BOUNDS ON DISTANCE-BASED TOPOLOGICAL INDICES IN GRAPHS

by

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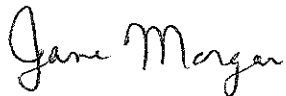University of KwaZulu-Natal

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To

My Rock and my Redeemer, the Lord Christ Jesus.

Preface and Declaration

The study described in this thesis was carried out in the School of Mathematics, Statistics and Computer Science, University of KwaZulu-Natal, Durban, during the period February 2009 to April 2012. This thesis was completed under the supervision of Doctor S. Mukwembi and Professor H. C. Swart.

This study represents original work by the author and has not been submitted in any form to another University nor has it been published previously. Where use was made of the work of others it has been duly acknowledged in the text.

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DETAILS OF CONTRIBUTION TO PUBLICATIONS that form part and/or include research presented in this thesis (include publications in preparation, submitted, *in press* and published and give details of the contributions of each author to the experimental work and writing of each publication.)

Publication 1.

M. J. Morgan, S. Mukwembi, H. C. Swart, On the eccentric connectivity index of a graph. Discrete Mathematics **311** (2011), 1229-1234.

Publication 2.

M. J. Morgan, S. Mukwembi, H. C. Swart, A lower bound on the eccentric connectivity index of a graph. Discrete Applied Mathematics **160** (2012), 248-258.

Publication 3.

P. Dankelmann, M. J. Morgan, S. Mukwembi, H. C. Swart, On the eccentric connectivity index and Wiener Index of a graph. Quaestiones Mathematicae (to appear).

Publication 4.

M. J. Morgan, S. Mukwembi, H. C. Swart, Extremal regular graphs for the eccentric connectivity index. (submitted).

Publication 5.

M. J. Morgan, S. Mukwembi, H. C. Swart, On a conjecture by Tomescu. (submitted).

Signed:

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Abstract

This thesis details the results of investigations into bounds on some distance-based topological indices.

The thesis consists of six chapters. In the first chapter we define the standard graph theory concepts, and introduce the distance-based graph invariants called *topological indices*. We give some background to these mathematical models, and show their applications, which are largely in chemistry and pharmacology. To complete the chapter we present some known results which will be relevant to the work.

Chapter 2 focuses on the topological index called the eccentric connectivity index. We obtain an exact lower bound on this index, in terms of order, and show that this bound is sharp. An asymptotically sharp upper bound is also derived. In addition, for trees of given order, when the diameter is also prescribed, tight upper and lower bounds are provided.

Our investigation into the eccentric connectivity index continues in Chapter 3. We generalize a result on trees from the previous chapter, proving that the known tight lower bound on the index for a tree in terms of order and diameter, is also valid for a graph of given order and diameter.

In Chapter 4, we turn to bounds on the eccentric connectivity index in terms of order and minimum degree. We first consider graphs with constant degree (regular graphs). Recently Došlić, Saheli & Vukičević, and Ilić posed the problem of determining extremal graphs with respect to our index, for regular (and more specifically, cubic) graphs. In addressing this open problem, we find upper and lower bounds

for the index. We also provide an extremal graph for the upper bound. Thereafter, the chapter continues with a consideration of minimum degree. For given order and minimum degree, an asymptotically sharp upper bound on the index is derived.

In Chapter 5, we turn our focus to the well-studied Wiener index. For trees of given order, we determine a sharp upper bound on this index, in terms of the eccentric connectivity index. With the use of spanning trees, this bound is then generalized to graphs.

Yet another distance-based topological index, the degree distance, is considered in Chapter 6. We find an asymptotically sharp upper bound on this index, for a graph of given order. This proof definitively settles a conjecture posed by Tomescu in 1999.

Contents

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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.
$r = \mathrm{rad}(G)$	radius of G.
$d = \mathrm{diam}(G)$	diameter of G.
$\mathrm{ec}_G(v)$	eccentricity of vertex $v \in V$.
$\mathrm{avec}(G)$	average eccentricity of G.
$(N[v])\ N(v)$	(closed) neighbourhood of vertex $v \in V$.
$(N[S])\ N(S)$	(closed) neighbourhood of subset $S \subseteq V$.
$D_G(v)$	total distance of vertex $v \in V$.
$C(G)$	the set of central vertices of G.
$A - B$	$\{x \in A \mid x \notin B\}$.
$|S|$	cardinality of a set S.
$G[S]$	subgraph induced by S in G, $S \subseteq V$.

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Chapter 1

Introduction and Preliminaries

1.1 Introduction

In this first chapter, we define the standard graph theoretical terms that will be used in the thesis, and introduce a mathematical model called a topological index. We then provide motivation for our work, and also present some relevant background results.

1.2 Graph Theory Terminology

A graph $G = (V, E)$, consists of a finite, non-empty set, V, of *vertices*, together with a (possibly empty) set, E, of unordered pairs of vertices, called *edges*. The number of elements in the vertex set V is called the *order* of G, and the number of elements in the edge set E is called its *size*. If G has an order of 1, then we say G is *trivial*; otherwise G is called *nontrivial*.

For $e \in E$, if edge $e = \{u, v\}$ (or, more simply $e = uv$,) we say that u and v are *adjacent* vertices, whereas e is said to be *incident* with u (or v). We also say that e *joins* vertices u and v. An edge with identical ends, $e = uu$ is called a *loop*. When two or more edges join the same pair of vertices, these are called *multiple edges*. A

graph is *simple* if it has no loops or multiple edges.

A *subgraph* of a graph G is a graph in which all its vertices belong to $V(G)$ and all its edges belong to $E(G)$. If a subgraph of G contains precisely all the vertices of G, it is called a *spanning* subgraph of G. For $S \subseteq V(G)$, the *induced subgraph* of S in G is the maximal subgraph of G which has vertex set S. For edge $e \in E(G)$, the subgraph $G - e$ is the graph obtained from G by deleting the edge e. Similarly, for vertex $u \in V(G)$, the subgraph $G - u$ is the graph obtained from G by deleting vertex u, along with all edges which are incident to u.

A *walk*, W, is a finite sequence $W : u_0, e_1, u_1, e_2, u_2, \ldots, e_k, u_k$ of terms which are alternately vertices and edges, where, for $i = 1, 2, \ldots, k$ the ends of edge e_i are u_{i-1} and u_i. The integer k is called the *length* of the walk. Since in a simple graph a walk can be uniquely determined by stating only its vertices, we can equivalently denote W by $u_0, u_1, u_2, \ldots, u_k$, instead of $u_0, e_1, u_1, e_2, u_2, \ldots, e_k, u_k$. If all the vertices (and hence, also all the edges) of a walk are distinct, we call it a *path*. A path P : $u_0, u_1, u_2, \ldots, u_k$ which starts at u_0 and finishes at u_k is called a $u_0 - u_k$ *path*. For $k \geq 3$, identifying the vertices u_0 and u_k in the path P yields a *cycle*, denoted by C_k.

A graph G is *connected* if every pair of vertices is connected by a path; otherwise it is *disconnected*. Disconnected graphs are thus split up into a number of connected subgraphs, called components. That is, a *component* of G is a maximal connected subgraph of G. A vertex of a connected graph is a *cut-vertex* if its removal disconnects the graph. More generally, for any simple graph G, v is a cut-vertex if $G - v$ has more components than the number of components in G. A *tree* is a connected graph with no cycles.

The degree of a vertex $w \in V(G)$, $\deg_G(w)$, is the number of edges incident to

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w. We denote by δ and Δ the minimum and maximum degrees of the vertices of G, respectively. A vertex of degree 1 is called an *end* vertex. A graph is *k-regular* if the degree of every vertex is k; and in particular, a 3-regular graph is called a *cubic* graph. And finally, a graph with a maximum vertex degree of four is known as a *chemical graph*, due to its application in the study of chemical molecules.

The *neighbours* of a vertex $v \in V(G)$ are the vertices adjacent to v. The *neighbourhood* of a vertex $v \in V(G)$, $N_G(v)$, is a set which consists of all vertices which are adjacent to v. So, $\deg(v) = |N_G(v)|$. We define the *closed neighbourhood*, $N_G[v]$, as $N_G[v] = \{v\} \cup N_G(v)$. Similarly, for $H \subseteq V(G)$, the neighbourhood of H, $N_G(H)$, is composed of the neighbours of all the vertices in H; while the closed neighbourhood of H, $N_G[H]$, consists of $N_G(H) \cup H$.

The *distance* between u and v in $V(G)$, $d_G(u, v)$, is the length of a shortest $u - v$ path in G. The *eccentricity*, $ec_G(u)$, of a vertex $u \in V(G)$ is the distance between u and a furthest vertex from u. The *diameter* of G, d, is defined as the maximum value of the eccentricities of the vertices of G. Similarly, the *radius* of G is defined as the minimum value of the eccentricities of the vertices of G. A spanning tree T of graph G is *radius-preserving* if the radius of T is equal to the radius of G. A shortest $u_0 - u_k$ path is called a *diametral path* if $k = d$, i.e., if $d_G(u_0, u_k) = d$, the diameter. It immediately follows that $ec(u_0) = ec(u_k) = d$. For vertex $v \in V(G)$, an *eccentric vertex of v* is a vertex which lies furthest away from v. A *central vertex* of G is any vertex whose eccentricity is equal to the radius of G. The *centre* of a graph is the subgraph induced by its central vertices. We denote by $C(G)$ the set of central vertices of G. The *average eccentricity*, $avec(G)$, of G is the mean eccentricity of the vertices in G, i.e.,

$$avec(G) = \frac{1}{n} \sum_{u \in V(G)} ec_G(u),$$

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where n is the order of G.

If no ambiguity is possible, the subscript G may be omitted in these notations.

We list here a few more of the most common classes of graphs. A $(n-1)$-regular graph of order n is called a *complete* graph, and is denoted by K_n. A graph is *bipartite* if its vertex set $V(G)$ can be partitioned into two subsets V_1 and V_2, and every edge has one end in V_1 and the other in V_2. In particular, if every vertex in V_1 is joined to every vertex in V_2, the graph is called a *complete bipartite* graph, and is denoted as $K_{a,b}$, where $|V_1| = a$ and $|V_2| = b$. Often the complete bipartite graph $K_{1,n-1}$ is called the *star* graph, S_n.

For terms not defined here, the reader is referred to any introductory Graph Theory book, such as [12]. More specialized terminology not presented here will be defined as needed, in the relevant chapter. Throughout this thesis, G will refer to a graph which is nontrivial, simple and connected.

1.3   Topological Indices

In this section, we introduce a graph parameter called a molecular descriptor or *topological index* (TI). It is a numerical value which is calculated from the molecular graph representation of a chemical compound, and is used to characterize the 'topology' of the molecule. Designed to find relationships between the structure of an organic molecule and its physical properties, it is valued as an important tool for predicting the physicochemical, biomedical, environmental and toxicological properties of a compound, directly from its molecular structure. Over a hundred such indices have been used in the literature [32, 38]. Here we present some of the most commonly cited TI's.

The oldest of these topological indices, dating back to 1947, is the well-known

Wiener index

$$W(G) := \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d(u,v) \quad = \sum_{\{u,v\} \subseteq V(G)} d(u,v).$$

Note that the factor of 1/2 is required in the first definition since each unordered pair $\{u,v\}, u \neq v$, appears twice in $\sum_{u \in V(G)} \sum_{v \in V(G)} d(u,v)$. This index was proposed by the chemist Harold Wiener [77] when he was analyzing the chemical properties of paraffins (alkanes). It is a distance-based index, and its mathematical properties have been much studied.

