(n-\kappa d)\left(n-c-c_1-h-\frac{\kappa}{2}d\right)\right) \\
&\quad + d(c-c_1)\left((c+h)\left(n-c-h-\frac{\kappa}{2}d\right) - c_1(c+h) + c\left(n-\frac{\kappa}{2}d-c\right)\right) + O(n^3).
\end{aligned}$$

For easy calculation in maximizing this term, we note that $c - c_1 \ge 0$, and that by (3.2), $n - c - h - \frac{\kappa}{2}d \ge 0$.

Hence the last term in the previous inequalities

$$d(c-c_1)\left((c+h)\left(n-c-h-\frac{\kappa}{2}d\right) - c_1(c+h) + c\left(n-\frac{\kappa}{2}d-c\right)\right)$$

is at most

$$d(c-c_1)\left((c+h+1)\left(n-c-h-\frac{\kappa}{2}d\right) - c_1(c+h) + c\left(n-\frac{\kappa}{2}d-c\right)\right).$$

It follows that

$$\begin{aligned}
D'(G) &\le dh\,(n-\kappa d - c)\left(n-c-c_1-h-\frac{\kappa}{2}d\right) \\
&\quad + c_1\left(d\,(n-\kappa d)\left(n-c-c_1-h-\frac{\kappa}{2}d\right)\right) \\
&\quad + d(c-c_1)\left((c+h+1)\left(n-c-h-\frac{\kappa}{2}d\right) - c_1(c+h)\right. \\
&\quad \left. + c\left(n-\frac{\kappa}{2}d-c\right)\right) + O(n^3).
\end{aligned}$$

Since κ is a fixed constant, the expression

$$\begin{aligned}
& dh\,(n-\kappa d-c)\left(n-c-c_1-h-\frac{\kappa}{2}d\right) \\
& +\ c_1\left(d\,(n-\kappa d)\left(n-c-c_1-h-\frac{\kappa}{2}d\right)\right) \\
& +\ d(c-c_1)\left((c+h+1)\left(n-c-h-\frac{\kappa}{2}d\right)-c_1(c+h)\right. \\
& \left.+\ c\left(n-\frac{\kappa}{2}d-c\right)\right)
\end{aligned}$$

is at most

$$\begin{aligned}
& dh\,(n-\kappa(d-1)-c)\left(n-c-c_1-h-\frac{\kappa}{2}d\right) \\
& +\ c_1\left(d\,(n-\kappa(d-1))\left(n-c-c_1-h-\frac{\kappa}{2}d\right)\right) \\
& +\ d(c-c_1)\left((c+h+1)\left(n-c-h-\frac{\kappa}{2}d\right)-c_1(c+h)\right. \\
& \left.+\ c\left(n-\frac{\kappa}{2}d-c\right)\right)+O(n^3);
\end{aligned}$$

hence,

$$\begin{aligned}
D'(G)\ \leq\ & dh\,(n-\kappa(d-1)-c)\left(n-c-c_1-h-\frac{\kappa}{2}d\right) \\
& +\ c_1\left(d\,(n-\kappa(d-1))\left(n-c-c_1-h-\frac{\kappa}{2}d\right)\right) \\
& +\ d(c-c_1)\left((c+h+1)\left(n-c-h-\frac{\kappa}{2}d\right)-c_1(c+h)\right. \\
& \left.+\ c\left(n-\frac{\kappa}{2}d-c\right)\right)+O(n^3).
\end{aligned}$$

Let $g(n,d,c,c_1)$ be the function

$$\begin{aligned}
g(n,d,c,c_1)\ :=\ & dh\,(n-\kappa(d-1)-c)\left(n-c-c_1-h-\frac{\kappa}{2}d\right) \\
& +\ d\,(n-\kappa(d-1))\left[c_1\left(n-c-c_1-h-\frac{\kappa}{2}d\right)\right] \\
& +\ d(c-c_1)\left[(c+h+1)\left(n-c-h-\frac{\kappa}{2}d\right)-c_1(c+h)\right. \\
& \left.+\ c\left(n-\frac{\kappa}{2}d-c\right)\right].
\end{aligned}$$

We first maximize g subject to c_1, keeping the other variables fixed.

Note that the derivative

$$\begin{aligned}\frac{dg}{dc_1} &= -dh\,(n-\kappa(d-1)) + dhc \\ &\quad + \; d\,(n-\kappa(d-1))\left[n-c-2c_1-h-\frac{\kappa}{2}d\right] \\ &\quad -d\left[(c+h+1)\left(n-c-h-\frac{\kappa}{2}d\right) + \; c\left(n-\frac{\kappa}{2}d-c\right) + (c-2c_1)(c+h)\right].\end{aligned}$$

From (3.2), $h = n-\kappa(d-1)-2c$. Using this, and the equation $n-\kappa(d-1) = h+2c$, we get, after simplification,

$$\frac{dg}{dc_1} = -d(h+c)^2 - dc(h+2c_1) - d\left(n-c-h-\frac{kd}{2}\right).$$

Note that since $d \geq 2$, we have

$$n-c-h-\frac{\kappa d}{2} = n-c-[n-\kappa(d-1)-2c] - \frac{\kappa d}{2} = c + k\left(\frac{d}{2}-1\right) > 0,$$

and so the derivative $\frac{dg}{dc_1}$ is negative. Therefore, g is decreasing in c_1. Thus, in conjunction with (3.2), we have

$$\begin{aligned} g(n,d,c,c_1) &\leq g(n,d,c,0) \\ &= dh\,(n-\kappa d-c)\left(n-c-h-\frac{\kappa}{2}d\right) \\ &\quad + \; dc\left((c+h+1)\left(n-c-h-\frac{\kappa}{2}d\right) + c\left(n-\frac{\kappa}{2}d-c\right)\right) \\ &= d\left((n-\kappa d-c)^2\left(c+\frac{\kappa}{2}d\right) + c^2\left(n-\frac{\kappa}{2}d-c\right)\right) + O(n^3). \end{aligned}$$

A simple differentiation with respect to c shows that the function

$$\begin{aligned} \theta(c) &:= (n-\kappa d-c)^2\left(c+\frac{\kappa}{2}d\right) + c^2\left(n-\frac{\kappa}{2}d-c\right) \\ &= (2\kappa d-n)c^2 + (n-\kappa d)(n-2\kappa d)c + \frac{1}{2}\kappa d(n-\kappa d)^2 \end{aligned}$$

has a critical value $c = \frac{1}{2}(n - \kappa d)$. Recall that $h \geq 2$ and from (3.2),

$$c = \frac{1}{2}(n - \kappa d - h) + \frac{\kappa}{2} \leq \frac{1}{2}(n - \kappa d) + \frac{\kappa}{2} - 1 = c^*.$$

Hence we obtain the domain of c, $0 \leq c \leq c^*$. Now we look at two cases.

Subcase A: $2\kappa d - n < 0$. Then the coefficient of c^2 in θ is negative. If on one hand $\kappa = 1$, then $\dfrac{1}{2}(n - \kappa d)$ is outside the domain of c. But the function θ is increasing for $c \leq \dfrac{1}{2}(n - \kappa d)$ and so

$$\theta(c) \leq \theta\left(\frac{1}{2}(n - \kappa d) - \frac{1}{2}\right) = \frac{1}{4}n(n - \kappa d)^2 + O(n^2).$$

If on the other hand $\kappa \geq 2$, then θ attains its maximum for $c = \frac{1}{2}(n - \kappa d)$ to give

$$\theta(c) \leq \theta\left(\frac{1}{2}(n - \kappa d)\right) = \frac{n}{4}(n - \kappa d)^2.$$

Hence, in both cases, $\theta(c) \leq \dfrac{n}{4}(n - \kappa d)^2 + O(n^2)$ to give

$$g(n, d, c, c_1) \leq \frac{1}{4}dn(n - \kappa d)^2 + O(n^3),$$

and so

$$\begin{aligned} D'(G) &\leq g(n, d, c, c_1) + O(n^3) \\ &\leq \frac{1}{4}dn(n - \kappa d)^2 + O(n^3). \end{aligned}$$

Subcase B: $d \geq \dfrac{n}{2\kappa}$. Then the coefficient of c^2 in θ is non-negative. Thus, θ is decreasing over the domain of c, so it is maximised at $c = 0$, and hence $\theta(c) \leq \theta(0) = \dfrac{1}{2}\kappa d(n - \kappa d)^2$. It follows that

$$D'(G) \leq \frac{\kappa}{2}d^2(n - \kappa d)^2 + O(n^3),$$

and the bound in Theorem 3.2 is proven.

To see that the bound is asymptotically sharp, when $d < \dfrac{n}{2\kappa}$, consider the graph $G_{n,d,\kappa} = G_0 + G_1 + \cdots + G_d$ where $G_0 = G_d = K_{\lceil \frac{1}{2}(n-\kappa d) \rceil}$, and $G_i = K_\kappa$ for $i = 1, 2, 3, \cdots, d-1$. Then $G_{n,d,\kappa}$ has diameter d, vertex-connectivity κ, and degree distance at least $\frac{1}{4} dn \left(n - \kappa d\right)^2$. For $d \geq \dfrac{n}{2\kappa}$, consider the graph $G_{n,d,\kappa} = G_0 + G_1 + \ldots + G_d$ where $G_i = K_\kappa$ for $i = 0, 1, 2, \ldots, d-1$ and $G_d = K_{n-\kappa d}$. □

Finally, the result below gives a strengthening of the bound in [10] and also settles completely a conjecture of Tomescu [57].

Corollary 3.3 *Let G be a connected graph of order n and vertex-connectivity κ. Then*

$$D'(G) \leq \frac{n^4}{27\kappa} + O(n^3).$$

Moreover, this inequality is asymptotically sharp.

Proof: Let d be the diameter of G. By the theorem above,

$$D'(G) \leq \begin{cases} \frac{1}{4} dn(n-\kappa d)^2 + O(n^3) & \text{if } d < \frac{n}{2\kappa}, \\ \\ \frac{1}{2}\kappa[d(n-\kappa d)]^2 + O(n^3) & \text{if } d \geq \frac{n}{2\kappa}. \end{cases}$$

The term $\frac{1}{4} dn \left(n - \kappa d\right)^2$ is maximized, with respect to d, for $d = \frac{n}{3\kappa}$, to give

$$\frac{1}{4} dn \left(n - \kappa d\right)^2 \leq \frac{n^4}{27\kappa}.$$

Hence $D'(G) \leq \dfrac{n^4}{27\kappa} + O(n^3)$ when $d < \dfrac{n}{2\kappa}$. If $d \geq \dfrac{n}{2\kappa}$, then the term $\dfrac{\kappa}{2} d^2 \left(n - \kappa d\right)^2$ is maximized, with respect to d, for $d = \dfrac{n}{2\kappa}$, to give

$$\frac{\kappa}{2} d^2 \left(n - \kappa d\right)^2 \leq \frac{n^4}{32\kappa} < \frac{n^4}{27\kappa}.$$

Therefore, in both cases, $D'(G) \leq \dfrac{n^4}{27\kappa} + O(n^3)$, as desired.