A modification is the *generalized Wiener index* (see [38])

$W_k(G) := \sum_{\{u,v\} \subseteq V(G)} [d(u,v)]^k$. In particular, for $k = -1$ it is called the 'reciprocal Wiener index' and for $k = -2$ it is the 'Harary index' or 'Harary number'. Sometimes the reciprocal Wiener index is also referred to as the Harary index.

Other topological indices based only on distance are the following (see [57]).

The *Szeged Index* $\mathrm{Sz}(G) := \sum_{uv \in E(G)} n_u(v) \, n_v(u),$

where $N_u(v) = \{w \in V \mid d(u,w) > d(v,w)\}$ and $n_u(v) = |N_u(v)|$;

and the *Padmakar-Ivan (PI) Index*, in which we find the sum over all edges $e = uv$ of G, of the number of edges which are not equidistant to the two ends of the edge e (vertices u and v). Precisely, $\mathrm{PI}(G) := \sum_{e=uv \in E(G)} n_u'(v) + n_v'(u),$ where

$N_u'(v) = \{e \in E \mid d'(u,e) > d'(v,e)\}, \quad n_u'(v) = |N_u'(v)|$

and for edge $e = ab$, $d'(u,e) = \min\{d(u,a), d(u,b)\}$.

Some popular indices (see [8]) which deal only with the degrees of vertices include the *Zagreb Index* $M(G) := \sum_{v \in V(G)} [\deg(v)]^2$, and the

Randić Index or *(Molecular) Connectivity Index*

$\chi(G) := \sum_{uv \in E(G)} [\deg(u) \deg(v)]^{-1/2}$. Related indices have been defined for exponents

other than $-1/2$.

The Schultz index includes both distance and degree in its definition. Described as a weighted version of the Wiener index, it was introduced independently by Dobrynin and Kochetova [21], and Gutman [36], in 1994.

Schultz Index or *Degree Distance*

$$D'(G) := \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} [\deg(u) + \deg(v)] \, d(u,v) = \sum_{\{u,v\} \subseteq V(G)} [\deg(u) + \deg(v)] \, d(u,v).$$

This index is also found in the *molecular topological index*, which had previously been defined by H. P. Schultz [72], and can be expressed as the sum of the Zagreb and Schultz indices.

A related index, which uses the product, rather than the sum of the degrees, is the

Gutman Index [36] $\text{Gut}(G) := \sum_{\{u,v\} \subseteq V(G)} [\deg(u) \cdot \deg(v)] \, d(u,v).$

A large part of this thesis deals with the eccentricity of vertices. Here we list the most commonly used topological indices which are eccentricity-based.

We begin with the *Eccentric Connectivity Index (ECI)*, which was put forward by Sharma, Goswami and Madan [73] in 1997.

$$\xi^C(G) := \sum_{v \in V(G)} \text{ec}_G(v) \deg_G(v).$$

It is called an *adjacency-cum-distance* index. Some refinements on the ECI are as follows.

1. AUGMENTED Eccentric Connectivity Index (see [6, 7]).

This sums the quotients of the product of adjacent vertex degrees, and the eccentricity of the concerned vertex. That is,

${}^A\xi^C(G) := \sum_{v \in V} \dfrac{M}{\text{ec}(v)},$ where M is the product of the degrees of all vertices in

the neighbourhood of v.

2. SUPERAUGMENTED Eccentric Connectivity Indices (see [23])

$${}^{SAc}\xi_k^C(G) := \sum_{v \in V} \frac{M}{[ec(v)]^{k+1}} \quad ; k = 1, 2, 3, \quad \text{where } M \text{ is defined as above.}$$

We mention three other indices which contain eccentricity in their definitions.

Connective Eccentricity Index (see [34]) $\quad C^\xi(G) := \sum_{v \in V(G)} \frac{\deg(v)}{ec(v)}.$

The eccentric distance sum was conceptualized by Gupta, Singh and Madan [35] in 2002.

Eccentric Distance Sum $\quad \xi^{DS}(G) := \sum_{v \in V(G)} ec(v) D(v),$

where $D(v) = \sum_{w \in V(G)} d(v, w)$ and finally, we have the

ADJACENT Eccentric Distance Sum [70] $\quad \xi^{SV}(G) := \sum_{u \in V(G)} \frac{ec(u) \cdot D(u)}{\deg(u)}.$

In this thesis, we focus much of our efforts on the eccentric connectivity index, although in the latter chapters we also investigate mathematical properties of the Wiener index and the Schultz index.

1.4 Literature Review

1.4.1 Motivation

Topological indices have important uses in medical, industrial and environmental research. Here we present some background material and give various applications, with emphasis on the ECI, Wiener and Schultz indices.

In chemistry, a *molecular graph* represents the topology of a molecule, by considering how the atoms are connected. This can be modelled by a graph, where the vertices represent the atoms, and the edges symbolize the covalent bonds between

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the atoms. Often these molecular graphs ignore or 'suppress' the hydrogen atoms, for example, as chemists often represent the benzene ring as a simple hexagon [4].

These graphs can be characterized by graph invariants, viz., parameters which are invariant under graph isomorphism. The invariant can be a polynomial, a sequence of numbers, or just a single number. When a single numerical value is used to characterize the structure of a molecule, this model is called a topological index [8]. Chemical graph theory uses these topological indices as a powerful tool for establishing relationships between the structure of the molecular graph, and its properties or activities. For instance, structural features such as size, shape, branching, symmetry, bonding patterns and the neighbourhood patterns of atoms in the molecules can be measured by a topological index [8, 9, 23, 54]. The Wiener index has successfully characterized properties such as the boiling point, density, critical pressure, refractive indices, heats of isomerizaton and vaporization of various hydrocarbons [21].

This quantitative relationship between the structure of a molecule and its properties (or activities) is the basis of the so-called Quantitative Structure versus Property (Activity) Relationship (QSPR, QSAR) studies. Here the term 'property' means physicochemical properties, whereas 'activity' refers to biological and pharmacological activities of the chemical compound [75]. When the emphasis is on the environmental hazard assessment of chemicals, rather than molecular design and pharmaceutical drug design, it is termed the Quantitative Structure versus Toxicity Relationship (QSTR) [1].

Much recent work in pharmaceutical drug design has focused on identifying properties of chemicals directly from their molecular structure. In pharmaceutical research, both trial and error synthesis of compounds and their random screening for

activity are time consuming and uneconomical [32]. So, preliminary investigations using QSAR/QSPR are done to select the most promising compounds for a desired property, and hence decrease the number of compounds which need to be synthesized during the process of designing new drugs [7, 32, 53].

Topological indices are 'one of the oldest and most widely used descriptors in QSAR' [28]. They have many advantages over other descriptors used in QSAR, such as geometrical, electrostatic, steric, electronic and quantum descriptors [25, 32]. TI's can be computed easily and rapidly for any known compound, or even one not yet synthesized. Many software programs, such as CODESSA, SciQSAR and POLLY are readily available for both the calculation of the descriptor values, and subsequent multivariate statistical analysis [32, 66]. Furthermore, not only are they powerful tools for drug design and environmental toxicology assessment, but they are also being used for virtual screening, lead optimization, isomer discrimination, chemical documentation and combinatorial library design [23].

First generation TI's are mathematical models which result in only integer outputs (e.g., Wiener, ECI). Indices such as the Harary index or the molecular connectivity index are considered to be second generation TI's, since they allow only integral graph parameters as variables, but might give a real output. Third generation indices allow input of real-valued graph parameters [23, 31]. For instance, the original 'topostructural' indices defined above are refined to 'topochemical' indices, which consider not only the topology (or connectivity of the atoms) of the molecule, but also the chemical nature of the atoms and bonds. A *heteroatom* is an atom, such as N, O or Cl, which is different from carbon or hydrogen [5]. When heteroatoms (vertices) are assigned their relative atomic weights (with respect to the carbon atom), this gives rise to calculations using 'chemical distances', 'chemical eccentric-

ities' and 'chemical degrees' [10, 23, 25]. Thus we have the Wiener topochemical index, eccentric connectivity topochemical index etc., which again have been successfully used in QSAR investigations [23, 24, 25, 26, 27]. Other third generation TI's consider the presence of multiple bonds. They weight the bonds (edges) according to the inverse of their bond order, so, for example, a value of 1/3 would be given to a triple bond [5].

In this thesis we investigate mathematical properties of some molecular descriptors, and more specifically, we study their extremal values. The investigation of extremal values is closely linked to isomer enumeration [55]. Suppose an integral index X (i.e., a first generation TI) is shown to have minimum and maximum values of X_m and X_M respectively, and that a particular class of chemical compounds under consideration has N isomers. If $N > (X_M - X_m)$, then two or more isomers will have the same value of the chosen index X. This type of (operational) 'degeneracy' is a serious problem encountered with topological indices [5].

Features such as low degeneracy, high sensitivity towards minor changes in the branching of molecules, and high discriminating power (such as X_M/X_m) are all considered measures of a 'good' TI [28, 70]. The eccentric connectivity index and its refinements, for instance, have been found to have low degeneracy [22], very high discriminating power [7], and extreme sensitivity towards branching [28].

Gutman and Tomivić [38] commented in 2000 that it would be valuable to demonstrate that some mathematical relations exist between various TI's being used in the chemical literature. Many such relationships, usually linear, have been identified. Inequalities relating the ECI with the eccentric distance sum, Schultz and Zagreb indices are given in [19, 40, 42, 81]. Khalifeh et al. [43] present relationships between the Wiener and Schultz indices. In the case of trees, the Wiener and Schultz indices

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actually determine each other (see, for example [18]).

$$D'(T) = 4W(T) - n(n-1), \qquad (1.1)$$

where T is a tree of order n. Considering the three TI's at the core of this work, we have the following relationships [81] which follow directly from the various definitions.

$$D'(G) \leq (n-1)\xi^C(G) \quad \text{and} \quad \xi^C(G) \geq \frac{2\delta}{n-1}W(G),$$

where G is a graph of order $n \geq 2$ and minimum degree δ.

In QSAR studies, no single TI has been identified as the best predictor for all the various chemicals investigated [5], and hence many indices have been proposed over the years. Indeed, since many are interrelated, they are typically used in various (linear) combinations in multivariate regression analyses [64, 65]. The chemical literature contains many studies comparing the degree of predictability of two or more different TI's. For instance, in drugs which counteract inflammation, the prediction of anti-inflammatory activity (of pyrazole carboxylic acid hydrazide analogues) using the eccentric connectivity index was found to be far superior to that using the Wiener index [33]. In [54] both the eccentric connectivity index and the Wiener index were found to have a high degree of prediction of HIV-protease inhibitory activity of tetrahydropyrimidin-2-ones, giving a vast potential for providing lead structures for the development of potent safe and potent anti-HIV compounds. Comparisons between these two topological models have been made for other drugs, such as those used in Alzheimer's disease [49], Huntington's disease and schizophrenia [52], hypertension [71], bacterial conditions [68], and as diuretics [69]. Other chemical compounds have been similarly considered in [47, 48, 50, 51].

Another active area of chemical research deals with nanotubes, nanotori, nanostars, and other dendrimers. These polymeric materials are of major chemical im-

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portance as they are finding applications in a variety of high technology uses, both biomedical (such as MRI diagnostics, coating agents to protect or deliver drugs to specific parts of the body, as anti-bacterial and anti-viral agents, as vectors in gene therapy) and industrial [44]. Explicit values for various topological indices, and in particular, the eccentric connectivity index, are being calculated for these classes of compounds (see, for example [2, 3, 67, 78]).

1.4.2 Relevant Background Results

In the first chapters of this thesis we focus on the eccentric connectivity index. In chapters 2 and 3 we derive some upper and lower bounds on the ECI, for both trees and graphs.

The following straightforward observations will be used in these chapters, and indeed, throughout the thesis. Consider a graph G of order n and diameter d, and let $P : v_0, v_1, \ldots, v_d$ be a diametral path. Then any vertex $x \notin V(P)$ can be adjacent to at most 3 (consecutive) vertices on P. Otherwise, a shorter path from v_0 to v_d, through x, could be found, which contradicts the definition of a diametral path.

Using similar reasoning, dividing the vertices on P into groups of 3, we claim that $N[v_i] \cap N[v_{i+3}] = \emptyset$. To show this claim, assume by contradiction that there exists a vertex u which lies in both these closed neighbourhoods. Then a shorter $v_0 - v_d$ path can be found going through u, again contradicting the definition of a diametral path.

The result $r \leq d \leq 2r$ which links the radius, r, and diameter, d, of a graph G, is well-known. The right hand inequality is easily shown by applying the triangle inequality to a central vertex c and a pair of vertices u, v for which $d_G(u, v) = d$. Thus,

Claim **1.1** *For all graphs G of radius r and diameter d,* $r \geq \lceil \frac{d}{2} \rceil$.

From this claim, in Chapter 3 we will observe that for any vertex w in a graph, $ec(w) \geq \lceil \frac{d}{2} \rceil$, since the radius is the lowest of all the eccentricities of the vertices of the graph.

In Chapter 4 we focus on a different graph invariant, the minimum degree, and find extremal values on the ECI for graphs of given order and minimum degree.

We will need the following bound proved by Dankelmann, Goddard and Swart [15] in 2004, on the average (mean) eccentricity of a graph.

Theorem 1.1 *Let G be a connected graph of order n and minimum degree δ. Then*

$$\text{avec}(G) \leq \frac{9n}{4(\delta + 1)} + \frac{15}{4}.$$

In the first part of this chapter we look specifically at graphs with constant degree, viz., regular graphs. Recently, Došlić, Saheli and Vukičević [22] stated that it would be interesting to determine extremal *cubic* graphs with respect to the eccentric connectivity index; and more generally, Ilić [40] has posed the same question for all *regular* graphs, with emphasis on cubic graphs. We completely solve this open problem for the upper bound.

Extremal graphs for the lower bound seem related to Moore graphs. If G has diameter d and maximum degree $\Delta \geq 2$, then an upper bound on the order of G can be found as follows [18, 58]. Let v be any vertex of G. There can be at most Δ vertices at a distance 1 from v. Then each of these Δ vertices can be adjacent to at most $(\Delta - 1)$ other vertices, at distance 2 from v. At a distance 3 from v there can be at most $\Delta(\Delta - 1)^2$ vertices, and so on. Recalling that the graph has diameter d, we add up this maximum number of vertices in each of the 'distance layers', to

arrive at the following upper bound on the number of vertices of G.

$$n \leq 1 + \Delta + \Delta(\Delta - 1) + \Delta(\Delta - 1)^2 + \ldots + \Delta(\Delta - 1)^{d-1} = 1 + \Delta \frac{(\Delta - 1)^d - 1}{\Delta - 2},$$

if $\Delta \geq 3$. (In the case when $\Delta = 2$, we have $n \leq 1 + 2d$.) The right hand side of this inequality is called the 'Moore bound', and is denoted by $M_{\Delta, d}$. Any extremal graph, i.e., a graph whose order is equal to the Moore bound, is called a *Moore Graph*. By the derivation of this bound, every Moore graph must be a regular graph. There are very few Moore graphs. For $d = 1$, we have the complete graphs $K_{\Delta+1}$. When $d = 2$, the Moore graphs are the cycle graph C_5 (with $\Delta = 2$), the Petersen graph ($\Delta = 3$) and the Hoffman-Singleton graph ($\Delta = 7$). The only other possible Moore graph of diameter two would be $\Delta = 57$-regular, and have order $n = 3250$; its existence is an outstanding problem in this field. Once $d \geq 3$, there are no Moore graphs, other than the cycle graphs C_{2d+1}. Hence, for all other values of d and Δ, graphs must be of order strictly less than the Moore bound. Finding graphs of maximum order which are close to this upper bound, viz., graphs of order $M_{\Delta, d} - \delta$, for some small integer value of $\delta \geq 1$ is called the *degree-diameter problem*, which is a topic of much research.

In our search for regular graphs which minimize the ECI, we derive a bound which uses the Moore bound. Hence, in the cubic case ($\Delta = 3$) the Petersen graph meets our lower bound. However, when the diameter is larger than 2, our bound clearly cannot be sharp, and our search for extremal graphs might be related to the degree-diameter problem in distances.

In the second part of Chapter 4 we generalize our investigations of the ECI to graphs of given order and minimum degree. Several authors have studied the average distance, a variant of the Wiener index. For instance, Kouider and Winkler

[46], Beezer, Riegsecker and Smith [11], and Dankelmann and Entringer [14] independently proved that the average distance of a connected graph of order n and minimum degree δ is at most $\frac{n}{\delta+1} + O(1)$. In terms of the Wiener index, this is equivalent to the bound

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

Thus we have an upper bound on the Wiener index in terms of order and minimum degree. In light of the comparisons between the Wiener and ECI being made in the pharmacological world, it is natural to ask how an upper bound on the eccentric connectivity index in terms of order and minimum degree would differ from this Wiener bound. We answer this question by deriving a corresponding bound for the ECI. For the derivation, we will need the following theorem presented in 1989 by Erdős, Pach, Pollack and Tuza [30].

Theorem 1.2 *Let G be a connected graph with n vertices, minimum degree, δ and diameter d. Then,*

$$d \leq \frac{3n}{\delta+1} - 1.$$

Proof. Let $P : v_0, v_1, \ldots, v_d$ be a diametral path. It was shown above that $N[v_i] \cap N[v_{i+3}] = \emptyset$. Define k as the integer for which $d = 3k + r$, where $r \in \{0, 1, 2\}$. Then, $N[v_0], N[v_3], N[v_6], \ldots, N[v_{3k}]$ are all pairwise disjoint sets. Further, note that $|N[v_i]| \geq \delta + 1$. A lower bound on the number of vertices of G is then

$$n \geq \sum_{i=0}^{k} |N[v_{3i}]| \geq (k+1)(\delta+1).$$

Solving for k, we have $k \leq \frac{n}{\delta+1} - 1$. But $k = \frac{d-r}{3} \geq \frac{d-2}{3}$, and upon simplification we have $d \leq \frac{3n}{\delta+1} - 1$. $\qquad\square$

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We remark that this upper bound is asymptotically sharp. For example, when $r = 0$, i.e., when $d = 3k$ for some integer k, consider the graph constructed as follows. Let $G_{\delta,d}$ be the graph with vertex set $V(G_{\delta,d}) = V_0 \cup V_1 \cup \cdots \cup V_{3k}$, where

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

and two distinct vertices $v \in V_i$, $v' \in V_j$ are joined by an edge if and only if $|j - i| \leq 1$. See Figure 1.1.
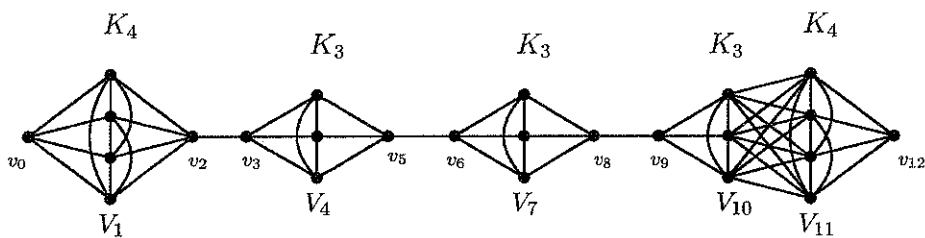

Figure 1.1: Example of an extremal graph, $G_{4,12}$

The graph $G_{\delta,d}$ has order $n = \frac{\delta+1}{3}(d + 3)$. Hence,

$$
d = \frac{3n}{\delta + 1} - 3 = \frac{3n}{\delta + 1} + O(1),
$$

and so it asymptotically meets the upper bound.

In the next chapter we use spanning trees of a graph to continue our studies comparing the ECI and the Wiener index. Spanning trees have been used by Dankelmann and Entringer [14] as an excellent tool for deriving upper bounds on the average distance, which is a variant of the Wiener index. Since the deletion of edges of a graph cannot decrease the distance between vertices, we have the following well-known property of the Wiener index.

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For any connected graph G, every spanning tree T of G satisfies the inequality

$$W(G) \leq W(T).$$

We investigate the relationship between the eccentric connectivity index of a graph and its spanning trees. Continuing in Chapter 5, we determine an upper bound on the Wiener index of a tree, in terms of its eccentric connectivity index. Applying our spanning tree relationship, this will imply an upper bound on the Wiener index of a general graph, in terms of the ECI.

In Chapter 6 we consider the degree distance (Schultz) topological index. Since it was proposed several years before the ECI, mathematical investigations into this index are more advanced. For example, in the case of unicyclic and bicyclic graphs, upper and lower bounds for the degree distance have been derived [39, 74], and their properties in terms of other graph parameters have been investigated [41]. In [13, 75], for specified order and size, the graph which attains the minimum value for the Schultz index is presented. For other results, see [18].

Studies into the relationship between the Wiener Index and the degree distance parameter abound (see, for example [20, 36, 37, 45]). For a given order, the Wiener index attains its minimum value for the complete graph, and maximum for the path. That is,

$$W(K_n) = \binom{n}{2} \leq W(G) \leq \binom{n+1}{3} = W(P_n).$$

(For a proof, see, for instance, [56].) When considering trees, the lower bound becomes the star graph, and we have

$$W(S_n) = (n-1)^2 \ \leq \ W(T) \ \leq \ W(P_n).$$

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Applying equation (1.1), it follows [75] that

$$D'(S_n) = 3n^2 - 7n + 4 \leq D'(T) \leq \frac{1}{3}n(n-1)(2n-1) = D'(P_n).$$

These two bounds on the degree distance have been derived using other approaches in [13, 43, 76]. However, extremal values on this index for graphs in general have proved to be more difficult to obtain. Indeed, in 1999, Tomescu [76] conjectured the asymptotic upper bound $D'(G) \leq \frac{1}{27}n^4 + O(n^3)$ for a connected graph G of order n. Nine years later, Bucicovschi and Cioabă [13] commented that Tomescu's conjecture 'seems difficult at present time.' In the following year Dankelmann, Gutman, Mukwembi and Swart [16] considered this problem and though they came close to proving the conjecture, their proof was inadequate to meet the $O(n^3)$ error term. In Chapter 6 we present an asymptotically tight upper bound on the Schultz index of a graph, in terms of order and diameter. Thereafter, a corollary will definitively confirm the Tomescu conjecture.

Chapter 2

The Eccentric Connectivity Index

2.1   Introduction

We begin by recalling the definition of the *eccentric connectivity index*, $\xi^C(G)$ of G, which was introduced in 1997 by Sharma, Goswami and Madan [73].

$$\xi^C(G) = \sum_{v \in V(G)} \mathrm{ec}(v) \deg(v),$$

where $\mathrm{ec}(v)$ and deg (v) are the eccentricity and degree of vertex v in G, respectively.

For several special classes of graphs, straightforward calculations give us the following useful values for our parameter. We begin with the complete graph K_n, and the complete bipartite graph $K_{a,b}$.