To see that the bound is asymptotically best possible, consider the graph $G_{n,d,\kappa}$ constructed above for the case $d < \dfrac{n}{2\kappa}$, with $d = \dfrac{n}{3\kappa}$. Note that

$$D'(G_{n,\frac{n}{3\kappa},\kappa}) > \frac{n^4}{27\kappa},$$

as claimed. □

Chapter 4

Degree distance and edge-connectivity

4.1 Introduction

In Chapter 2 we showed that

$$D'(G) \leq \frac{n^4}{9(\delta + 1)} + O(n^3), \tag{4.1}$$

where δ is the minimum degree of G. Moreover, for a fixed δ, the inequality is asymptotically sharp. In Chapter 3, we continued this study and improved the upper bound (4.1) for graphs with fixed vertex-connectivity. Precisely, we proved the asymptotically tight upper bound:

$$D'(G) \leq \frac{n^4}{27\kappa} + O(n^3), \tag{4.2}$$

for a κ-connected graph G of order n. The two bounds, (4.1) and (4.2), solve completely the problem of bounding degree distance in terms of order and two classical connectivity measures, namely, minimum degree, and vertex-connectivity. In this chapter, we are concerned with finding upper bounds on degree distance in terms order and the third connectivity measure, edge-connectivity.

For $\lambda \geq 8$, the bound is a direct consequence of (4.1) while the cases $\lambda \leq 7$ are more complicated. Thus for $\lambda \geq 8$, an application of the inequality, $\delta \geq \lambda$, to (4.1) yields the following proposition.

Proposition 4.1 *Let G be a λ-edge-connected graph, $\lambda \geq 8$, of order n. Then*

$$D'(G) \leq \frac{n^4}{9(\lambda+1)} + O(n^3).$$

Moreover, for a fixed λ, this inequality is asymptotically sharp.

The problem to get better upper bounds of the degree distance in terms of order and edge-connectivity λ, where $2 \leq \lambda \leq 7$, turns out to be harder and requires some additional ideas apart from the standard method of treating degree distance that was introduced in [10]. We will therefore consider this problem separately as the subject of this chapter. Thus here we completely solve the problem of relating degree distance to order and each of the three classical connectivity measures, namely, minimum degree, vertex-connectivity and edge-connectivity.

4.2 Results

We first illustrate that the bound presented in Proposition 4.1 is, for a fixed λ, asymptotically sharp. For positive integers n, λ and k with $k \equiv 1 \mod 3$, consider the graph $G_{n,k,\lambda} = G_1 + G_2 + \cdots + G_k$, where $G_1 = K_{\lceil \frac{1}{2}(n - \frac{(k-2)(\lambda+1)}{3}) \rceil}$, $G_k = K_{\lfloor \frac{1}{2}(n - \frac{(k-2)(\lambda+1)}{3}) \rfloor}$, $G_2 = K_\lambda = G_{k-1}$ and for $3 \leq i \leq k-2$,

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

Then $D'(G_{n,k,\lambda}) = \dfrac{n^4}{9(\lambda+1)} + O(n^3)$, when $k = \frac{n}{\lambda+1} + O(1)$, confirming that the bound presented in Proposition 4.1 is, for a fixed λ, asymptotically sharp.

The following discussion is useful in this chapter:

Discussion 1 *Let G be a graph, $V_1, V_2 \subset V(G)$ with $V_1 \cap V_2 = \emptyset$. Clearly, $|E(V_1, V_2)| \leq |V_1||V_2|$. If $E(V_1, V_2)$ is a disconnecting set of G, then $|E(V_1, V_2)| \geq \lambda(G)$ so that $|V_1||V_2| \geq \lambda(G)$. Let $v \in V(G)$. Then $k_i k_{i+1} \geq \lambda$ for all $i = 1, 2, \ldots, ec_G(v) - 1$.*

The following lemma follows from $ab \leq (\frac{a+b}{2})^2$. In other words, the geometric mean of two (positive) real numbers never exceeds their arithmetic mean.

Lemma 4.1 *For positive integers a and b,*

(a) $ab \geq 2$ implies that $a + b \geq 3$.

(b) $ab \geq 3$ implies that $a + b \geq 4$.

(c) $ab \geq 4$ implies that $a + b \geq 4$.

(d) $ab \geq 5$ implies that $a + b \geq 5$.

(e) $ab \geq 6$ implies that $a + b \geq 5$.

(f) $ab \geq 7$ implies that $a + b \geq 6$.

We now present a very simple, but important observation.

Fact 4.1 *Let G be a 2-edge-connected graph of order n and diameter d. If $v \in V(G)$, then*

$$d \leq \frac{2}{3}(n - \deg\ v) + \frac{4}{3}.$$

Proof of Fact 4.1: Let v_0 be a vertex of G of eccentricity d and let $N_i = N_i(v_0)$. Let $v \in V(G)$. Then $v \in N_i$ for some $i \in \{0, 1, 2, \ldots, d\}$. Thus, $N(v) \subset N_{i-1} \cup N_i \cup N_{i+1}$ and recall by Lemma 4.1 (a) that $|N_j \cup N_{j+1}| \geq 3$ for all $j = 1, 2, \ldots, d-1$. Hence,

$$\begin{aligned} n &\geq |\cup_{j=0}^{i-2} N_j| + \deg\, v + 1 + |\cup_{j=i+2}^{d} N_j| \\ &\geq \deg\, v + 1 + 3\left(\frac{d-2}{2}\right) \\ &\geq \deg\, v + \frac{3}{2}d - 2. \end{aligned}$$

Hence, $d \leq \frac{2}{3}(n - \deg\, v) + \frac{4}{3}$, as required. □

We will need the following useful result.

Proposition 4.2 *Let G be a 2-edge-connected graph of order n and diameter d. If $v \in V(G)$, then*

$$D(v) \leq d(n - \frac{3}{4}d - \deg\, v) + O(n).$$

Proof: Let $v \in V(G)$, denote the eccentricity of v by e. For all $i = 1, 2, , \ldots, e$, let $N_i = N_i(v)$ and $|N_i| = k_i$. Clearly, $k_1 = \deg\, v$. Since G is 2-edge-connected, then for all $i = 1, 2, \ldots, e-1$, $k_i k_{i+1} \geq 2$ and thus by Lemma 4.1 (a), $k_i + k_{i+1} \geq 3$. Hence,

$$\begin{aligned} D(v) &= 1k_1 + 2k_2 + \cdots + ek_e \\ &\leq \begin{cases} \deg\, v + 2\cdot 1 + 3\cdot 2 + \cdots + (e-2)\cdot 1 + (e-1)\cdot 2 \\ +e(n - \frac{3}{2}e - \deg\, v + 2) + O(n) \qquad \text{if } e \text{ is even}, \\ \\ \deg\, v + 2\cdot 1 + 3\cdot 2 + \cdots + (e-2)\cdot 2 + (e-1)\cdot 1 \\ +e(n - \frac{3}{2}e - \deg\, v + \frac{5}{2}) + O(n) \qquad \text{if } e \text{ is odd}, \end{cases} \\ &\leq e\left(n - \frac{3}{4}e - \deg\, v\right) + O(n). \end{aligned}$$

Now consider $f(x) := x(n - \frac{3}{4}x - \deg\, v)$, where $x = e$. The function f is increasing on $\left[1, \dfrac{2}{3}(n - \deg\, v)\right]$. Using Fact 4.1 and $1 \le e \le d$, we consider two cases. First if $d \le \dfrac{2}{3}(n - \deg\, v)$, then $D(v) \le f(d) + O(n) = d\left(n - \frac{3}{4}d - \deg\, v\right) + O(n)$. Secondly, if by Fact 4.1, $d = \dfrac{2}{3}(n - \deg\, v) + c$, where $0 \le c \le \dfrac{4}{3}$, then $f \le f\left(\dfrac{2}{3}(n - \deg\, v)\right) = f(d - c)$. But

$$\begin{aligned} f(d-c) &= (d-c)\left(n - \frac{3}{4}(d-c) - \deg\, v\right) \\ &= d\left(n - \frac{3}{4}d - \deg\, v\right) + O(n). \end{aligned}$$

Hence, in both cases $D(v) \le d\left(n - \dfrac{3}{4}d - \deg\, v\right) + O(n)$, as required. □

The standard technique of dealing with bounding degree distance presented in [10] does not account for the relationship between degree distance and edge-connectivity. In the next theorem, we will refine the vertex partitions used in [10] to adequately account for edge-connectivity. Once again, the diameter plays a crucial role and provides us with the following intermediate result.

Theorem 4.2 *Let G be a 2-edge-connected graph of order n and diameter d. Then*

$$D'(G) \le \begin{cases} \frac{1}{4}dn(n - \frac{3}{2}d)^2 + O(n^3) & \text{if } d < \frac{n}{3}, \\ \frac{3}{4}d^2(n - \frac{3}{2}d)^2 + O(n^3) & \text{if } d \ge \frac{n}{3}. \end{cases}$$

Moreover, this inequality is asymptotically sharp.

Proof: Let v_0 be a vertex of G of eccentricity d and let $N_j = N_j(v_0)$. Recall that $|N_j \cup N_{j+1}| \ge 3$ for all $j = 0, 1, 2, \ldots, d-1$. For each set $B_i \in \{N_0 \cup N_1, N_2 \cup N_3, N_4 \cup$

$N_5, \ldots\}$ choose any three elements $u_{i1}, u_{i2}, u_{i3} \in B_i$ and denote the set $\{u_{i1}, u_{i2}, u_{i3}\}$ by A_i, $i = 1, 2, \ldots, \lceil \frac{d+1}{2} \rceil$. Let $N := \cup_{i=1}^{\lceil \frac{d+1}{2} \rceil} A_i$.

Claim 13 *Let N be as above. Then*

$$\sum_{u \in N} D'(u) \leq O(n^3).$$

Proof of Claim 13: Partition N as $N = U_1 \cup U_2 \cup \cdots \cup U_9$, where

$$U_1 = \{u_{11}, u_{41}, u_{71}, \ldots\},$$

$$U_2 = \{u_{12}, u_{42}, u_{72}, \ldots\},$$

$$U_3 = \{u_{13}, u_{43}, u_{73}, \ldots\},$$

$$U_4 = \{u_{21}, u_{51}, u_{81}, \ldots\},$$

$$U_5 = \{u_{22}, u_{52}, u_{82}, \ldots\},$$

$$U_6 = \{u_{23}, u_{53}, u_{83}, \ldots\},$$

$$U_7 = \{u_{31}, u_{61}, u_{91}, \ldots\},$$

$$U_8 = \{u_{32}, u_{62}, u_{92}, \ldots\},$$

$$U_9 = \{u_{33}, u_{63}, u_{93}, \ldots\}.$$

Then,

$$\sum_{u \in N} D'(u) = \sum_{u \in U_1} D'(u) + \sum_{u \in U_2} D'(u) + \ldots + \sum_{u \in N_9} D'(u).$$

For each $x, y \in U_i$, $i = 1, 2, \ldots, 9$, since $d(x, y) \geq 5$ we have $N(x) \cap N(y) = \emptyset$. It follows that $\sum_{x \in U_i} \deg x \leq n$ for $i = 1, 2, \ldots, 9$. From Proposition 4.2,

$$\begin{aligned} D(x) &\leq d\left(n - \frac{3}{4}d - \deg x\right) + O(n) \\ &= O(n^2). \end{aligned}$$

Thus,

$$\begin{aligned}
\sum_{u \in N} D'(u) &= \sum_{u \in N} D(u)\text{deg } u \\
&\leq O(n^2)\left(\sum_{u \in U_1} \text{deg } u + \sum_{u \in U_2} \text{deg } u + \ldots + \sum_{u \in U_9} \text{deg } u\right) \\
&\leq O(n^2)(9n) \\
&= O(n^3),
\end{aligned}$$

and Claim 13 is proven.