$\xi^C(K_n) = n(n-1)$ (for $n \geq 2$) ;

$\xi^C(K_{a,b}) = 4\,a\,b$ (for $a,\, b \neq 1$)

and the index reaches its maximum for $K_{a,b}$ when $a = b = n/2$.

For the star, cycle and paths of order n,

$\xi^C(S_n) = \xi^C(K_{1,n-1}) = 3(n-1)$ (for $n \geq 3$) ;

$$\xi^C(C_n) = \begin{cases} n^2 & \text{for } n \text{ even} \\ n(n-1) & \text{for } n \text{ odd;} \end{cases}$$

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$$\xi^C(P_n) = \begin{cases} \frac{1}{2}\left(3n^2 - 6n + 4\right) & \text{for } n \text{ even} \\ \frac{3}{2}\left(n - 1\right)^2 & \text{for } n \text{ odd.} \end{cases}$$

Furthermore, we calculate the eccentric connectivity index for three other classes of graphs which will be important in our theorems. Recall that d denotes the diameter of the graph.

The *broom* graph $B_{n,d}$ consists of a path P_d, together with $(n - d)$ end vertices all adjacent to the same end vertex of P_d. The *lollipop* graph $L_{n,d}$ 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}. See Figure 2.1.
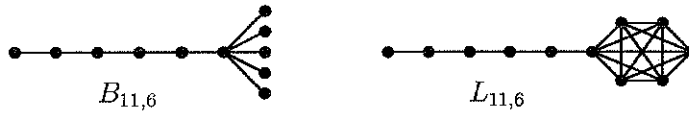
Figure 2.1: Graphs $B_{11,6}$, $L_{11,6}$

Particularly relevant to our studies is the *volcano* graph $V_{n,d}$. It is the graph obtained from a path P_{d+1} and a set S of $n - d - 1$ vertices, by joining each vertex in S to a central vertex of P_{d+1}. Note that for a fixed value of n, when d is even, the volcano graph $V_{n,d}$ is unique; whereas when d is odd, there may be several non-isomorphic volcano graphs $V_{n,d}$. See Figure 2.2.

Figure 2.2: Volcano Graphs $V_{15,9}$, and $V_{11,6}$

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Straightforward calculations show that

$$\xi^C(B_{n,d}) = \begin{cases} 2dn - n - d^2/2 - d + 1 & \text{for } d \text{ even} \\ \frac{1}{2}\left(3 - 2d - d^2 - 2n + 4dn\right) & \text{for } d \text{ odd;} \end{cases}$$

$$\xi^C(L_{n,d}) = \begin{cases} \frac{1}{2}\left(2 - 2d + d^2 + 2d^3 - 2n + 2dn - 4d^2n + 2dn^2\right) & \text{for } d \text{ even} \\ \frac{1}{2}\left(3 - 2d + d^2 + 2d^3 - 2n + 2dn - 4d^2n + 2dn^2\right) & \text{for } d \text{ odd;} \end{cases}$$

$$\xi^C(V_{n,d}) = \begin{cases} nd + n + d^2/2 - 2d - 1 & \text{for } d \text{ even} \\ nd + 2n + d^2/2 - 3d - 3/2 & \text{for } d \text{ odd.} \end{cases}$$

We now present upper and lower bounds on our index, initially for general graphs G, and then for trees T. (See [62].)

2.2   Bounds for General Graphs

Our first theorem shows that the eccentric connectivity index is minimized with the star graph.

Theorem 2.1 *Let $G = (V, E)$ be a connected graph of order n, $n \geq 4$. Then*

$$\xi^C(G) \geq 3(n-1),$$

and the bound is tight.

Proof. Let $A = \{v \in V \mid \deg(v) = n - 1\}$, $B = \{v \in V \mid n - 2 \geq \deg(v) \geq 2\}$ and $C = \{v \in V \mid \deg(v) = 1\}$. Then letting $|A| = a$, $|B| = b$ and $|C| = c$, we obtain

$$a + b + c = n \tag{2.1}$$

Since $\deg(v) \leq n - 2$ for every vertex v in $B \cup C$, it follows that, for $n \geq 4$,

$$\text{ec}(v) \geq 2 \quad \text{for all } v \in B \cup C. \tag{2.2}$$

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CASE 1 $A \neq \emptyset$; i.e., $a \geq 1$. Then (2.1) and (2.2) in conjunction with $n > 3$, give

$$
\begin{aligned}
\xi^C(G) &= \sum_{v \in A} ec(v) \deg(v) + \sum_{v \in B \cup C} ec(v) \deg(v) \\
&\geq \sum_{v \in A} 1 \cdot (n-1) + \sum_{v \in B \cup C} 2 \cdot 1 \\
&= a(n-1) + 2(b+c) \\
&= 2n + a(n-3) \\
&\geq 2n + n - 3,
\end{aligned}
$$

as claimed.

CASE 2 $A = \emptyset$; i.e., $a = 0$. We claim that for all $v \in C$, $ec(v) \geq 3$. To see this, if there exists an $x \in C$ for which $ec(x) = 2$, its neighbour would have to have degree $(n-1)$, a contradiction to $A = \emptyset$. Otherwise, $ec(x) = 1$, which implies $n = 2$, a contradiction to our assumption that $n \geq 4$. Hence, $ec(v) \geq 3$ for all $v \in C$. This, together with (2.1) and (2.2) yields

$$
\begin{aligned}
\xi^C(G) &= \sum_{v \in B} ec(v) \deg(v) + \sum_{v \in C} ec(v) \deg(v) \\
&\geq \sum_{v \in B} 2 \cdot 2 + \sum_{v \in C} 3 \cdot 1 \\
&= 4b + 3c \\
&= 3n + b,
\end{aligned}
$$

and the bound is established. The bound is attained by the star graph.   □

We now derive an asymptotic upper bound on the ECI, when G has order n. We initially consider a graph of given order and diameter, and thereafter obtain, as a corollary, an upper bound of the ECI in terms of order.

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Theorem 2.2 *Let G be a connected graph of order n and diameter d. Then*

$$\xi^C(G) \leq d(n-d)^2 + O(n^2),$$

and this bound is best possible.

Proof. Let $P : u_0, u_1, \ldots, u_d$ be a diametral path, and let $M \subseteq V$ be the set of the remaining vertices which are not on P. Call $m = |M|$.

Claim **2.1** $\quad \sum_{x \in V(P)} ec(x) \deg(x) \leq O(n^2).$

Proof of Claim 2.1: We partition the vertices of P as $V(P) = V_0 \cup V_1 \cup V_2$, where V_0, V_1 and V_2 are defined as follows:

$$V_0 = \{u_0, u_3, u_6, \ldots\},$$

$$V_1 = \{u_1, u_4, u_7, \ldots\},$$

$$V_2 = \{u_2, u_5, u_8, \ldots\}.$$

Let $x, y \in V_i$, for some $i = 0, 1, 2$. Since the distance between x and y along P is at least 3, and P is a diametral path, we have that $N[x] \cap N[y] = \emptyset$, where $N[v]$ is the closed neighbourhood of v in G. Thus $\sum_{x \in V_i} \deg(x) \leq n - |V_i|$, for each $i = 0, 1, 2$.

Now

$$\sum_{x \in V(P)} ec(x) \deg(x) = \sum_{x \in V_0} ec(x) \deg(x) + \sum_{x \in V_1} ec(x) \deg(x) + \sum_{x \in V_2} ec(x) \deg(x)$$

$$\leq \sum_{x \in V_0} d \deg(x) + \sum_{x \in V_1} d \deg(x) + \sum_{x \in V_2} d \deg(x)$$

$$= d \left(\sum_{x \in V_0} \deg(x) + \sum_{x \in V_1} \deg(x) + \sum_{x \in V_2} \deg(x) \right)$$

$$\leq d \left(n - |V_0| + n - |V_1| + n - |V_2| \right)$$

$$= d \left(3n - d - 1 \right)$$

$$= O(n^2).$$

Thus Claim 2.1 is proven.

Claim **2.2** $\mathrm{ec}(v)\deg(v) \le d(n-d) + O(n)$ *for all* $v \in M$.

Proof of Claim 2.2: Since P is a diametral path, $v \in M$ is adjacent to at most 3 vertices of P. Hence, $\deg(v) \le n - d + 1$ and so

$$\mathrm{ec}(v)\deg(v) \le d(n-d+1) \le d(n-d) + O(n),$$

as required.

Finally, combining Claims 2.1 and 2.2 we obtain

$$\begin{aligned}
\xi^C(G) &= \sum_{v \in M} \mathrm{ec}(v)\deg(v) + \sum_{x \in P} \mathrm{ec}(x)\deg(x) \\
&\le m\left[d(n-d) + O(n)\right] + O(n^2) \\
&= (n-d-1)d(n-d) + O(n^2) \\
&= d(n-d)^2 + O(n^2).
\end{aligned}$$

which proves the bound.

Our bound is sharp, since the lollipop graph attains this upper value. In fact, straightforward calculation of the ECI value shows that

$$\xi^C(L_{n,d}) = d(d-n)^2 + O(n^2). \qquad \square$$

Differentiating with respect to the diameter, the bound in Theorem 2.2 results in a maximum ECI value at $d = n/3$, and hence we have

Corollary 2.3 *Let G be a connected graph of order n. Then*

$$\xi^C(G) \le \frac{4}{27}n^3 + O(n^2),$$

and the bound is sharp.

Again, the lollipop graph, $L_{n,n/3}$ shows that this bound is best possible.

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2.3 Bounds for Trees

Turning now to trees, we show that the path gives the maximum eccentric connectivity index value, amongst all trees of a given order. We will need the following fact and lemma.

Fact 2.1 *Let T be a tree and x a vertex of T. If $\mathrm{ec}(x) = d(x,y)$ for some y in T, then y must be an end vertex.*

To show this fact, let $P : x, v_1, v_2, \ldots, v_k, y$ be the unique $x - y$ path in T. If, by contradiction, $\deg(y) \geq 2$, then there exists a vertex z, $z \neq v_k$, which is adjacent to y. Then $d(x,z) = d(x,y) + d(y,z) = \mathrm{ec}(x) + 1$, which contradicts the definition of the eccentricity of x as the maximum distance between x and any other vertex of the graph. Therefore, y must be an end vertex.

Lemma 2.4 *Let T be a tree, w a vertex of T, and let $P : v_0, v_1, \ldots, v_d$ be a diametral path of T. Then $\mathrm{ec}(w) = \max\{d(w, v_0), d(w, v_d)\}$.*

Proof. First, note by the definition of eccentricity, that $\mathrm{ec}(w) \geq d(w, v_0), d(w, v_d)$. By way of contradiction, suppose that

$$\mathrm{ec}(w) > d(w, v_0) \quad \text{and} \quad \mathrm{ec}(w) > d(w, v_d). \tag{2.3}$$

Let a be an eccentric vertex of w, i.e., $\mathrm{ec}(w) = d(w, a)$. Thus,

$$d(w, a) = \mathrm{ec}(w) > d(w, v_0) \quad \text{and} \quad d(w, a) > d(w, v_d). \tag{2.4}$$

By Fact 2.1, a is an end vertex. But, by (2.4), we have that $a \neq v_0, v_d$. So, a is not on P.

We consider two cases separately.

CASE 1 w is on P

By (2.4) and the definition of a diametral path, $w \neq v_0, v_d$. Since w is on P, we have $w = v_i$, for some $i = 1, 2, \ldots, d - 1$. Let v_j be the vertex on P closest to a. Assume, without loss of generality, that $j \geq i$. Then

$$
\begin{aligned}
d(v_0, a) &= d(v_0, w) + d(w, a) \\
&= d(v_0, w) + d(w, a) + d(w, v_d) - d(w, v_d) \\
&= [d(v_0, w) + d(w, v_d)] + [d(w, a) - d(w, v_d)] \\
&= d + [d(w, a) - d(w, v_d)].
\end{aligned}
$$

But from (2.4), $d(w, a) - d(w, v_d) > 0$. Thus, $d(v_0, a) > d$, a contradiction to the fact that T has diameter d.

CASE 2 w is not on P

Then, for some $i = 1, 2, \ldots, d - 1$, let v_i be the vertex on P closest to w. Since a is an end vertex, it cannot lie on the $w - v_i$ path. Let v_j be the vertex on P closest to a. Assume, without loss of generality, that $j \geq i$. Again, since $d(w, a) - d(w, v_d) > 0$, we have

$$
\begin{aligned}
d(v_0, a) &= d(v_0, v_j) + d(v_j, a) \\
&= d(v_0, v_j) + d(v_j, a) + d(w, v_d) - d(w, v_d) \\
&= d(v_0, v_j) + d(v_j, a) + [d(w, v_i) + d(v_i, v_j) + d(v_j, v_d)] - d(w, v_d) \\
&= [d(v_0, v_j) + d(v_j, v_d)] + d(v_j, a) + d(w, v_i) + d(v_i, v_j) - d(w, v_d) \\
&= d + [d(w, v_i) + d(v_i, v_j) + d(v_j, a)] - d(w, v_d) \\
&\geq d + d(w, a) - d(w, v_d) \\
&> d,
\end{aligned}
$$

and again we find that $d(v_0, a) > d$, a contradiction to the fact that T has diameter d.

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Thus (2.3) is impossible, so either $\mathrm{ec}(w) = d(w, v_0)$ or $\mathrm{ec}(w) = d(w, v_d)$. Using the definition of eccentricity, the lemma follows. $\quad\square$

Theorem 2.5 *Let T be a tree of order n, $n \geq 2$. Then*

$$\xi^C(T) \leq \xi^C(P_n) = \begin{cases} \frac{1}{2}(3n^2 - 6n + 4) & \text{for } n \text{ even} \\ \frac{3}{2}(n-1)^2 & \text{for } n \text{ odd.} \end{cases} \tag{2.5}$$

Proof. (By reverse induction on the diameter d of T.) If $d = n - 1$, then $T = P_n$ and the theorem is true. Hence, we need only to consider trees other than the path, and thus it follows that T contains at least 3 end vertices. The theorem also holds for $n = 2$ or 3. So, assume that $n \geq 4$, $d \leq n - 2$. The induction hypothesis is that (2.5) holds if $d = k + 1$, for some k, $2 \leq k \leq n - 3$.

Now, consider a tree T with diameter $d = k$. Let $P : x_0, x_1, \ldots, x_d$ be a diametral path in T and let y be an end vertex of T, where $y \notin \{x_0, x_d\}$. Let v be the unique neighbour of y in T. By Lemma 2.4, assume, without loss of generality, that $\mathrm{ec}_T(v) = d_T(v, x_0)$.

Consider the tree T' obtained from T by 'moving' y and attaching it to x_0, i.e., $T' = (T - vy) \cup yx_0$. Then $d(T') = k + 1$ and $|V(T')| = n$, so by the induction hypothesis

$$\xi^C(T') \leq \xi^C(P_n). \tag{2.6}$$

Fact 2.2 (i) *If $z \in V(T) - \{v, y\}$, then $\mathrm{ec}_{T'}(z) \geq \mathrm{ec}_T(z)$,*

(ii) $\mathrm{ec}_{T'}(v) \geq \mathrm{ec}_T(v) + 1$,

(iii) $\mathrm{ec}_{T'}(y) \geq \mathrm{ec}_T(y) + 1$,

(iv) $\deg_{T'}(v) = \deg_T(v) - 1$; $\deg_{T'}(x_0) = \deg_T(x_0) + 1$,

(v) $\deg_{T'}(x) = \deg_T(x)$ *for all* $x \in V(T) - \{x_0, v\}$.

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To see that (i) holds, let $z \in V(T) - \{v, y\}$. Then by Lemma 2.4, $\mathrm{ec}_T(z) = d_T(z, x_0)$ or $\mathrm{ec}_T(z) = d_T(z, x_d)$. In the former case, we have $\mathrm{ec}_{T'}(z) \geq d_{T'}(y, z) = d_{T'}(y, x_0) + d_{T'}(x_0, z) = 1 + d_T(x_0, z) = 1 + \mathrm{ec}_T(z)$, and (i) follows. In the latter, we have $\mathrm{ec}_{T'}(z) \geq d_{T'}(z, x_d) = d_T(z, x_d) = \mathrm{ec}_T(z)$, as desired.

We now prove (ii). Recall that $\mathrm{ec}_T(v) = d_T(v, x_0)$. It follows that $\mathrm{ec}_{T'}(v) \geq d_{T'}(v, y) = d_{T'}(v, x_0) + d_{T'}(x_0, y) = d_T(v, x_0) + 1 = \mathrm{ec}_T(v) + 1$, and (ii) is proven. Next, we note that $\mathrm{ec}_{T'}(y) \geq d_{T'}(y, x_d) = d + 1 \geq \mathrm{ec}_T(y) + 1$, and so (iii) holds. Finally, by the construction of T', (iv) and (v) hold, and so the fact is proven.

Letting $S = \{v, y, x_0\}$, and using Fact 2.2 (i) and (v), we have

$$\sum_{u \in V(T) - S} [\mathrm{ec}_{T'}(u) \deg_{T'}(u) - \mathrm{ec}_T(u) \deg_T(u)] \geq 0. \tag{2.7}$$

Summing over the set S, and using Fact 2.2 (i), (ii), (iii) and (iv), and $\deg_T(v) \geq 2$, we have

$$
\begin{aligned}
\sum_{u \in S} [\mathrm{ec}_{T'}(u) \deg_{T'}(u) - \mathrm{ec}_T(u) \deg_T(u)] \ = \ & [\mathrm{ec}_{T'}(v) \deg_{T'}(v) - \mathrm{ec}_T(v) \deg_T(v)] \\
& + [\mathrm{ec}_{T'}(y) \deg_{T'}(y) - \mathrm{ec}_T(y) \deg_T(y)] \\
& + [\mathrm{ec}_{T'}(x_0) \deg_{T'}(x_0) - \mathrm{ec}_T(x_0) \deg_T(x_0)] \\
\geq \ & [\deg_T(v) - \mathrm{ec}_T(v) - 1] + [1] + [\mathrm{ec}_T(x_0)] \\
\geq \ & [2 - \mathrm{ec}_T(v) - 1] + [1] + [d] \\
= \ & 2 - \mathrm{ec}_T(v) + d \\
\geq \ & 2.
\end{aligned}
$$

This, in conjunction with (2.7), yields

$$\xi^C(T') - \xi^C(T) = \sum_{u \in V(T)-S} [\mathrm{ec}_{T'}(u) \deg_{T'}(u) - \mathrm{ec}_T(u) \deg_T(u)]$$

$$+ \sum_{u \in S} [\mathrm{ec}_{T'}(u) \deg_{T'}(u) - \mathrm{ec}_T(u) \deg_T(u)]$$

$$\geq 2.$$

Combining this inequality with (2.6), we conclude that $\xi^C(T) < \xi^C(T') \leq \xi^C(P_n)$, and the proof of the theorem is complete. $\qquad\square$

We complete this chapter by finding upper and lower bounds on our parameter for a tree T, when both the order and diameter are prescribed. We begin with the upper bound.

Theorem 2.6 *If T is a tree of order n and diameter d, then $\xi^C(T) \leq \xi^C(B_{n,d})$.*

Proof. Let $P : x_0, x_1, \ldots, x_d$ be a diametral path in T.

If $T = B_{n,d}$, then there is nothing to be proved; so assume that there exists an end vertex v of T, $v \neq x_0$, such that v is adjacent to a vertex u, where $u \neq x_{d-1}$. (It is possible that u lies on P.) Denote by $\{v_1, v_2, \ldots, v_k\}$ the set of end vertices which are adjacent to u; and $v_i \neq x_0$ for $i = 1, 2, \ldots, k$. Let $\deg(u) = r + k$, for some $r \geq 1$.

Form another tree, T', by replacing the k edges $u v_i$ with $x_{d-1} v_i$ for $i = 1, 2, \ldots, k$. Note that T' has the same order and diameter as T.

We show that T' has a larger eccentric connectivity index than T.

$$\xi^C(T) = \sum_{i=1}^k \mathrm{ec}_T(v_i) \deg_T(v_i) + \mathrm{ec}_T(u) \deg_T(u) + (d-1) \deg_T(x_{d-1}) + N$$

$$\leq k \cdot (d)(1) + \mathrm{ec}_T(u)(r+k) + (d-1) \deg_T(x_{d-1}) + N,$$

where $N = \sum_{x \in V(T)-\{v_1,v_2,\ldots,v_k,u,x_{d-1}\}} \mathrm{ec}_T(x) \deg_T(x)$.

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In comparison,

$$\xi^C(T') = k \cdot (d)(1) + \mathrm{ec}_T(u)\, r + (d-1)(k + \deg_T(x_{d-1})) + N.$$

So, since $\mathrm{ec}(u) \leq d - 1$,

$$\xi^C(T') - \xi^C(T) \geq -k\,\mathrm{ec}_T(u) + k(d-1) \geq 0.$$

Continue this procedure, forming new trees, until all the end vertices in $V(T) - \{x_0\}$ are adjacent to x_{d-1}. Thus, a broom $B_{n,d}$ is obtained, of order n and diameter d, with the property that $\xi^C(B_{n,d}) \geq \xi^C(T)$. This completes the proof. $\qquad\square$

Theorem 2.7 *If T is a tree of order $n \geq 3$ and diameter d, then*

$$\xi^C(T) \geq \xi^C(V_{n,d}). \tag{2.8}$$

Proof. The inequality (2.8) holds if $n = 3$ or 4. It also holds if $d = n - 1$, since in this case $T = V_{n,d} = P_n$, i.e., T is a path. Let us assume that there exists a tree T with $\xi^C(T) < \xi^C(V_{n,d})$, where d is the diameter of T and, of such counterexamples to (2.8), choose T to have the smallest possible order, n.

Let $P : x_0, x_1, \ldots, x_d$ be a diametral path in T. Since T is not the path graph, let x be an end vertex in $V(T) - V(P)$. Label as y the vertex adjacent to x, and let $T' = T - x$. Then, since $n(T') < n(T)$ we have

$$\xi^C(T') \geq \xi^C(V_{n-1,d}) \quad \text{while} \quad \xi^C(T) < \xi^C(V_{n,d}).$$

Hence $\xi^C(T) - \xi^C(T') < \xi^C(V_{n,d}) - \xi^C(V_{n-1,d}) \leq \begin{cases} d+1 & \text{for } d \text{ even} \\ d+2 & \text{for } d \text{ odd}. \end{cases}$

However,
$$\xi^C(T) - \xi^C(T') \geq ec(x) \cdot 1 + ec(y) \cdot 1$$

$$\geq (\lceil d/2 \rceil + 1) + \lceil d/2 \rceil$$

$$\geq \begin{cases} d+1 & \text{for } d \text{ even} \\ \\ d+2 & \text{for } d \text{ odd.} \end{cases}$$

This is a contradiction, and the theorem is proven.   □

An extension of the result of Theorem 2.7 will be presented in the next chapter.[1]

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[1]We remark that soon after the publication of the results presented in this chapter, we learnt that [22, 79, 81] also independently, obtained results similar to some of our bounds.