From here on-wards we partition the remaining vertices of G analogously to the standard partitioning developed in [10]. Let $\mathcal{C}$ be a maximum set of disjoint pairs of vertices from $V - N$ which lie at a distance at least 3, i.e., if $\{a, b\} \in \mathcal{C}$, then $d(a, b) \geq 3$. If $\{a, b\} \in \mathcal{C}$ we say a and b are partners. Finally, let K be the remaining vertices of G, i.e., $K = V - N - \{x : x \in \{a, b\} \in \mathcal{C}\}$. Let $|K| = k$, and $|\mathcal{C}| = c$. Then

$$n = 3\left\lceil \frac{d+1}{2} \right\rceil + 2c + k. \tag{4.3}$$

Fact 4.2 *Let* $\{a, b\} \in \mathcal{C}$. *Then* $\deg a + \deg b \leq n - \frac{3}{2}d + O(1)$.

Proof of Fact 4.2: Note that, since $d(a, b) \geq 3$, $N[a] \cap N[b] = \emptyset$. Also, each of the two vertices, a and b, can be adjacent to at most 9 vertices in N. Thus,

$$\begin{aligned}
n &\geq \deg a + 1 + \deg b + 1 + |N| - 18 \\
&\geq \deg a + \deg b + \frac{3}{2}d + \frac{3}{2} - 16 \\
&= \deg a + \deg b + \frac{3}{2}d + O(1),
\end{aligned}$$

and rearranging the terms completes the proof of Fact 4.2.

Now consider two cases.

Case 1: $k \leq 1$. For $x \in K$, $D(x) \leq (n-1)^2$, so $D'(x) \leq (n-1)^3$. Thus $\sum_{x \in K} D'(x) = O(n^3)$.

Claim 14 *If $\{a, b\} \in \mathcal{C}$, then $D'(a) + D'(b) \leq \frac{1}{2}dn(n - \frac{3}{2}d) + O(n^2)$.*

Proof of Claim 14: By Proposition 4.2, $D(a) \leq d\left(n - \dfrac{3}{4}d - \deg a\right) + O(n)$. Hence,

$$D'(a) \leq \deg a \left(d\left(n - \frac{3}{4}d - \deg a\right)\right) + O(n^2).$$

Similarly, $D'(b) \leq \deg b \left(d\left(n - \dfrac{3}{4}d - \deg b\right)\right) + O(n^2)$. Thus,

$$\begin{aligned} D'(a) + D'(b) &\leq \deg a \left(d\left(n - \frac{3}{4}d - \deg a\right)\right) + \deg b \left(d\left(n - \frac{3}{4}d - \deg b\right)\right) + O(n^2) \\ &= d\left((\deg a + \deg b)\left(n - \frac{3}{4}d\right) - \left((\deg a)^2 + (\deg b)^2\right)\right) + O(n^2) \\ &\leq d\left((\deg a + \deg b)\left(n - \frac{3}{4}d\right) - \frac{1}{2}(\deg a + \deg b)^2\right) + O(n^2). \end{aligned}$$

Let $x = \deg a + \deg b$ and let $f(x) := d\left(x\left(n - \frac{3}{4}d\right) - \frac{1}{2}x^2\right)$. Then by Fact 4.2, $x \leq n - \dfrac{3}{2}d + O(1)$. A simple differentiation shows that f is increasing for all $x \leq n - \frac{3}{4}d$. Hence, f attains its maximum for $x = n - \dfrac{3}{2}d + O(1)$. Thus,

$$\begin{aligned} D'(a) + D'(b) &\leq f\left(n - \frac{3}{2}d + O(1)\right) \\ &= \frac{1}{2}dn\left(n - \frac{3}{2}d)\right) + O(n^2), \end{aligned}$$

and Claim 14 is proven.

From (4.3), we have $c = \frac{1}{2}\left(n - 3\lceil\frac{d+1}{2}\rceil - k\right)$. Hence since $k \leq 1$, we have $c = \frac{1}{2}\left(n - \frac{3}{2}d\right) + O(1)$. This, in conjunction with Claim 14, yields

$$\begin{aligned}\sum_{\{a,b\}\in\mathcal{C}} (D'(a) + D'(b)) &\leq c\left(\frac{1}{2}dn\left(n - \frac{3}{2}d\right) + O(n^2)\right)\\ &= \left(\frac{1}{2}\left(n - \frac{3}{2}d\right) + O(1)\right)\left(\frac{1}{2}dn\left(n - \frac{3}{2}d\right) + O(n^2)\right)\\ &= \frac{1}{4}dn\left(n - \frac{3}{2}d\right)^2 + O(n^3).\end{aligned}$$

Hence,

$$\begin{aligned}D'(G) &= \sum_{\{a,b\}\in\mathcal{C}} (D'(a) + D'(b)) + \sum_{x\in K} D'(x) + \sum_{u\in N} D'(u)\\ &\leq \frac{1}{4}dn\left(n - \frac{3}{2}d\right)^2 + O(n^3) + O(n^3) + O(n^3)\\ &= \frac{1}{4}dn\left(n - \frac{3}{2}d\right)^2 + O(n^3),\end{aligned}$$

which establishes the bound in the theorem for Case 1 and for $d < \frac{n}{3}$. For $d \geq \frac{n}{3}$,

$$\frac{1}{4}nd(n - \frac{3}{2}d)^2 \leq \frac{3}{4}d^2(n - \frac{3}{2}d)^2 + O(n^3),$$

and so the theorem is proved for Case 1.

Case 2: $k \geq 2$. Now the pairs of vertices in $\mathcal{C}$ will be partitioned further. Fix a vertex $z \in K$. For each pair $\{a,b\} \in \mathcal{C}$, choose a vertex closer to z; if $d(a,z) = d(b,z)$ arbitrarily choose one of the vertices. Let A be the set of all these vertices closer to z, and B be the set of partners of these vertices in A, so $|A| = |B| = c$. Furthermore, let $A_1(B_1)$ be the set of vertices $w \in A(B)$ whose partner is at a distance at most 9 from w. Let $c_1 = |A_1| = |B_1|$.

Claim 15 *For all $u, v \in A \cup K$, $d(u,v) \leq 8$.*

Proof of Claim 15: Since $\mathcal{C}$ is a maximum set of pairs of vertices of distance at least 3, any two vertices of K must be at a distance of at most 2. We show that $d(a,z) \le 4$ for all $a \in A$. Suppose, to the contrary, that there exists a vertex $a \in A$ for which $d(a,z) \ge 5$. Let b be the partner of a. By definition of A, $d(z,b) \ge 5$. Now consider another vertex $z' \in K, \quad z \ne z'$. Since $d(z,z') \le 2$ we have $5 \le d(b,z) \le d(b,z') + d(z,z') \le d(b,z') + 2$ which implies $d(b,z') \ge 3$. This contradicts the maximality of $\mathcal{C}$ since $\{a,b\}$ will be replaced by $\{a,z\}$ and $\{b,z'\}$. Hence $d(a,z) \le 4$, for each $a \in A$. Thus for $u,v \in A, \quad d(u,v) \le d(u,z) + d(z,v) \le 8$.

Claim 16 *For all $x \in K$,*

$$D'(x) \le d\left(n - \frac{3}{2}d - c\right)\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n^2).$$

Proof of Claim 16: By Claim 15, all $c+k$ vertices in $A \cup K$ lie within a distance of 8 from each vertex $x \in K$. This implies that all the c_1 vertices in B_1 lie within a distance of $9+8$ from x. Thus, as in Proposition 4.2,

$$\begin{aligned} D(x) \quad &\le \quad \begin{cases} 8(c+k) + 17c_1 + 18 + 2\cdot 19 + 20 + \cdots + d - 1 \\ + \, d\left(n - c - c_1 - k - \frac{3}{2}d\right) \qquad \text{if } \ d \text{ is odd,} \\ \\ 8(c+k) + 17c_1 + 18 + 2\cdot 19 + 20 + \cdots + 2(d-1) \\ + \, d\left(n - c - c_1 - k - \frac{3}{2}d\right) \qquad \text{if } \ d \text{ is even,} \end{cases} \\ &= \quad d\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n^2). \end{aligned}$$

In order to find a bound on the degree of x we use a counting argument. Note that x can have at most 9 neighbours in N. By definition of A and B, x cannot be adjacent to two vertices, w and z, where $w \in A$ is a partner of $z \in B$ since

$d(w,z) \geq 3$. Thus, x is adjacent to at most c vertices in $A \cup B$. It follows that

$$\begin{aligned} n &\geq \deg x + |N| - 9 + |A \cup B| - c \\ &= \deg x + \frac{3}{2}d + \frac{3}{2} - 9 + c. \end{aligned}$$

Hence $\deg x \leq n - \frac{3}{2}d - c + \frac{15}{2}$. Therefore,

$$\begin{aligned} D'(x) &= \deg x D(x) \\ &\leq d\left(n - \frac{3}{2}d - c\right)\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n^2), \end{aligned}$$

and this proves Claim 16.

We now turn to finding an upper bound on the contribution of the pairs in $\mathcal{C}$ to the degree distance. We abuse notation and write $\{a,b\} \in A_1 \cup B_1$ if a and b are partners, i.e., $\{a,b\} \in \mathcal{C}$, with $a \in A_1$ and $b \in B_1$. Note that

$$\sum_{\{a,b\}\in\mathcal{C}} (D'(a)+D'(b)) = \sum_{\{a,b\}\in A_1\cup B_1} (D'(a)+D'(b)) + \sum_{\{a,b\}\in(A-A_1)\cup(B-B_1)} (D'(a)+D'(b)).$$

We first consider the set $A_1 \cup B_1$.

Claim 17 *Let $\{a,b\} \in \mathcal{C}$. If $d(a,b) \leq 9$, i.e., if $\{a,b\} \in A_1 \cup B_1$, then*

$$D'(a) + D'(b) \leq d\left(n - \frac{3}{2}d\right)\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n^2).$$

Proof of Claim 17: We first show that any two vertices in $A \cup K \cup B_1$ lie within a distance of 26 from each other. By Claim 15, any two vertices in $A \cup K$ lie within a distance of 8 from each other. Now assume that $b, v \in B_1$, and let a and u be the partners of b and v in A_1, respectively. Then $d(b,v) \leq d(b,a) + d(a,u) + d(u,v) \leq 9 + 8 + 9 = 26$. Thus any two vertices in B_1 are within a distance of 26 from each other. Now let $a \in A \cup K$ and $b \in B_1$, and let u be the partner of b in $A_1 \subseteq A$. Then $d(a,b) \leq d(a,u) + d(u,b) \leq 8 + 9 < 26$. Hence any two vertices in $A \cup K \cup B_1$ lie within a distance of 26 from each other.

Now let $w \in A_1 \cup B_1$. Since w is in $A \cup Y \cup B_1$, all the $c + k + c_1 - 1$ vertices in $A \cup K \cup B_1$ lie within a distance of 26 from w. It follows, as in Proposition 4.2, that

$$
\begin{aligned}
D(w) &\leq \begin{cases} 26(c+k+c_1-1) + 27 + 2 \cdot 28 + \cdots + d - 1 \\ +d\left(n - c - c_1 - k - \dfrac{3}{2}d\right) \qquad \text{if } d \text{ is even,} \\ \\ 26(c+k+c_1-1) + 27 + 2 \cdot 28 + \cdots + 2(d-1) \\ +d\left(n - c - c_1 - k - \dfrac{3}{2}d\right) \qquad \text{if } d \text{ is odd,} \end{cases} \\
&= d\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n).
\end{aligned}
$$

Thus, if $\{a, b\}$ is a pair in $A_1 \cup B_1$, then

$$
\begin{aligned}
D'(a) + D'(b) &\leq \deg a \left(d\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n)\right) \\
&\quad + \deg b \left(d\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n)\right) \\
&= (\deg a + \deg b)\left(d\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n^2)\right).
\end{aligned}
$$

By Fact 4.2, $\deg a + \deg b \leq n - \frac{3}{2}d + O(1)$. Therefore,

$$
\begin{aligned}
D'(a) + D'(b) &\leq \left(n - \frac{3}{2}d + O(1)\right)\left(d\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n^2)\right) \\
&= d\left(n - \frac{3}{2}d\right)\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n^2),
\end{aligned}
$$

and Claim 17 is proven.