Chapter 3

A Lower Bound on the Eccentric Connectivity Index

3.1 Introduction

In the previous chapter, we presented a tight lower bound on the eccentric connectivity index for a tree, in terms of order and diameter. We proved that if T is a tree of order $n \geq 3$ and diameter d, then

$$\xi^C(T) \geq \xi^C(V_{n,d}). \tag{3.1}$$

In this chapter we generalize this result, proving that the volcano graph, $V_{n,d}$, achieves the lowest value for the eccentric connectivity index over all general graphs (rather than only trees), of fixed order n and diameter d. (See [59].)

This simple generalization has been quite challenging to prove. The difficulty in achieving the sharp bound lies with some 'problem vertices'.

From Claim 1.1 and the observation that the eccentricity of any vertex is bounded below by the radius of the graph, we have that

$$\text{for all vertices } w \in V(G), \quad ec(w) \geq \lceil d/2 \rceil. \tag{3.2}$$

The problem vertices have degree two, and precisely meet this eccentricity lower

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bound.

Notation

Given a connected graph G with diameter d, we denote by $t(G)$ the number of vertices in G of degree 2 and eccentricity precisely $\lceil d/2 \rceil$, i.e.,

$$t(G) := |\{x \in V(G) \mid \deg(x) = 2 \text{ and } \mathrm{ec}(x) = \lceil d/2 \rceil\}|.$$

Consider a connected graph G of order n and diameter d. If $d = 2$, note that from Theorem 2.1, $\xi^C(G) \geq \xi^C(S_n) = \xi^C(V_{n,2})$.

Hence from now onwards in this chapter, we only consider $d \geq 3$.

Theorem 3.1 *Let $G = (V, E)$ be a connected graph of order n, and diameter $d \geq 3$. Then*

$$\xi^C(G) \geq \xi^C(V_{n,d}).$$

Proof.

Due to the complexity of this proof, we subdivide it into two parts, according to whether G contains at least one problem vertex (Part A), or has none (Part B). In Part A, we subdivide the proof further, when the diameter is even or odd.

3.2 Eccentric Connectivity Index in the Presence of Problem Vertices

Part A

We first prove that the theorem holds when G contains at least one problem vertex. So, assume that $t(G) \geq 1$. We must show that $\xi^C(G) \geq \xi^C(V_{n,d})$.

Suppose, to the contrary, that there exists a counterexample G, for which $t(G) \geq 1$ and

$$\xi^C(G) < \xi^C(V_{n,d}). \tag{3.3}$$

Of all such counterexamples, choose G to have the smallest possible order, n. Hence, any graph G' with diameter d', at least one problem vertex, and $n' < n$ vertices, will satisfy

$$\xi^C(G') \geq \xi^C(V_{n',d'}).\tag{3.4}$$

Let $P : v_0, v_1, \ldots, v_d$ be a diametral path in G, and define $S = V - V(P)$.

We will need two general properties of the distance from a vertex $w \in G$ to v_0 or v_d, for any arbitrary graph G.

For all vertices $w \in V(G)$, $\quad d(w, v_0) \geq \lceil d/2 \rceil$ or $d(w, v_d) \geq \lceil d/2 \rceil$. $\tag{3.5}$

To see that (3.5) holds, suppose, by contradiction, that both $d(w, v_0) < \lceil d/2 \rceil$ and $d(w, v_d) < \lceil d/2 \rceil$. By the triangle inequality, $d = d(v_0, v_d) \leq d(v_0, w) + d(w, v_d)$ which implies

$$d \leq (\lceil d/2 \rceil - 1) + (\lceil d/2 \rceil - 1) = 2 \lceil d/2 \rceil - 2 = \begin{cases} d - 2 & \text{for } d \text{ even} \\ \\ d - 1 & \text{for } d \text{ odd,} \end{cases}$$

which is impossible, and (3.5) is proven.

It follows from the definition of eccentricity, and (3.5), that

for $w \in V(G)$, if $\mathrm{ec}(w) = \lceil d/2 \rceil$, then $d(w, v_0) = \lceil d/2 \rceil$ or $d(w, v_d) = \lceil d/2 \rceil$. $\tag{3.6}$

We will apply these two general properties of graphs to our counterexample graph G.

Claim **3.1** *There are no end vertices in S.*

Proof of Claim 3.1: Suppose to the contrary, that S contains an end vertex x, and let y be the neighbour of x. Form G' by removing the vertex x, viz. set $G' = G - x$.

Fact 3.1 *(i) The diameter of G' is d, since x is not on the diametral path P.*

(ii) $n(G') = n - 1 < n(G)$.

(iii) $t(G') \geq 1$.

To establish (iii), we show that G' indeed has a problem vertex. Since $t(G) \geq 1$, let z be a problem vertex of G, i.e., $\deg_G(z) = 2$ and $\mathrm{ec}_G(z) = \lceil d/2 \rceil$. We first show that $z \neq y$. If z is equal to y, then $\deg_G(y) = 2$. Let w be the other neighbour of y. Note that any path from $\{v_0, v_d\}$ to y must pass through w. We can assume, without loss of generality, that $d_G(w, v_d) \geq d_G(w, v_0)$. Then, by (3.5),

$$\mathrm{ec}_G(y) \ \geq \ d_G(y, v_d) \ = \ d_G(y, w) + d_G(w, v_d) \ \geq \ 1 + \lceil d/2 \rceil,$$

and this contradicts the fact that $\mathrm{ec}_G(y) = \mathrm{ec}_G(z) = \lceil d/2 \rceil$. Thus, $z \neq y$, and this implies that $\deg_{G'}(z) = 2$.

Since $\mathrm{ec}_G(z) = \lceil d/2 \rceil$, (3.6) implies that in G, z is at distance $\lceil d/2 \rceil$ from one of v_0 or v_d, say, v_d. Then, since x is not on any such shortest path between z and v_d, $\lceil d/2 \rceil = d_G(z, v_d) = d_{G'}(z, v_d)$. So, $\mathrm{ec}_{G'}(z) \geq \lceil d/2 \rceil$. But the removal of an end vertex cannot increase the eccentricity of any other vertex in the graph ($\mathrm{ec}_{G'}(z) \leq \mathrm{ec}_G(z)$), so we conclude that $\mathrm{ec}_{G'}(z) = \lceil d/2 \rceil$, and hence z is a problem vertex of G'. This completes the proof of Fact 3.1.

From Fact 3.1, G' is not a counterexample, and thus by (3.4)

$$\xi^C(G') \ \geq \ \xi^C(V_{n-1,d}). \tag{3.7}$$

Note that for all $u \in V(G') - \{y\}$, $\deg_G(u) = \deg_{G'}(u)$, and $\mathrm{ec}_G(u) \geq \mathrm{ec}_{G'}(u)$. Also, $\mathrm{ec}_G(y) = \mathrm{ec}_{G'}(y)$. These observations, as well as (3.2), imply

$$\xi^C(G) - \xi^C(G') \ \geq \ \deg_G(x)\,\mathrm{ec}_G(x) + \deg_G(y)\,\mathrm{ec}_G(y) - \deg_{G'}(y)\,\mathrm{ec}_{G'}(y)$$

$$= \ 1 \cdot \mathrm{ec}_G(x) + \deg_G(y)\,\mathrm{ec}_G(y) - (\deg_G(y) - 1)\,\mathrm{ec}_{G'}(y)$$

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$$= \mathrm{ec}_G(x) + 1 \cdot \mathrm{ec}_G(y)$$

$$\geq (\lceil d/2 \rceil + 1) + \lceil d/2 \rceil$$

$$= 2(\lceil d/2 \rceil) + 1.$$

Thus

$$\xi^C(G') + 2(\lceil d/2 \rceil) + 1 \leq \xi^C(G).$$

Combining this with (3.7) yields

$$\xi^C(V_{n-1,d}) + 2(\lceil d/2 \rceil) + 1 \leq \xi^C(G),$$

and since G is a counterexample, (3.3) gives

$$\xi^C(V_{n-1,d}) + 2(\lceil d/2 \rceil) + 1 \leq \xi^C(G) < \xi^C(V_{n,d}). \tag{3.8}$$

But, straightforward calculations yield

$\xi^C(V_{n-1,d}) + 2(\lceil d/2 \rceil) + 1$

$$= \begin{cases} (n-1)(d+1) + d^2/2 - 2d - 1 + (d+1) & \text{for } d \text{ even} \\ \\ (n-1)(d+2) + d^2/2 - 3d - 3/2 + (d+2) & \text{for } d \text{ odd} \end{cases}$$

$$= \begin{cases} n(d+1) + d^2/2 - 2d - 1 & \text{for } d \text{ even} \\ \\ n(d+2) + d^2/2 - 3d - 3/2 & \text{for } d \text{ odd} \end{cases}$$

$$= \xi^C(V_{n,d}).$$

So (3.8) reduces to $\xi^C(V_{n,d}) < \xi^C(V_{n,d})$, a contradiction. Therefore, Claim 3.1 is proven.

Fact 3.2 *Every vertex in G has degree at least 2, except possibly for v_0 and v_d.*

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To see that Fact 3.2 holds, recall that $V = S \cup \{v_1, v_2, \ldots, v_{d-1}\} \cup \{v_0, v_d\}$. Then, observe that by Claim 3.1, every vertex in S has degree at least 2. Also, for every v_i, $i = 1, \ldots, (d-1)$, on P, we have $\deg(v_i) \geq 2$, and hence, Fact 3.2 is established.

We now look at two cases separately, depending on the parity of d. In each case we will partition the vertex set of the counterexample graph G into several sets, in order to calculate a lower bound on the eccentric connectivity index of G in terms of the index value of the volcano graph $V_{n,d}$, to thus arrive at a contradiction.

3.2.1 Even Diameter

CASE 1 d is even

Here $\lceil d/2 \rceil = d/2$. Let Q be the set of problem vertices, i.e.,

$$Q := \{x \in V(G) \mid \deg(x) = 2, \; \mathrm{ec}(x) = d/2\}.$$

Claim 3.2 Every vertex $u \in Q$ is adjacent to some vertex u' satisfying

$$\mathrm{ec}(u') \geq (d/2) + 1.$$

Proof of Claim 3.2: Consider a problem vertex $u \in Q$. Since $\mathrm{ec}(u) = \lceil d/2 \rceil$, (3.6) implies that u is at a distance $d/2$ from one of v_0 or v_d, say, v_d. Consider a shortest path connecting u and v_d : $u, u_1, u_2, \ldots, v_d$. Since $d(u, v_d) = d/2$, and $u, u_1, u_2, \ldots, v_d$ is a shortest path, then $d(u_1, v_d) = (d/2) - 1$. We show that $d(u_1, v_0) \geq (d/2) + 1$. If not, then by the triangle inequality,

$$d = d(v_0, v_d) \leq d(v_0, u_1) + d(u_1, v_d) \leq (d/2) + ((d/2) - 1) = d - 1$$

which is impossible. Thus, $d(u_1, v_0) \geq (d/2) + 1$, and hence $\mathrm{ec}(u_1) \geq (d/2) + 1$. Setting $u' = u_1$, completes the proof of Claim 3.2.

For every $u \in Q$, choose a vertex u' as found in Claim 3.2, and denote it by $f(u)$.

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Let $Q' := \{f(u) \mid u \in Q\}$, and set $|Q| = q$ and $|Q'| = q'$. Since the mapping $f(u) = u'$ is not necessarily injective, we have that $q' \leq q$.