Now consider pairs $\{a, b\}$ of vertices in $\mathcal{C}$ which are not in $A_1 \cup B_1$.

Claim 18 *Let $\{a,b\} \in \mathcal{C}$. If $d(a,b) \geq 10$, i.e., if $\{a,b\} \in (A-A_1) \cup (B-B_1)$, then*

$$D'(a) + D'(b) \leq d(c+k)\left(n - c - c_1 - k - \frac{3}{4}d\right) + cd\left(n - \frac{3}{4}d - c\right) + O(n^2).$$

Proof of Claim 18: We consider vertices from $A - A_1$ and from $B - B_1$ separately. Let $a \in A - A_1$. Then as in Claim 17, all the $c + k - 1$ vertices in $A \cup K$ lie at a distance of 8 from a and all the c_1 vertices in B_1 lie within a distance of $9 + 8 = 17$ from a. Thus, as in Proposition 4.2,

$$\begin{aligned} D(a) \quad &\leq \quad \begin{cases} 8(c+k-1) + 17c_1 + 18 + 2\cdot 19 + 20 + 2\cdot 21 + \cdots + d - 1 \\ +d\left(n - c - c_1 - k - \frac{3}{2}d\right) \qquad \text{if } \ d \text{ is odd,} \\ \\ 8(c+k-1) + 17c_1 + 18 + 2\cdot 19 + 20 + 2\cdot 21 + \cdots + 2(d-1) \\ +d\left(n - c - c_1 - k - \frac{3}{2}d\right) \qquad \text{if } \ d \text{ is even,} \end{cases} \\ &= \quad d\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n). \end{aligned}$$

We now find a bound on the degree of a. By definition of $\mathcal{C}$, a cannot be adjacent to both w and u, where $w \in A$ is a partner of $u \in B$ since $d(w,u) \geq 3$. Hence a is adjacent to at most $c-1$ vertices in $A \cup B$. Further, a is adjacent to at most 9 vertices in N and has at most k neighbours in K. Thus,

$$\deg a \leq c - 1 + 9 + k = c + k + 8.$$

It follows that

$$\begin{aligned} D'(a) \quad &= \quad \deg a D(a) \\ &\leq \quad (c+k+8)\left(d\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n)\right) \\ &= \quad d(c+k)\left(n - c - c_1 - k - \frac{3}{4}d\right) + O(n^2). \qquad (4.4) \end{aligned}$$

Now let $b \in B - B_1$. By Proposition 4.2, we have

$$D(b) \leq d\left(n - \frac{3}{4}d - \deg b\right) + O(n),$$

and so

$$D'(b) \leq \deg b\left(d\left(n - \frac{3}{4}d - \deg b\right)\right) + O(n^2). \tag{4.5}$$

We first maximize $\deg b\left(d\left(n - \frac{3}{4}d - \deg b\right)\right)$ with respect to $\deg b$. Let

$$f(x) := x\left(d\left(n - \frac{3}{4}d - x\right)\right),$$

where $x = \deg b$. A simple differentiation shows that f is increasing for $x \leq \frac{1}{2}\left(n - \frac{3}{4}d\right)$. We find an upper bound on x, i.e., on $\deg b$. Note that as above, b can be adjacent to at most $c-1$ vertices in $A \cup B$, and has at most 9 neighbours in N. We show that b cannot be adjacent to any vertex in K. Suppose to the contrary that $y \in K$ and $d(b,y) = 1$. Recall that a is the partner of b and $d(a,b) \geq 10$. By Claim 15, $d(a,y) \leq 8$. Hence $10 \leq d(a,b) \leq d(b,y) + d(y,a) \leq 1+8$, a contradiction. Thus, b cannot be adjacent to any vertex in K. We conclude that

$$\deg b \leq c - 1 + 9 = c + 8.$$

We look at two cases separately. First assume that $\deg b = c + 8$. Then

$$\begin{aligned} f(\deg b) &= f(c+8) \\ &= (c+8)\left(d\left(n - \frac{3}{4}d - (c+8)\right)\right) \\ &= cd\left(n - \frac{3}{4}d - c\right) + O(n^2). \end{aligned} \tag{4.6}$$

Second, assume that $\deg b \leq c$. From (4.3) and the fact that $k \geq 2$, we have

$$c \leq \frac{1}{2}\left(n - \frac{3}{2}d - \frac{3}{2} - k\right) + O(1) \leq \frac{1}{2}\left(n - \frac{3}{2}d - \frac{7}{2}\right).$$

Notice that

$$\frac{1}{2}\left(n-\frac{3}{2}d-\frac{7}{2}\right) \leq \frac{1}{2}\left(n-\frac{3}{2}d\right),$$

and so f is increasing in $[1,c]$. Therefore,

$$f(\deg b) \leq f(c) = cd\left(n-\frac{3}{4}d-c\right),$$

for this case. Comparing this with (4.6), we get that

$$f(\deg b) \leq cd\left(n-\frac{3}{4}d-c\right)+O(n^2).$$

Thus, from (4.5), we have

$$D'(b) \leq cd\left(n-\frac{3}{4}d-c\right)+O(n^2).$$

Combining this with (4.4), we get

$$D'(a)+D'(b) \leq d(c+k)\left(n-c-c_1-k-\frac{3}{4}d\right)+cd\left(n-\frac{3}{4}d-c\right)+O(n^2),$$

and Claim 18 is proven.

Using Claims 13, 16, 17, and 18 we have

$$\begin{aligned} D'(G) &= \sum_{u\in N} D'(u) + \sum_{x\in K} D'(x) + \sum_{\{a,b\}\in \mathcal{C}} (D'(a)+D'(b)) \\ &\le dk\left(n-\frac{3}{2}d-c\right)\left(n-c-c_1-k-\frac{3}{4}d\right) \\ &+ c_1\left(d\left(n-\frac{3}{2}d\right)\left(n-c-c_1-k-\frac{3}{4}d\right)\right) \\ &+ (c-c_1)\left(d(c+k)\left(n-c-c_1-k-\frac{3}{4}d\right)+cd\left(n-\frac{3}{4}d-c\right)\right)+O(n^3) \\ &= dk\left(n-\frac{3}{2}d-c\right)\left(n-c-c_1-k-\frac{3}{4}d\right) \\ &+ c_1\left(d\left(n-\frac{3}{2}d\right)\left(n-c-c_1-k-\frac{3}{4}d\right)\right) \\ &+ d(c-c_1)\left((c+k)\left(n-c-k-\frac{3}{4}d\right)-c_1(c+k)+c\left(n-\frac{3}{4}d-c\right)\right)+O(n^3). \end{aligned}$$

For easy calculation in maximizing this term, we note that $c-c_1\ge 0$, and that by (4.3), $n-c-k-\frac{3}{4}d\ge 0$. Hence the last term in the previous inequalities

$$d(c-c_1)\left((c+k)\left(n-c-k-\frac{3}{4}d\right)-c_1(c+k)+c\left(n-\frac{3}{4}d-c\right)\right)$$

is at most

$$d(c-c_1)\left((c+k+4)\left(n-c-k-\frac{3}{4}d\right)-c_1(c+k)+c\left(n-\frac{3}{4}d-c\right)\right).$$

It follows that

$$
\begin{aligned}
D'(G) \;\leq\; & dk\left(n-\frac{3}{2}d-c\right)\left(n-c-c_1-k-\frac{3}{4}d\right) \\
& + \; c_1\left(d\left(n-\frac{3}{2}d\right)\left(n-c-c_1-k-\frac{3}{4}d\right)\right) \\
& + \; d(c-c_1)\left((c+k+4)\left(n-c-k-\frac{3}{4}d\right)-c_1(c+k)\right. \\
& + \; \left.c\left(n-\frac{3}{4}d-c\right)\right)+O(n^3).
\end{aligned}
$$

Let $g(n,d,c,c_1)$ be the function

$$
\begin{aligned}
g(n,d,c,c_1) \;:=\; & dk\left(n-\frac{3}{2}d-c\right)\left(n-c-c_1-k-\frac{3}{4}d\right) \\
& + \; c_1\left(d\left(n-\frac{3}{2}d\right)\left(n-c-c_1-k-\frac{3}{4}d\right)\right) \\
& + \; d(c-c_1)\left((c+k+4)\left(n-c-k-\frac{3}{4}d\right)-c_1(c+k)\right. \\
& + \; \left.c\left(n-\frac{3}{4}d-c\right)\right).
\end{aligned}
$$

We first maximize g subject to c_1, keeping the other variables fixed. We show that the derivative of g with respect to c_1 is negative. Note that the derivative is

$$\begin{aligned}
\frac{dg}{dc_1} &= -dk\left(n-\frac{3}{2}d-c\right)+d\left(n-\frac{3}{2}d\right)\left(n-c-c_1-k-\frac{3}{4}d\right)\\
&-c_1d\left(n-\frac{3}{2}d\right)\\
&-d\left[(c+k+4)\left(n-c-k-\frac{3}{4}d\right)-c_1(c+k)+c\left(n-\frac{3}{4}d-c\right)\right]\\
&-d(c-c_1)(c+k)
\end{aligned}$$

$$\begin{aligned}
&= -dk\left(n-\frac{3}{2}d-c\right)-c_1d\left(n-\frac{3}{2}d\right)\\
&-d\left[(c+k+4)\left(n-c-k-\frac{3}{4}d\right)+c\left(n-\frac{3}{4}d-c\right)\right]\\
&+c_1d(c+k)-d(c-c_1)(c+k)\\
&+d\left(n-\frac{3}{2}d\right)\left(n-c-c_1-k-\frac{3}{4}d\right)
\end{aligned}$$

$$\begin{aligned}
&= -dk\left(n-\frac{3}{2}d-c\right)-c_1d\left[n-\frac{3}{2}d-c-k\right]\\
&-d\left[(c+k+4)\left(n-c-k-\frac{3}{4}d\right)+c\left(n-\frac{3}{4}d-c\right)\right]\\
&-d(c-c_1)(c+k)\\
&+d\left(n-\frac{3}{2}d\right)\left(n-c-c_1-k-\frac{3}{4}d\right)
\end{aligned}$$

$$\begin{aligned}
= \quad & -dk\left(n-\frac{3}{2}d-c\right)-c_1d\left[n-\frac{3}{2}d-c-k\right] \\
& -d(c+k+4)\left(n-c-k-\frac{3}{4}d\right)-dc\left(n-\frac{3}{4}d-c\right) \\
& -d(c-c_1)(c+k)-c_1d\left(n-\frac{3}{2}d\right) \\
& +d\left(n-\frac{3}{2}d\right)\left(n-c-k-\frac{3}{4}d\right)
\end{aligned}$$

$$\begin{aligned}
= \quad & -dk\left(n-\frac{3}{2}d-c\right)-c_1d\left[n-\frac{3}{2}d-c-k\right] \\
& -dc\left(n-\frac{3}{4}d-c\right) \\
& -d(c-c_1)(c+k)-c_1d\left(n-\frac{3}{2}d\right) \\
& +d\left(n-c-k-\frac{3}{4}d\right)\left[n-\frac{3}{2}d-c-k-4\right]
\end{aligned}$$

$$\begin{aligned}
= \quad & -dk\left(n-\frac{3}{2}d-c\right)-c_1d\left[n-\frac{3}{2}d-c-k\right] \\
& -dc\left(n-\frac{3}{4}d-c-k\right)-dck \\
& -d(c-c_1)(c+k)-c_1d\left(n-\frac{3}{2}d\right) \\
& +d\left(n-c-k-\frac{3}{4}d\right)\left[n-\frac{3}{2}d-c-k-4\right]
\end{aligned}$$

$$\begin{aligned} &= -dk\left(n-\frac{3}{2}d-c\right)-c_1d\left[n-\frac{3}{2}d-c-k\right] \\ &\quad -dck \\ &\quad -d(c-c_1)(c+k)-c_1d\left(n-\frac{3}{2}d\right) \\ &\quad +d\left(n-c-k-\frac{3}{4}d\right)\left[n-\frac{3}{2}d-2c-k-4\right]. \end{aligned}$$

From (4.3), $n-\frac{3}{2}d-2c-k \leq 3$. Thus, since $n-c-k-\dfrac{3}{4}d \geq 0$, the last term above is negative. From (4.3), $n-\frac{3}{2}d-2c-k \geq \frac{3}{2}$, and so it follows that the terms

$$n-\frac{3}{2}d-c, \quad n-\frac{3}{2}d-c-k, \quad \text{and } n-\frac{3}{2}d,$$

are all positive. Further, $c-c_1 \geq 0$.

It follows that the derivative

$$\begin{aligned} \frac{dg}{dc_1} &= -dk\left(n-\frac{3}{2}d-c\right)-c_1d\left[n-\frac{3}{2}d-c-k\right] \\ &\quad -dck \\ &\quad -d(c-c_1)(c+k)-c_1d\left(n-\frac{3}{2}d\right) \\ &\quad +d\left(n-c-k-\frac{3}{4}d\right)\left[n-\frac{3}{2}d-2c-k-4\right] \end{aligned}$$

is negative. Therefore, g is decreasing in c_1. Thus, in conjunction with (4.3), we have

$$\begin{aligned} g(n,d,c,c_1) &\leq g(n,d,c,0) \\ &= dk\left(n-\frac{3}{2}d-c\right)\left(n-c-k-\frac{3}{4}d\right) \\ &\quad + dc\left((c+k+4)\left(n-c-k-\frac{3}{4}d\right)+c\left(n-\frac{3}{4}d-c\right)\right) \\ &= d\left(\left(n-\frac{3}{2}d-c\right)^2\left(c+\frac{3}{4}d\right)+c^2\left(n-\frac{3}{4}d-c\right)\right)+O(n^3). \end{aligned}$$

A simple differentiation with respect to c shows that the function

$$\begin{aligned} \phi(c) :&= \left(n-\frac{3}{2}d-c\right)^2\left(c+\frac{3}{4}d\right)+c^2\left(n-\frac{3}{4}d-c\right) \\ &= (3d-n)c^2+\left(n-\frac{3}{2}d\right)(n-3d)c+\frac{3}{4}d\left(n-\frac{3}{2}\right)^2, \end{aligned}$$

has a critical point at $c=\frac{1}{2}\left(n-\frac{3}{2}d\right)$. Recall that $k\geq 2$ and from (4.3),

$$c=\frac{1}{2}(n-\frac{3}{2}d-k)+O(1)\leq\frac{1}{2}(n-\frac{3}{2}d)-\frac{3}{2}=c^*.$$

Hence, we obtain the domain of c, $0\leq c\leq c^*$. Now we look at two cases.

SUBCASE A: For $d<\frac{n}{3}$, the function ϕ is increasing for $c\leq\frac{1}{2}\left(n-\frac{3}{2}d\right)$ and so

$$\phi\leq\phi\left(\frac{1}{2}\left(n-\frac{3}{2}d\right)-\frac{3}{2}\right)=\frac{n}{4}\left(n-\frac{3}{2}d\right)^2+O(n^2)$$

and so

$$D'(G)\leq\frac{1}{4}dn(n-\frac{3}{2}d)^2+O(n^3).$$

SUBCASE B: If $d\geq\frac{n}{3}$, then ϕ is decreasing over the domain of c so it is maximised at $c=0$, and hence $\phi(c)\leq\phi(0)=\dfrac{3}{4}d\left(n-\dfrac{3}{2}d\right)$. It follows that

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

and Theorem 4.2 is proven.

To see that the bound is asymptotically sharp, when $d < \frac{n}{3}$ and for $\lambda = 2$, consider the graph $G_{n,d,\lambda} = G_0 + G_1 + \cdots + G_d$ where $G_0 = G_d = K_{\lceil \frac{1}{2}(n-\frac{3}{2}d)\rceil}$ and for $i = 1, 2, 3, \ldots, d-1$,

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

Then $G_{n,d,2}$ is 2-edge-connected and has diameter d and degree distance at least $\frac{1}{4}dn\left(n - \frac{3}{2}d\right)^2$. For $d \geq \frac{n}{3}$, consider the graph $G_{n,d,2} = G_0 + G_1 + \cdots + G_d$ where $G_d = K_{\lceil (n-\frac{3}{2}d)\rceil}$ and for $i = 0, 1, 2, \ldots, d-1$,

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

□

Corollary 4.3 *Let G be a 2-edge-connected graph of order n. Then*

$$D'(G) \leq \frac{2n^4}{81} + O(n^3).$$

Moreover, this inequality is asymptotically sharp.

Proof: Let d be the diameter of G. By the theorem above,

$$D'(G) \leq \begin{cases} \frac{1}{4}dn(n-\frac{3}{2}d)^2 + O(n^3) & \text{if } d < \frac{n}{3}, \\ \\ \frac{3}{4}d^2(n-\frac{3}{2}d)^2 + O(n^3) & \text{if } d \geq \frac{n}{3}. \end{cases}$$

The term $\frac{1}{4}dn\left(n - \frac{3}{2}d\right)^2$ is maximized, with respect to d, for $d = \frac{2n}{9}$, to give

$$\frac{1}{4}dn\left(n - \frac{3}{2}d\right)^2 \leq \frac{2n^4}{81}.$$

Hence,

$$D'(G) \leq \frac{2n^4}{81} + O(n^3).$$

The term $\frac{3}{4}d^2\left(n - \frac{3}{2}d\right)^2$ is maximized, with respect to d, for $d = \frac{n}{3}$, to give

$$\frac{3}{4}d^2\left(n - \frac{3}{2}d\right)^2 \leq \frac{n^4}{48} < \frac{2n^4}{81}.$$

Therefore, in both cases

$$D'(G) = \frac{2n^4}{81} + O(n^3),$$

as desired.

To see that the bound is asymptotically best possible consider the graph $G_{n,d,\lambda}$ constructed above with $d = \frac{2n}{9}$. Note that

$$D'(G_{n,\frac{2n}{9},\lambda}) = \frac{2n^4}{81} + O(n^3),$$

as claimed. □

Using similar proofs as for Theorem 4.2 we obtain the following results.

Theorem 4.4 *Let G be a 3-and 4-edge-connected graph of order n and diameter d. Then*

$$D'(G) \leq \begin{cases} \frac{1}{4}dn(n-2d)^2 + O(n^3) & \text{if } d < \frac{n}{4}, \\ d^2(n-2d)^2 + O(n^3) & \text{if } d \geq \frac{n}{4}. \end{cases}$$

Moreover, this inequality is asymptotically sharp.

To see that the bound is asymptotically sharp, for $d < \frac{n}{4}$ and for $\lambda = 3, 4$ consider the graph $G_{n,d,\lambda} = G_0 + G_1 + \cdots + G_d$ where $G_0 = G_d = K_{\lceil \frac{1}{2}(n-2d) \rceil}$ and $G_i = K_2$ for $i = 1, 2, \ldots, d-1$. For $d \geq \frac{n}{4}$, and when $\lambda = 3$, consider the graph $G_{n,d,3} = G_0 + G_1 + \cdots + G_d$ where $G_d = K_{\lceil (n-2d) \rceil}$, $G_0 = K_1$, $G_1 = K_3$ and $G_i = K_2$

for $i = 2, 3, \ldots, d-1$. For $\lambda = 4$ consider the graph $G_{n,d,4} = G_0 + G_1 + \cdots + G_d$ where $G_d = K_{\lceil (n-2d-1) \rceil}$, $G_0 = K_1$, $G_1 = K_4$ and $G_i = K_2$ for $i = 2, 3, \ldots, d-1$.

Corollary 4.5 *Let G be a 3-and 4-edge-connected graph of order n. Then*

$$D'(G) \leq \frac{n^4}{54} + O(n^3).$$

Moreover, this inequality is asymptotically sharp.

To see that the bound is asymptotically best possible consider the graph $G_{n,d,\lambda}$ constructed above with $d = \frac{n}{6}$. Note that

$$D'(G_{n,\frac{n}{6},\lambda}) = \frac{n^4}{54} + O(n^3),$$

as claimed. □

Theorem 4.6 *Let G be a 5-and 6-edge-connected graph of order n and diameter d. Then*

$$D'(G) \leq \begin{cases} \frac{1}{4}dn(n-\frac{5}{2}d)^2 + O(n^3) & \text{if } d < \frac{n}{5}, \\ \\ \frac{5}{4}d^2(n-\frac{5}{2}d)^2 + O(n^3) & \text{if } d \geq \frac{n}{5}. \end{cases}$$

Moreover, this inequality is asymptotically sharp.

To see that the bound is asymptotically sharp, for $d < \frac{n}{5}$ and for $\lambda = 5, 6$ consider the graph $G_{n,d,\lambda} = G_0 + G_1 + \cdots + G_d$ where $G_0 = G_d = K_{\lceil \frac{1}{2}(n-\frac{5}{2}d) \rceil}$ and for $i = 1, 2, \ldots, d-1$,

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

For $d \geq \frac{n}{5}$ and for $\lambda = 5$ consider the graph $G_{n,d,5} = G_0 + G_1 + \cdots + G_d$ where $G_d = K_{\lceil (n-\frac{5}{2}d) \rceil}$, $G_0 = K_1$, $G_1 = K_5$ and for $i = 2, 3, \ldots, d-1$,

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

For $\lambda = 6$ consider the graph $G_{n,d,6} = G_0 + G_1 + \cdots + G_d$ where $G_d = K_{\lceil (n - \frac{5}{2}d - 1)\rceil}$, $G_0 = K_1$, $G_1 = K_6$ and for $i = 2, 3, \ldots, d-1$,

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

Corollary 4.7 *Let G be a 5-and 6-edge-connected graph of order n. Then*

$$D'(G) \leq \frac{2n^4}{135} + O(n^3).$$

Moreover, this inequality is asymptotically sharp.

To see that the bound is asymptotically best possible consider the graph $G_{n,d,\lambda}$ constructed above with $d = \frac{2n}{15}$. Note that

$$D'(G_{n,\frac{2n}{15},\lambda}) = \frac{2n^4}{135} + O(n^3),$$

as claimed. □

Theorem 4.8 *Let G be a 7-edge-connected graph of order n and diameter d. Then*

$$D'(G) \leq \begin{cases} \frac{1}{4}dn(n-3d)^2 + O(n^3) & \text{if } d < \frac{n}{6}, \\ \\ \frac{3}{2}d^2(n-3d)^2 + O(n^3) & \text{if } d \geq \frac{n}{6}. \end{cases}$$

Moreover, this inequality is asymptotically sharp.