Observe that Claim 3.2 gives $\text{ec}(f(u)) \geq (d/2) + 1$, and this implies that Q' cannot contain any problem vertices. Therefore, $Q \cap Q' = \emptyset$.

Fact 3.3 $\deg(u') \geq 2$ *for all* $u' \in Q'$.

To prove this fact, it suffices, by Fact 3.2, to show that if $u' \in Q'$, then $u' \notin \{v_0, v_d\}$. Suppose, to the contrary, that $u' \in \{v_0, v_d\}$. Then $\text{ec}(u') = d$. Also, since $u' \in Q'$, u' is a neighbour of some problem vertex $u \in Q$. Thus $|\text{ec}(u') - \text{ec}(u)| \leq 1$, i.e., $|d - d/2| \leq 1$, which contradicts the fact that $d \geq 3$. Hence, Fact 3.3 is proven.

We now find a lower bound for $\sum_{w \in Q'} \text{ec}(w) \deg(w)$.

By Fact 3.3, $\sum_{w \in Q'} \deg(w) \geq 2 q'$. On the other hand, since every vertex in Q is adjacent to some vertex in Q', we have $\sum_{w \in Q'} \deg(w) \geq q$. Summing these two inequalities gives $2 \sum_{w \in Q'} \deg(w) \geq 2 q' + q$. Therefore,

$$\sum_{w \in Q'} \deg(w) \geq q' + q/2. \tag{3.9}$$

For $w \in Q'$, by Claim 3.2, we have that $\text{ec}(w) \geq (d/2) + 1$. This, in conjunction with (3.9), yields

$$
\begin{aligned}
\sum_{w \in Q'} \text{ec}(w) \deg(w) &\geq \sum_{w \in Q'} ((d/2) + 1) \deg(w) \\
&= ((d/2) + 1) \sum_{w \in Q'} \deg(w) \\
&\geq ((d/2) + 1) (q' + q/2).
\end{aligned}
$$

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Hence, from the definition of Q, and the above inequality, we have

$$
\begin{aligned}
\sum_{v \in (Q \cup Q')} ec(v) \deg(v) &= \sum_{v \in Q} ec(v) \deg(v) + \sum_{w \in Q'} ec(w) \deg(w) \\
&\geq 2q\,(d/2) + ((d/2) + 1)\,(q' + q/2) \\
&= q \cdot ((5d+2)/4) + q' \cdot ((d/2) + 1).
\end{aligned} \tag{3.10}
$$

Next, set $P' := \{v_0, \ldots, v_{(d/2)-2},\ v_{(d/2)+2}, \ldots, v_d\}$. (If $d = 4$, then $P' := \{v_0, v_4\}$.)

It can be seen that Q, Q' and P' are all pairwise disjoint. Note that $|P'| = d - 2$.

A bound for the eccentric connectivity index of P' can be found by direct calculation. If $d \geq 6$ we have:

$$
\begin{aligned}
\sum_{v \in P'} ec(v) \deg(v) &= ec(v_0) \deg(v_0) + ec(v_d) \deg(v_d) \\
&\quad + \sum_{i=1}^{(d/2)-2} ec(v_i) \deg(v_i) + \sum_{i=(d/2)+2}^{d-1} ec(v_i) \deg(v_i) \\
&\geq d \cdot 1 + d \cdot 1 + 2 \sum_{i=1}^{(d/2)-2} (d - i) \cdot 2 \\
&= 2d + 4 \cdot \sum_{i=1}^{(d/2)-2} (d - i) \\
&= 3\,d^2/2 - 3d - 4.
\end{aligned} \tag{3.11}
$$

(And if $d = 4$, (3.11) still holds.)

Define $S' = V - (P' \cup Q \cup Q')$.

Since v_0, $v_d \in P'$, then v_0, $v_d \notin S'$, and it follows from Fact 3.2 that S' has no end vertices. This allows us to partition S' as follows:

let $A = \{x \in S' \mid \deg(x) = 2\}$, $B = \{x \in S' \mid \deg(x) \geq 3\}$. Setting $|A| = a$, and $|B| = b$, we obtain

$$
a + b + (d - 2) + q + q' = n. \tag{3.12}
$$

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Combining (3.2) with the fact that there are no problem vertices in S', we have that for all vertices x in A, $ec(x) \geq (d/2) + 1$. Applying this inequality, (3.2), (3.10) and (3.11), we calculate

$$
\begin{aligned}
\xi^C(G) \;=\; & \sum_{x \in A} ec(x) \deg(x) \;+\; \sum_{u \in B} ec(u) \deg(u) \\
& + \sum_{v \in P'} ec(v) \deg(v) \;+\; \sum_{v \in Q} ec(v) \deg(v) \;+\; \sum_{w \in Q'} ec(w) \deg(w)
\end{aligned}
$$

$$
\begin{aligned}
\geq \;\; & 2a\,(d/2 + 1) + 3b\,(d/2) + (3\,d^2/2 - 3d - 4) + q \cdot ((5d + 2)/4) + q' \cdot ((d/2) + 1) \\
= \;\; & a\,(d + 2) + b\,(3d/2) + (3\,d^2/2 - 3d - 4) + q\,((5d + 2)/4) + q'\,(\tfrac{1}{2}d + 1). \quad (3.13)
\end{aligned}
$$

We will minimize (3.13) by optimizing the coefficients a, b, q and q' in two stages. First, recall that $q' \leq q$. Fixing a and b, the sum of the last two terms in (3.13) is as small as possible when q' is as large as possible, i.e., when $q' = q$. This gives

$$
\xi^C(G) \geq a(d + 2) + b(3d/2) + (3/2)\,d^2 - 3d - 4 + q \cdot ((7d + 6)/4), \qquad (3.14)
$$

and now (3.12) has been reduced to $a + b + 2q = n - d + 2$.

Second, if $d \geq 4$, (3.14) is minimized for $b = 0$, $q = 0$, and $a = n - d + 2$. Thus,

$$
\begin{aligned}
\xi^C(G) \;\geq\; & (n - d + 2)(d + 2) + (3/2)\,d^2 - 3d - 4 \\
= \;\; & n(d + 1) + n - d^2 - 2d + 2d + 4 + (3/2)\,d^2 - 3d - 4 \\
= \;\; & n(d + 1) + d^2/2 - 2d - 1 + n - d + 1 \\
= \;\; & \xi^C(V_{n,d}) + n - d + 1.
\end{aligned}
$$

Since $n \geq d + 1 > d - 1$, we have $\xi^C(G) \geq \xi^C(V_{n,d}) + n - d + 1 > \xi^C(V_{n,d})$, which contradicts (3.3). It follows that for d even, $\xi^C(G) \geq \xi^C(V_{n,d})$.

Continuing in Part A, we now turn to the case with d odd.

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3.2.2 Odd Diameter

CASE 2 d is odd

Here $\lceil d/2 \rceil = (d+1)/2$. In this case, a class of problem vertices with both neighbours in the centre of the graph, will require special attention. So, it will now be necessary to partition the vertex set of the counterexample graph G into even more sets than were needed in the d even case.

Let $R = \{x \in V \mid \deg(x) = 2, \ ec(x) = \lceil d/2 \rceil\}$. So R is the set of problem vertices of G, and clearly, $|R| = t \geq 1$.

Partition R as follows: $R = Q \cup H$, where

$Q := \{x \in R \mid x \text{ is adjacent to a vertex outside } C(G)\}$ and

$H := \{x \in R \mid \text{both neighbours of } x \text{ are in } C(G)\}$.

Since they partition R, we have that

$$Q \cap H = \emptyset. \tag{3.15}$$

Claim 3.3 Every vertex $u \in Q$ is adjacent to some vertex u' satisfying

$$ec(u') \geq ((d+1)/2) + 1.$$

Proof of Claim 3.3: Consider $u \in Q$. By the definition of Q, the problem vertex u is adjacent to a vertex, u', which is not a central vertex. So, $ec(u') \geq (d+1)/2 + 1$, and Claim 3.3 is proven.

For every $u \in Q$, choose a vertex u' as found in Claim 3.3, and denote it by $f(u)$.

Let $Q' := \{f(u) \mid u \in Q\}$, and set $|Q| = q$ and $|Q'| = q'$. Since the mapping $f(u) = u'$ is not necessarily injective, we have that $q' \leq q$. Also, Claim 3.3 gives $ec(f(u)) \geq ((d+1)/2) + 1$, while all vertices in Q have eccentricity $(d+1)/2$, so

$$Q \cap Q' = \emptyset. \tag{3.16}$$

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Claim **3.4**

$$\sum_{w \in Q'} \text{ec}(w) \ \deg(w) \ \geq \ q((d+3)/4) + q'((d+3)/2) - 3. \qquad (3.17)$$

Proof of Claim 3.4: Since every vertex in Q is adjacent to some vertex in Q', we have

$$\sum_{w \in Q'} \deg(w) \geq |Q| = q. \qquad (3.18)$$

Then, Claim 3.3 and (3.18) give

$$\sum_{w \in Q'} \text{ec}(w) \ \deg(w) \ \geq \ (((d+1)/2) + 1) \ q. \qquad (3.19)$$

Observe that by Fact 3.2, Q' can contain at most 2 end vertices, possibly v_0 or v_d. We look at three cases, separately:

(i) If Q' contains no end vertices, then $\sum_{w \in Q'} \deg(w) \geq \sum_{w \in Q'} 2 \ = \ 2q'$. Summing this inequality with (3.18) gives $2 \sum_{w \in Q'} \deg(w) \geq q + 2q'$, and therefore

$\sum_{w \in Q'} \deg(w) \geq q/2 + q'$. From this result, and Claim 3.3, it follows that

$$
\begin{aligned}
\sum_{w \in Q'} \text{ec}(w) \ \deg(w) \ &\geq \ \sum_{w \in Q'} (((d+1)/2) + 1) \ \deg(w) \\
&\geq \ (((d+1)/2) + 1) \ (q/2 + q') \\
&= \ q((d+3)/4) + q'((d+3)/2) \\
&> \ q((d+3)/4) + q'((d+3)/2) - 3
\end{aligned}
$$

and (3.17) holds for case (i).

(ii) If Q' contains exactly one end vertex, say, without loss of generality, v_0, then, by Claim 3.3,

$$\sum_{w \in Q'} \text{ec}(w) \ \deg(w) \ = \ \text{ec}(v_0) \deg(v_0) + \sum_{w \in Q' - \{v_0\}} \text{ec}(w) \ \deg(w)$$

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$$\geq d \cdot 1 + 2 \cdot (q' - 1)(((d+1)/2) + 1).$$

Summing this with (3.19) gives

$$2 \sum_{w \in Q'} \text{ec}(w) \deg(w) \geq d + 2 \cdot (q' - 1)((d+1)/2 + 1) + q\left(((d+1)/2) + 1\right)$$

$$= q'(d+3) + q((d+3)/2) - 3$$

and this simplifies to

$$\sum_{w \in Q'} \text{ec}(w) \deg(w) \geq q((d+3)/4) + q'((d+3)/2) - 3/2$$

$$> q((d+3)/4) + q'((d+3)/2) - 3$$

and (3.17) holds for case (ii).

The final case is

(iii) if both v_0 and v_d are in Q', and they both have degree 1. Proceeding as in case (ii), we have that

$$\sum_{w \in Q'} \text{ec}(w) \deg(w) \geq 2d + 2 \cdot (q' - 2)(((d+1)/2) + 1).$$

Summing this with (3.19) gives

$$2 \sum_{w \in Q'} \text{ec}(w) \deg(w) \geq 2d + 2 \cdot (q' - 2)((d+1)/2 + 1) + q((d+3)/2)$$

and this simplifies to

$$\sum_{w \in Q'} \text{ec}(w) \deg(w) \geq q((d+3)/4) + q'((d+3)/2) - 3,$$

which completes case (iii), and hence, Claim 3.4 is proven.