To see that the bound is asymptotically sharp, for $d < \frac{n}{6}$ and for $\lambda = 7$ consider the graph $G_{n,d,\lambda} = G_0 + G_1 + \cdots + G_d$ where $G_0 = G_d = K_{\lceil \frac{1}{2}(n-3d)\rceil}$ and $G_i = K_3$, for $i = 1, 2, \ldots, d-1$. For $d \geq \frac{n}{6}$ and for $\lambda = 7$ consider the graph $G_{n,d,7} = G_0 + G_1 + \cdots + G_d$ where $G_d = K_{\lceil (n-3d-2)\rceil}$, $G_0 = K_1$, $G_1 = K_7$ and $G_i = K_3$, for $i = 2, 3, \ldots, d-1$.

Corollary 4.9 *Let G be a 7-edge-connected graph of order n. Then*

$$D'(G) \leq \frac{n^4}{81} + O(n^3).$$

Moreover, this inequality is asymptotically sharp.

To see that the bound is asymptotically best possible consider the graph $G_{n,d,\lambda}$ constructed above with $d = \frac{n}{9}$. Note that

$$D'(G_{n,\frac{n}{9},\lambda}) = \frac{n^4}{81} + O(n^3),$$

as claimed. □

Chapter 5

Radius, diameter, size and vertex-connectivity

5.1 Introduction

This chapter is a continuation of the work that was started in [46] where upper bounds on the size 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 tight upper bound on the size in terms of order, diameter and vertex-connectivity. The bound, for fixed vertex-connectivity, is a strengthening of Ore's theorem [49], which we state below.

Theorem 5.1 *Let G be a connected graph of order n, diameter d and size m. Then*

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

5.2 Results

Let G be a finite connected graph of order n, size m and diameter d. From now on-wards $v_0 \in V(G)$ is a fixed vertex of eccentricity d and for each $i = 0, 1, 2, 3, \ldots, d$,

$$N_i := \{x \in V(G) | d_G(x, v_0) = i\}.$$

The following result is a strengthening of Ore's theorem if vertex-connectivity is prescribed.

Theorem 5.2 *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.

Proof. Assume the notation for v_0 and N_i given above. Note that since G is κ-connected, we have $|N_i| \geq \kappa$ for all $i = 1, 2, \ldots, d-1$. For each N_i, $i = 1, 2, \ldots, d-1$, choose any κ vertices, $u_{i1}, u_{i2}, \ldots, u_{i\kappa}$. For each $j = 1, 2, \ldots, \kappa$, let $P_j := \{u_{1j}, u_{2j}, u_{3j}, \ldots, u_{d-1j}\}$ and denote $\cup_{j=1}^{\kappa} P_j$ by $N = \cup_{j=1}^{\kappa} P_j$. Then,

$$|N| = \kappa(d-1). \tag{5.1}$$

Claim 19 *Let N be as above. Then $\sum_{x \in N} \deg x \leq O(n)$.*

Proof of Claim 19: First consider P_j. Partition P_j as follows:
$P_j = U_1 \cup U_2 \cup U_3$, where

$$U_1 = \{u_{1j}, u_{4j}, u_{7j}, \ldots\},$$

$$U_2 = \{u_{2j}, u_{5j}, u_{8j}, \ldots\}, \text{ and}$$

$$U_3 = \{u_{3j}, u_{6j}, u_{9j}, \ldots\}.$$

Note that for any $x, y \in U_i, i = 1, 2, 3$, we have $N[x] \cap N[y] = \emptyset$, where $N[v]$ denotes the closed neighbourhood of vertex v in G. It follows that

$$n \geq |\cup_{x \in U_i} N[x]| = \sum_{x \in U_i} \deg x + |U_i|, \text{ for each } i = 1, 2, 3.$$

Therefore,

$$\begin{aligned} 3n &\geq \sum_{x \in U_1} \deg x + \sum_{x \in U_2} \deg x + \sum_{x \in U_3} \deg x + |U_1| + |U_2| + |U_3| \\ &= \sum_{x \in P_j} \deg x + |P_j|. \end{aligned}$$

Thus, $\sum_{x \in P_j} \deg x \leq 3n - |P_j|$. We conclude that

$$\begin{aligned} \sum_{x \in N} \deg x &= \sum_{j=1}^{\kappa} \left(\sum_{x \in P_j} \deg x \right) \\ &\leq \sum_{j=1}^{\kappa} (3n - |P_j|) \\ &\leq 3n\kappa - |N| \\ &= O(n), \end{aligned}$$

and Claim 19 is proven.

Now let $Q = V - N$. Then from (5.1),

$$|Q| = n - \kappa(d-1). \tag{5.2}$$

Claim 20 *Let* $x \in Q$. *Then* $\deg x \leq n - \kappa d + O(1)$.

Proof of Claim 20: Let $x \in Q$. Then x can only be adjacent to vertices from at most 3 of the sets $N_i, i = 1, 2, 3, \ldots, d-1$. Hence x is adjacent to at most 3κ vertices from N. It follows that

$$\begin{aligned} \deg x &\leq |Q| + 3\kappa \\ &= n - \kappa(d-1) - 1 + 3\kappa \\ &= n - \kappa d + 4\kappa - 1, \end{aligned}$$

and Claim 20 is proven.

By Claim 20, and from (5.2), we have

$$\begin{aligned}\sum_{x\in Q}\deg x &\le \sum_{x\in Q}(n-\kappa d+O(1)) \\ &\le (n-\kappa(d-1))\,(n-\kappa d+O(1)) \\ &= (n-\kappa d)^2+O(n).\end{aligned}$$

Combining this and Claim 19, we get

$$\begin{aligned}\sum_{x\in V}\deg x &= \sum_{x\in N}\deg x+\sum_{x\in Q}\deg x \\ &\le (n-\kappa d)^2+O(n).\end{aligned}$$

It follows, by the Handshaking Lemma, that

$$m=\frac{1}{2}\sum_{x\in V}\deg x\le\frac{1}{2}(n-\kappa d)^2+O(n),$$

and the bound in the theorem is proven.

To see that the bound is asymptotically sharp, consider the sequential join graph

$$G_{n,d,\kappa}=G_0+G_1+\cdots+G_d,$$

where $G_i=K_\kappa$ for $i=0,1,2,3,\ldots,d-1$ and $G_d=K_{n-\kappa d}$. □

Using the counting technique employed in Theorem 5.2, we obtain the following theorem which is an improvement of Vizing's theorem [60] if vertex-connectivity is prescribed.

Theorem 5.3 *Let G be a κ-connected graph of order n, radius r and size m. Then*

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

Moreover, this inequality is, for a fixed κ, asymptotically tight. □

Chapter 6

Radius, diameter and the leaf number

6.1 Introduction

To date neither upper bounds on radius and diameter in terms of the leaf number nor lower bounds on the leaf number in terms of radius and diameter have been reported on. In this chapter, we contribute towards filling this gap. Further, using a technique developed by Dankelmann and Entringer [9], we prove a lower bound on the leaf number of a graph of given order and minimum degree.

We use the following terminology and notation. Let $e = uv$ be an edge of G. By *subdividing* the edge e we mean removing e from G and adding a new vertex w together with edges uw and wv to G. A *subdivided star* is a graph obtained by the following recursive rule: (i) the star graph, i.e., $K_{1,n-1}$, is a subdivided star, and (ii) a subdivided star with $n+1$ vertices can be obtained from some subdivided star H with n vertices by subdividing one edge of H. Thus, in any subdivided star, there is at most one vertex of degree at least 3. If H is a subgraph of a graph G, we write $H \leq G$. Let S be a subset of $V(G)$. The distance between a vertex u and S is defined as $\min\limits_{v \in S} d_G(u,v)$ and is denoted by $d_G(u,S)$. The closed neighbourhood of a vertex u of G is the set $\{x \in V : d_G(x, u) \leq 1\}$ and is denoted by $N_G[u]$. The closed neighbourhood, $N_G[S]$, of S is the set $\cup_{u \in S} N_G[u]$. The open neighbourhood, $N_G(S)$, of S is the set of all vertices adjacent to some vertex of S. Where there is no danger of confusion, we will drop the subscript G. A *2-packing* of G is a subset $A \subseteq V(G)$ with $d_G(u, v) > 2$ for all $u, v \in A$.

6.2 Results

Let G be a connected graph. Recall that the leaf number of G is denoted by $L(G)$. We begin by presenting a simple, but handy, lemma showing that any tree T', $T' \leq G$, is extendable into a spanning tree T of G such that $L(T) \geq L(T')$. We need some notation. Let H be a subgraph of G and v a vertex in H. Let G_v be the connected component containing v in the graph obtained from G by removing all vertices of H except v, i.e., $V(H) - \{v\}$. Denote by $H \bullet v$ the union of H and a breast first search tree of G_v rooted at v.

Lemma 6.1 *Let G be a connected graph and $T' \leq G$ a tree. Then there exists a spanning tree T of G such that $T' \leq T$ and $L(T) \geq L(T')$.*

Proof: Let the vertex set of T' be $\{u_1, u_2, \ldots, u_k\}$. Construct trees $T_1, T_2, \ldots, T_k$ by the following recursive formula: $T_1 = T' \bullet u_1,\ T_2 = T_1 \bullet u_2$, and for $i = 3, \ldots, k$, $T_i = T_{i-1} \bullet u_i$. Then $T = T_k$ satisfies the required properties. □

Theorem 6.2 *Let G be a connected graph with leaf number L and minimum degree $\delta > 2$. Then the diameter of G satisfies*

$$d \leq \frac{3(L-2)}{\delta - 2} + 2,$$

and this bound is tight.

Proof. Let $P : v_0, v_1, \ldots, v_d$ be a diametral path of G. Let q and l be the unique integers satisfying $d = 3q + l$, $0 \le l < 3$. We consider each of the three cases, as determined by l, separately.

Case A: $l = 0$. Let S be the set $S = \{v_{3i+1} \mid i = 0, 1, \ldots, q-1\}$. Consider the tree $T' \le G$ with vertex set $V(T') = \cup_{x \in S} N[x]$ and edge set

$$E(T') = E(P) \cup \{uv \in E(G) \mid u \in S \text{ and } v \in N[u]\}.$$

Clearly, since for all $x, y \in S$, $N[x] \cap N[y] = \emptyset$, we have

$$\begin{aligned} L(T') &= \deg_{T'}(v_1) - 1 + \sum_{i=1}^{q-1} [\deg_{T'}(v_{3i+1}) - 2] + 1 \\ &\ge \delta + (q-1)(\delta - 2) \\ &= \frac{d}{3}(\delta - 2) + 2. \end{aligned}$$

By Lemma 6.1, let T be a spanning tree of G with $L(T) \ge L(T')$. It follows that $L(G) \ge L(T) \ge \frac{d}{3}(\delta - 2) + 2$, and the theorem follows up on rearranging the terms.

Case B: $l = 1$. As above let S be the set $S = \{v_{3i+1} \mid i = 0, 1, \ldots, q\}$. Consider the tree $T' \le G$ with vertex set $V(T') = \cup_{x \in S} N[x]$ and edge set

$$E(T') = E(P) \cup \{uv \in E(G) \mid u \in S \text{ and } v \in N[u]\}.$$

Then

$$\begin{aligned} L(T') &= \deg_{T'}(v_1) - 1 + \sum_{i=1}^{q-1} [\deg_{T'}(v_{3i+1}) - 2] + \deg_{T'}(v_{3q+1}) - 1 \\ &\ge \delta - 1 + (q-1)(\delta - 2) + \delta - 1 \\ &= \frac{d-1}{3}(\delta - 2) + \delta. \end{aligned}$$

As above, $d \le \frac{3(L-2)}{\delta - 2} + 1 < \frac{3(L-2)}{\delta - 2} + 2$, as desired.

Case C: $l = 2$, is treated similarly and the bound in the theorem is established. To see that the bound is tight, let $d > 1$, $d \equiv 2 \pmod 3$, and $\delta > 2$ be two integers. Let $G_{\delta,d}$ be the graph with vertex set $V(G_{\delta,d}) = V_0 \cup V_1 \cup \cdots \cup V_d$, where

$$|V_i| = \begin{cases} 1 & \text{if } i \equiv 0 \text{ or } 2 \pmod 3, \\ \delta & \text{if } i = 1 \text{ or } d-1, \\ \delta - 1 & \text{otherwise,} \end{cases}$$

where uv, $u \in V_i$ and $v \in V_j$, is an edge of $G_{\delta,d}$ if and only if $|i - j| \leq 1$. Then $d(G_{\delta,d}) = \frac{3(L(G_{\delta,d})-2)}{\delta-2} + 2$, and the theorem is proven. □

We now turn to finding an upper bound on the radius. We use an observation made by Erdös, Pach, Pollack and Tuza [24]. First we need a definition and some notation.

Definition 1 *Let $G = (V, E)$ be a connected graph with minimum degree $\delta \geq 3$ and radius $r \geq 6$. Let z be a fixed central vertex of G, and so $r = \mathrm{ec}_G(z)$. For each $i = 0, 1, \ldots, r$, we define $N_i = \{v \in V \mid d_G(v, z) = i\}$. Hence, $V = N_0 \cup N_1 \cup \cdots \cup N_r$ is a partition of V. We denote by $N_{\leq j}$ and $N_{\geq j}$ the sets $\cup_{0 \leq i \leq j} N_i$ and $\cup_{j \leq i \leq r} N_i$, respectively. Let T be a spanning tree of G that is distance-preserving from z; that is, $d_T(v, z) = d_G(v, z)$ for all vertices $v \in V$. For vertices $u, v \in V$, let $T(u, v)$ denote the (unique) u–v path in T. Let $z_r \in N_r$. We say that a vertex $y \in V$ is* related *to the vertex z_r if there exist vertices $u, v \in V$, where $u \in V(T(z, z_r)) \cap N_{\geq 5}$ and $v \in V(T(z, y)) \cap N_{\geq 5}$ such that $d_G(u, v) \leq 2$.*

We are now in a position to state the result due to Erdös et al.

Fact 6.1 (Erdös et al. [24]) *Let G be a connected graph with minimum degree $\delta \geq 3$ and radius $r \geq 6$ and let z be a central vertex of G. For each vertex $z_r \in N_r$, there exists a vertex in $N_{\geq r-5}$ which is not related to z_r.*

Theorem 6.3 *Let G be a connected graph of radius $r \geq 6$, leaf number L, and minimum degree $\delta \geq 3$. Then*

$$r \leq \frac{3(L-2)}{2(\delta-2)} + \frac{17}{2}.$$

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

Proof. Let z, z_r and N_i, $i = 0, 1, \ldots, r$ be as above. By Fact 6.1, let $y_t \in N_t$, $t \geq r-5$, be a vertex not related to z_r. Let z_5 be the unique vertex in $V(T(z, z_r)) \cap N_5$ and let $T(z_5, z_r) = z_5, z_6, \ldots, z_r$. Let y_5 be the unique vertex in $V(T(z, y_t)) \cap N_5$ and let $T(y_5, y_t) = y_5, y_6, \ldots, y_t$. Let q and l be the unique integers satisfying $r - 4 = 3q + l$, $0 \leq l < 3$. Let S' be the set $S' = \{z_{3i-1} \mid i = 2, 3, \ldots, q+1\}$. Let q' and l' be the unique integers satisfying $t - 4 = 3q' + l'$, $0 \leq l' < 3$. Let S'' be the set $S'' = \{y_{3i-1} \mid i = 2, 3, \ldots, q'+1\}$. Note that since y_t and z_r are not related for $x, y \in S' \cup S''$, $x \neq y$, we have $N[x] \cap N[y] = \emptyset$. Consider the tree $T' \leq G$ with vertex set $V(T') = \cup_{x \in S' \cup S''} N[x] \cup V(T(z_5, y_5))$ and edge set

$$E(T(z_5, z_r)) \cup E(T(y_5, y_t)) \cup E(T(z_5, y_5)) \cup \{uv \in E(G) \mid u \in S' \cup S'' \text{ and } v \in N[u]\}.$$

Then

$$\begin{aligned}
L(T') &\geq \delta - 1 + (q + q' - 2)(\delta - 2) + \delta - 1 \\
&= \frac{(r + t - 8 - l - l')}{3}(\delta - 2) + 2 \\
&\geq \frac{(r + t - 12)}{3}(\delta - 2) + 2 \\
&\geq \frac{(r + r - 5 - 12)}{3}(\delta - 2) + 2 \\
&= \frac{(2r - 17)}{3}(\delta - 2) + 2.
\end{aligned}$$

The bound in the theorem follows by an application of Lemma 6.1 and rearranging terms. To see that the bound is, apart from the value of an additive constant, best possible, consider the graph $G_{\delta,d}$ constructed in Theorem 6.2. □

To date no non-trivial lower bound on the radius in terms of other graph parameters has been reported on. In the next theorem, we present a lower bound on the radius in terms of order and the leaf number.

Theorem 6.4 *Let G be a connected graph of order n, radius r and leaf number L. Then*

$$r \geq \frac{n-1}{L}.$$

Moreover, this bound is tight.

Proof. We first prove that for every tree T of order n, and radius r,

$$L(T) \geq \frac{n-1}{r}. \tag{6.1}$$

Let us assume that there exists a tree T of order n, and radius r which is a counterexample to (6.1), i.e.,

$$L(T) < \frac{n-1}{r}. \tag{6.2}$$

Of such counterexamples to (6.1), choose T to have the smallest possible order, n. Clearly, T is not the path. Let $P : v_0, v_1, \ldots, v_d$ be a diametral path of T. Fix a centre vertex u of T. Thus, u is necessarily on P. We first prove that u is the only vertex in T of degree at least 3. This is shown by proving that for each end vertex x a vertex of degree at least 3 closest to x is u.

Claim 21 *Let x be an end vertex of T, $x \notin \{v_0, v_d\}$. If x' is a vertex of degree at least 3 closest to x, then $x' = u$.*

Proof of Claim 21: Suppose to the contrary that $x' \neq u$ and let $T(x, x') : x = x_1, x_2, \ldots, x_k, x'$ be the path on T joining x and x'. Since u is on P and $x \notin \{v_0, v_d\}$, u cannot be on $T(x, x')$, otherwise $\deg_T u \geq 3$ and $d_T(x, u) < d_T(x, x')$, a contradiction. Let $T' = T - \{x_1, x_2, \ldots, x_k\}$. Since the degree of x' in T is at least 3, $L(T') = L(T) - 1$. Furthermore, T' has radius r and order $n - k$. Since u has eccentricity r, we have

$$d_T(u, x) = d_T(u, x') + d_T(x', x) = d_T(u, x') + k \leq r.$$

It follows that $k \leq r - d_T(u, x') \leq r - 1$. By minimality of T, we have that $L(T') \geq \frac{(n-k)-1}{r}$. Hence

$$L(T) = L(T') + 1 \geq \frac{n-k-1}{r} + 1 = \frac{n+r-k-1}{r} \geq \frac{n+(k+1)-k-1}{r} > \frac{n-1}{r};$$

a contradiction to (6.2), and the claim is proven.

A repeated application of Claim 21 to end vertices shows that u is the only vertex of degree at least 3, and all other vertices have degree 2 or 1. This, in conjunction with the fact that u has eccentricity r, each of the $\deg_T(u)$ components say $T_1, T_2, \ldots, T_{\deg_T(u)}$ of $T - u$ is a path of order at most r and so $L(T) = \deg_T(u)$. We now have

$$n - 1 = |V(T_1)| + |V(T_2)| + \cdots + |V(T_{\deg_T(u)})| \leq r \cdot \deg_T(u) = r \cdot L(T),$$

from which it follows that $L(T) \geq \frac{n-1}{r}$, a contradiction to (6.2). This completes the proof of the bound (6.1).

Now let G be a graph of order n and radius r. Let T be a radius-preserving spanning tree of G. Then by definition of the leaf number, in conjunction with (6.1),

$$L(G) \geq L(T) \geq \frac{n-1}{r},$$

as desired.

To see that the bound is tight, let n and r be positive integers, with $1 \leq r \leq \frac{n}{2}$. Let q and ε, $0 \leq \varepsilon < r$, be the unique integers such that $n-1 = qr+\varepsilon$. Let $G_{n,r}$ be a subdivided star with a centre vertex u where q end vertices are at distance exactly r from u, and one end vertex at distance ε from u, if $\varepsilon \neq 0$. Then $L(G_{n,r}) = \frac{n-1}{r}$, if $\varepsilon = 0$, and $L(G_{n,r}) = \frac{n-1}{r} + 1 - \frac{\varepsilon}{r}$, if $\varepsilon \neq 0$. □

Theorem 6.3, in conjunction with Theorem 6.4, yields the following lower bound on the leaf number in terms of order and minimum degree.

Corollary 6.5 *Let G be a connected graph of order n and minimum degree $\delta \geq 3$. If the radius of G is at least 6, then the leaf number L of G satisfies*

$$L \geq \sqrt{\frac{2}{3}(\delta-2)(n-1)} + O(\delta). \qquad \square$$

It is reported in [51] that Linial's Conjecture fails for sufficiently large δ. We now prove a new bound, whose flavour is that of Linial's bound, on the leaf number in terms of order and minimum degree. We point out here that for $\delta \geq 8$, the new bound presented below improves on Griggs and Wu's theorem, Theorem 6.2, whereas for $\delta \to \infty$ the result proves Theorem 6.3.

Theorem 6.6 *Let G be a connected graph of order n and minimum degree δ. Then the leaf number of G satisfies*

$$L(G) \geq \frac{\delta-2}{2\delta-1}n + \frac{2(\delta+1)}{2\delta-1}.$$

Proof. We first find a maximal 2-packing A of G using the following procedure. Choose a vertex v of G and let $A = \{v\}$. If there exists a vertex u of G with

$d(u, A) = 3$, add u to A. Add vertices u with $d(u, A) = 3$ to A until each of the vertices not in A is within distance two of A. Let T'' be the forest with vertex set $N[A]$ and whose edge set consists of all edges incident with a vertex of A.

Clearly, the number of end vertices $s(T'')$ in T'' is $s(T'') = \sum_{x \in A} \deg_G(x)$. By our construction of A, there exist $|A| - 1$ edges in G, each of them joining two neighbours of distinct elements of A, whose addition to T'' yields a tree $T' \leq G$. Since each of the $|A| - 1$ edges added to T'' to get T' joins two end vertices of T'', we have

$$s(T') \geq s(T'') - 2(|A| - 1) = \sum_{x \in A} \deg_G(x) - 2|A| + 2. \tag{6.3}$$

Let B be the vertices of G not in T'. By our construction, each vertex in B is within distance one of $N(A)$. Further $V = A \cup N(A) \cup B$ is a partition of V. Therefore, $n = |A| + |N(A)| + |B| = |A| + \sum_{x \in A} \deg_G(x) + |B|$. This, in conjunction with (6.3), yields

$$\begin{aligned} L(T') &= s(T') \geq \sum_{x \in A} \deg_G(x) - 2|A| + 2 \\ &= n - 3|A| - |B| + 2. \end{aligned}$$

From $n = |A| + \sum_{x \in A} \deg_G(x) + |B|$, we have $(\delta + 1)|A| \leq n - |B|$, and so $|A| \leq \frac{n - |B|}{\delta + 1}$. It follows that

$$L(T') \geq n - 3\frac{n - |B|}{\delta + 1} - |B| + 2 = \frac{\delta - 2}{\delta + 1} n - \frac{\delta - 2}{\delta + 1}|B| + 2. \tag{6.4}$$

We look at two cases separately.

If on one hand $|B| \leq \frac{\delta - 2}{2\delta - 1} n + \frac{2(\delta + 1)}{2\delta - 1}$, then from (6.4), we have $L(T') \geq \frac{\delta - 2}{2\delta - 1} n + \frac{2(\delta + 1)}{2\delta - 1}$, and the bound in the theorem follows by an application of Lemma 6.1.

If on the other hand $|B| > \frac{\delta - 2}{2\delta - 1} n + \frac{2(\delta + 1)}{2\delta - 1}$, then we extend the tree T' to a tree T with a larger number of leaf vertices as follows. Note that each vertex x in B is adjacent to some vertex x' in $N(A)$. Let T be the spanning tree of G with edge set $E(T') \cup \{xx' \mid x \in B\}$. Then

$$L(G) \geq L(T) = s(T) \geq |B| > \frac{\delta - 2}{2\delta - 1}n + \frac{2(\delta + 1)}{2\delta - 1},$$

and the theorem is proven. □

Conclusion

In this thesis we have completely solved the problem of determining upper bounds on degree distance, in terms of order, and the three classical connectivity measures minimum degree, vertex-connectivity and edge-connectivity.

We also gave an asymptotically sharp upper bound on the size of a graph G in terms of order, diameter and vertex-connectivity. The result is a strengthening of an old classical theorem of Ore [49] if vertex-connectivity is prescribed and constant.

In the last chapter of the thesis we gave tight upper bounds for the maximum radius and diameter of a graph G in terms of minimum degree and the leaf number. We also gave a tight lower bound on the radius in terms of order, and the leaf number. Equivalently, the result provide lower bounds on the leaf number of a graph G in terms of order and radius and, in terms of minimum degree and diameter. We proved a lower bound on the leaf number which essentially solves a conjecture of Linial reported in [17].

Bibliography

[1] P. Ali, S. Mukwembi, S. Munyira, Degree distance and vertex-connectivity. *Discrete Appl. Math.* **161** (2013), 2802–2811.

[2] M. O. Ball, Computing network reliability. *Operations Research* **27** (1979), 823–838.

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

[4] F. R. K. Chung, The average distance and the independence number. *J. Graph Theory.* **12** (1988) 229-235.

[5] F. Dai and J. Wu, An extended localized algorithm for connected dominating set formation in ad hoc wireless networks. *IEEE Trans. Parallel Distrib. Sysy.*, **15**(10) (2004), 908–920.

[6] P. Dankelmann, G. Dlamini, and H. C. Swart, Upper bounds on distance measures in $K_{2,l}$-free graphs. (submitted)

[7] P. Dankelmann, G. Dlamini, and H. C. Swart, Upper bounds on distance measures in $K_{3,3}$-free graphs. *Util. Math.* **67** (2005), 205–222.

[8] P. Dankelmann, G. S. Domke, W. Goddard, P. Grobler J.H. Hattingh, H.C Swart, Maximum sizes of graphs with given domination parameters. *Discrete Math.* **281** (2004), 137–148.

[9] P. Dankelmann, R. C. Entringer, Average distance, minimum degree and spanning trees. *J. Graph Theory* **33** (2000), 1–13.

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

[11] P. Dankelmann, M. J. Morgan, S. Mukwembi and H. C. Swart, On the Eccentric Connectivity Index and Wiener Index of a Graph. (submitted).

[12] P. Dankelmann and S. Mukwembi, The Distance Concept and Distance in Graphs, in B. Furtula and I. Gutman (eds), *Distance in Molecular Graphs - Theory* , (2011), 2–48.

[13] P. Dankelmann, S. Mukwembi and H. C. Swart, An upper bound on the radius of a 3-edge-connected graph. *Util. Math.* **73** (2007), 207–215.

[14] P. Dankelmann, H. C. Swart, and P. van den Berg, Diameter and inverse degree. *Discrete Math.* **308** (2008), 670–673.

[15] P. Dankelmann, L. Volkmann, Minimum size of a graph or digraph of given radius, *Inform. Process. Lett.* **109** (2009), 971–973.

[16] E. DeLaViña and B. Waller, Spanning trees with many leaves and average distance. *Electron. J. Combin.* **15** (2008), 1–16.

[17] G. Ding, T. Johnson and P. Seymour, Spanning Trees with Many Leaves. *J. Graph Theory* **37** (2001), 189-197.

[18] M. V Diudea, I. Gutman, L. Jäntschi, Molecular Topological, Nova, Huntington, New york, 2001.

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

[20] Z. Du and B. Zhou, Maximum degree distance of graphs with exactly two cycles, *Bull. Math. Soc. Sci. Math. Roumanie (N.S)* **54 (102)** (2011), 119-136.

[21] Z. Du and B. Zhou, Degree distance of unicyclic graphs, *Filomat* **24** (2010), 95-120.

[22] Y. Egawa and K. Inoue, Radius of $(2k-1)$-connected graphs. *Ars Combin.* **51** (1999), 89-95.

[23] P. Erdős, J. Pach, and J. Spencer, On the mean distance between points of a graph, *Congr. Numer.* **64** (1988), 121–124.

[24] P. Erdös, J. Pach, R. Pollack and Z. Tuza, Radius, diameter, and minimum degree. *J. Combin. Theory B* **47** (1989), 73-79.

[25] P. Erdös, M. Sachs and V. Sos, Maximum Induced Trees in Graphs, *J. Combin. Theory B*, **41** (1986), 61-79.

[26] S. Fajtlowicz and W. Waller, On two Conjectures of Graffiti, *Congr. Numer.*, **55** (1986), 51-56.

[27] O. Favaron, Radius and independence of a graph, *Preprint* (1986).

[28] D. B. Goldsmith, B. Manvel and V. Faber, A lower bound for the order of a graph in terms of the diameter and minimum degree. *J. Combin. Inform. System Sciences* **6** (1981), 315-319.

[29] J. R. Griggs, D. J. Kleitman and A. Shastri, Spanning trees with many leaves in cubic graphs. *J. Graph Theory* **13** (1989), 669-695.

[30] J. Griggs and M. Wu, Spanning trees in graphs of minimum degree 4 or 5. *Discrete Math.* **104** (1992), 167-183.

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

[32] J. Harant, An upper bound for the radius of a 3-connected graph. *Discrete Math.* **122** (1993), 335-341.

[33] J. Harant and H. Walther, On the radius of graphs. *J. Combin. Theory Ser. B* **30** (1981), 113-117.

[34] F. Harary, The maximum connectivity of a graph. *Proc. Nat. Acad. Sci. USA* **48** (1962), 1142–1146.

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

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

[37] D. J. Klein, Z. Mihalić, D. Plavšić and N. Trinajstić, Molecular topological index, a relation with the Wiener index. *J. Chem. Inf. Comput. Sci.* **32** (1992), 304-305.

[38] D. J. Kleitman and D. B. West, Spanning trees with many leaves. *SIAM J. Discrete Math.* **4** (1991), 99–106.

[39] M. Kouider and P. Winkler, Mean distance and minimum degree. *J. Graph Theory* **25** (1997) 95-99.

[40] W. Liang, Constructing minimum-energy broadcast trees in wireless ad hoc networks. In *Proc. of 3rd MobiHoc*, New York, (2002), 112-122.

[41] Z. Mihalić, S. Nikolić, and N. Trinajstić, Comparative Study of Molecular Descriptors Derived from the Distance Matrix. *J. Chem. Inf. Comput. Sci.* **32** (1992) 28-37.

[42] J. W. Moon, On the diameter of a graph. *Michigan Math. J.* **12** (1965), 349-351.

[43] M. J. Morgan, S. Mukwembi and H. C. Swart, On a Conjecture by Tomescu. *Utilitas Mathematica* (to appear).

[44] S. Mukwembi, On diameter and inverse degree of a graph. *Discrete Math.* **310** (2010), 940–946.

[45] S. Mukwembi, A note on diameter and the degree sequence of a graph. *Appl. Math. Lett.* **25** (2012), 175–178.

[46] S. Mukwembi, On size, order, diameter and minimum degree. *Indian J. Pure Appl. Math.* **44** (2013), 467–472.

[47] S. Mukwembi, On size, radius and minimum degree. *Discrete Mathematics and Theoretical Computer Science* **16**(1) (2014), 1-6.

[48] S. Mukwembi and S. Munyira, Degree distance and minimum degree. *Bull. Aust. Math. Soc.* **87** (2013), 255-271.

[49] O. Ore, Diameters in graphs. *J. Combin. Theory* **5** (1968), 75–81.

[50] Z. Tao, X. Junming and L. Jun, On diameters and average distance of graphs. *Or Transactions* **8** (2004), 1–6.

[51] K. Ozeki and T. Yamashita, Spanning trees: a survey. *Graphs and Combinatorics* **27** (2011), 1–26.

[52] M. A. Park, J. Willson, C. Wang, M. Thai, W. Wu, and A. Farago, A dominating and absorbent set in a wireless ad-hoc network with different transmission ranges. In *Proc. of 8th MobiHoc*, New York, (2007), 22-31.

[53] H. P. Schultz, E. B. Schultz, and T. P Schultz, Topological Organic Chemistry. 7. Graph Theory and Molecular Topological Indices of Unsaturated and Aromatic Hydrocarbons. *J. Chem. Inf. Comput. Sci.* **33** (1993), 863–867.

[54] J. A. Storer, Constructing full spanning trees for cubic graphs. *Inform Process Lett.* **13** (1981), 8–11.

[55] Z. Tao, X. Junming and L. Jun, On diameters and average distance of graphs, *Or Transactions* **8** (2004), 1–6.

[56] M. Thai, F. Wang, D. Liu, S. Zhou, and D. Du, Connected dominating sets in wireless networks with different transmission ranges. *IEEE Trans. Mob. Comput.,* **6**(7) (2007), 721–730.

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

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

[59] A. Tripathi and S. Vijay, On the least size of a graph with a given degree set. *Discrete Appl. Math.* **154** (2006), 2530–2536.

[60] V. Vizing, The number of edges in a graph of given radius. *Soviet. Math. Dokl* **8** (1967), 535-536.

[61] H. Wiener, Structural determination of the paraffin boiling points. *J. Amer. Chem. Soc.* **69** (1947), 17-20.

[62] W. Zhou, S. Hau and H. Ma, A note on tricylic graphs with minimum degree distance. *Discrete Math. Algorithms Appl.* **3** (2011), 25–32.