Thus, from the fact that $Q \subseteq R$, and Claim 3.4,

$$\sum_{v \in (Q \cup Q')} \text{ec}(v) \deg(v) = \sum_{v \in Q} \text{ec}(v) \deg(v) + \sum_{v \in Q'} \text{ec}(v) \deg(v)$$

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$$\geq \quad 2q((d+1)/2) + q((d+3)/4) + q'((d+3)/2) - 3$$

$$= \quad q((5d+7)/4) + q'((d+3)/2) - 3. \tag{3.20}$$

Next we consider the extra vertex set H and define its neighbourhood, $H' :=$ $N(H)$. Note that by the definition of H, $N(H) \subseteq C(G)$. Set $|H| = h$ and $|H'| = h'$. Since each vertex in H has degree 2, and H' is the neighbourhood of H, we have that $h' \leq 2h$. Also note that by Claim 3.3, $\text{ec}(u') \geq ((d+1)/2) + 1$, for each $u' \in Q'$; whereas all the vertices in H, and in H' are central vertices. This implies that

$$Q' \cap (H \cup H') = \emptyset. \tag{3.21}$$

In order to find a bound on the degrees of the vertices in H', we need the following two claims.

Claim **3.5** *Let $x \in H$. Then its two neighbours each have degree at least 3.*

Proof of Claim 3.5: Let w and y be the two neighbours of x. So, by the definition of H, they are both central vertices, i.e., $\text{ec}(w) = (d+1)/2 = \text{ec}(y)$. This immediately implies

$$d(w, v_0), \quad d(w, v_d) \leq (d+1)/2. \tag{3.22}$$

Also, by (3.6) we have that y lies at a distance $(d+1)/2$ from v_0 or v_d. Assume, without loss of generality, that

$$d(y, v_d) = (d+1)/2. \tag{3.23}$$

First, we show that $d(w, v_0) \geq (d-1)/2$. If not, then by (3.22) and the triangle inequality

$$d = d(v_0, v_d) \leq d(v_0, w) + d(w, v_d) \leq ((d-1)/2 - 1) + ((d+1)/2) = d - 1,$$

which is impossible. So,

$$d(w, v_0) \geq (d-1)/2. \tag{3.24}$$

Similarly,

$$d(w, v_d) \geq (d-1)/2. \tag{3.25}$$

Now, continuing the proof of Claim 3.5, assume by contradiction, that $\deg(y) \leq 2$.

Since $y \in C(G)$, $y \neq v_0$, v_d, and hence, by Fact 3.2, $\deg(y) \neq 1$.

It follows that $\deg(y) = 2$. Then label as z, the second neighbour of y.

If $z = w$, then w is a cut-vertex, since its removal would disconnect the edge xy from the rest of the graph. Thus, every path from $\{v_0, v_d\}$ to y must go through w. But then (3.5) implies that $\mathrm{ec}(y) \geq 1 + \max\{d(w, v_0), d(w, v_d)\} \geq 1 + (d+1)/2$, which contradicts the fact that $\mathrm{ec}(y) = (d+1)/2$. So, $z \neq w$.

Next, by (3.24) and (3.25), any shortest path from $\{v_0, v_d\}$ to y which goes through w and x, has length at least $(d-1)/2 + d(w, x) + d(x, y) = (d+1)/2 + 1$. Hence, since $\mathrm{ec}(y) = (d+1)/2$, we have that any shortest $\{v_0, v_d\}$ to y path cannot pass through w and x. Note again that since $y \in C(G), y \neq v_0, v_d$. Hence, any shortest path from y to $\{v_0, v_d\}$ must pass through z. Thus, from (3.23), and since any shortest $y - v_d$ path must pass through z, we have that $d(z, v_d) = (d+1)/2 - 1$. However, this then gives that $d(z, v_0) \geq (d+1)/2$, since otherwise, by the triangle inequality

$$d = d(v_0, v_d) \leq d(v_0, z) + d(z, v_d) \leq ((d+1)/2 - 1) + (((d+1)/2) - 1) = d - 1$$

which is impossible. So, $d(z, v_0) \geq (d+1)/2$, which in turn implies that a shortest $y - v_0$ path which passes through z must have length at least $((d+1)/2) + 1$, contrary to the fact that $\mathrm{ec}(y) = (d+1)/2$. Therefore, a shortest $v_0 - y$ path cannot pass through z, a contradiction. So, $\deg(y) \neq 2$.

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Thus, $\deg(y) \nleq 2$, i.e., $\deg(y) \geq 3$. By an equivalent argument, $\deg(w) \geq 3$, which completes the proof of Claim 3.5.

From Claim 3.5 we have that all the vertices of H' have degree at least 3; whereas all the vertices in H and Q have degree 2, since they are problem vertices. Thus,

$$H' \cap (Q \cup H) = \emptyset. \tag{3.26}$$

Summarizing, thus far, by (3.15), (3.16), (3.21) and (3.26) we have shown that Q, Q', H and H' are all pairwise disjoint.

Claim **3.6** $\sum_{x \in H'} \deg(x) \geq h + (3/2)h'$.

Proof of Claim 3.6: On the one hand, since by Claim 3.5, $\deg(x) \geq 3$, for all $x \in H'$, we have that $\sum_{x \in H'} \deg(x) \geq 3h'$. On the other hand, since every vertex in H has two neighbours in H', we have $\sum_{x \in H'} \deg(x) \geq 2h$. Summing these two inequalities, we get $2 \sum_{x \in H'} \deg(x) \geq 2h + 3h'$, and upon division by 2, Claim 3.6 is proven.

Claim 3.6, and the definitions of H and H', give a lower bound for the eccentric connectivity index over $H \cup H'$ as follows:

$$\begin{aligned}
\sum_{x \in (H \cup H')} \mathrm{ec}(x)\deg(x) &= \sum_{x \in H} \mathrm{ec}(x)\deg(x) + \sum_{x \in H'} \mathrm{ec}(x)\deg(x) \\
&= h((d+1)/2) \cdot 2 + ((d+1)/2) \sum_{x \in H'} \deg(x) \\
&\geq h(d+1) + ((d+1)/2)(h + (3/2)h') \\
&= h(3(d+1)/2) + h'(3(d+1)/4). \tag{3.27}
\end{aligned}$$

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Next, set $P' := \{v_0, \ldots, v_{(d-5)/2}, v_{(d+5)/2}, \ldots, v_d\}$. (If $d = 3$, then $P' := \emptyset$; whereas if $d = 5$, then $P' := \{v_0, v_5\}$.)

It can be seen that $P' \cap (Q \cup Q' \cup H \cup H') = \emptyset$. Note that $|P'| = d - 3$.

A bound for the eccentric connectivity index of P' can be found by direct calculation. If $d \geq 7$, we have:

$$
\begin{aligned}
\sum_{v \in P'} \mathrm{ec}(v)\deg(v) \;=\;& \mathrm{ec}(v_0)\deg(v_0) \;+\; \mathrm{ec}(v_d)\deg(v_d) \\[2mm]
& +\; \sum_{i=1}^{(d-5)/2} \mathrm{ec}(v_i)\deg(v_i) \;+\; \sum_{i=(d+5)/2}^{d-1} \mathrm{ec}(v_i)\deg(v_i) \\[2mm]
\geq\;& d \cdot 1 + d \cdot 1 + 2 \sum_{i=1}^{(d-5)/2} (d-i) \cdot 2 \\[2mm]
=\;& 2d + 4 \cdot \sum_{i=1}^{(d-5)/2} (d-i) \\[2mm]
=\;& 3\,d^2/2 - 4d - 15/2.
\end{aligned}
\tag{3.28}
$$

(And (3.28) also holds for $d = 5$.)

For $d = 3$, we have

$$
\sum_{v \in P'} \mathrm{ec}(v)\deg(v) \;=\; 0.
\tag{3.29}
$$

Define $S' = V - (Q \cup Q' \cup H \cup H' \cup P')$.

For now, assume that $d \geq 5$. (We will consider the case for $d = 3$, below.) Since $v_0, v_d \in P'$, then $v_0, v_d \notin S'$. It follows from Fact 3.2, that S' has no end vertices, and this allows us to partition S' as follows:

let $A = \{x \in S' \mid \deg(x) = 2\}, \quad B = \{x \in S' \mid \deg(x) \geq 3\}$. Setting $|A| = a$, and $|B| = b$, we obtain

$$
a + b + q + q' + h + h' + (d - 3) = n.
\tag{3.30}
$$

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Combining (3.2) with the fact that there are no problem vertices in S', we have that for all vertices x in A, $\mathrm{ec}(x) \geq ((d+1)/2) + 1$.

Applying this inequality, and (3.2), an upper bound for the index over the vertices of S' is

$$\sum_{x \in A} \mathrm{ec}(x)\deg(x) \; + \; \sum_{u \in B} \mathrm{ec}(u)\deg(u) \;\; \geq \;\; 2a((d+1)/2+1) + 3b((d+1)/2)$$

$$= \; a(d+3) + b(3(d+1)/2).$$

Combining this inequality, (3.20), (3.27) and (3.28) we have

$$\xi^C(G) \;=\; \sum_{x \in A} \mathrm{ec}(x)\deg(x) \;+\; \sum_{u \in B} \mathrm{ec}(u)\deg(u)$$

$$+ \sum_{v \in Q} \mathrm{ec}(v)\deg(v) \;+\; \sum_{w \in Q'} \mathrm{ec}(w)\deg(w) \;+\; \sum_{v \in H} \mathrm{ec}(v)\deg(v)$$

$$+ \sum_{v \in H'} \mathrm{ec}(v)\deg(v) \;+\; \sum_{v \in P'} \mathrm{ec}(v)\deg(v)$$

$$\geq \; a(d+3) + b(3(d+1)/2) + q((5d+7)/4) + q'((d+3)/2) - 3$$

$$+ h(3(d+1)/2) + h'(3(d+1)/4) \;+\; 3\,d^2/2 - 4d - 15/2. \qquad (3.31)$$

We will minimize (3.31) by optimizing the coefficients a, b, q, q', h, and h' in three stages. First, recall that $q' \leq q$. Fixing a, b, h and h', (3.31) is as small as possible when q' is as large as possible, i.e., when $q' = q$. This gives

$$\xi^C(G) \;\geq\; a(d+3) + b(3(d+1)/2) + q((7d+13)/4) - 3$$

$$+ h(3(d+1)/2) + h'(3(d+1)/4) \;+\; 3\,d^2/2 - 4d - 15/2 \qquad (3.32)$$

and now (3.30) has been reduced to

$$a + b + 2q + h + h' = n - d + 3. \qquad (3.33)$$

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Second, recall that $h' \leq 2h$. Fixing a, b and q, (3.32) is as small as possible when h' is as large as possible, i.e., when $h' = 2h$. This gives

$$
\begin{aligned}
\xi^C(G) \;\geq\; & a(d+3) + b(3(d+1)/2) + q((7d+13)/4) - 3 \\
& + h\,(3(d+1)) + 3\,d^2/2 - 4d - 15/2
\end{aligned}
\tag{3.34}
$$

and now (3.33) has been reduced to $\;a + b + 2q + 3h = n - d + 3$.

Third, if $d \geq 3$, (3.34) is minimized for $b = q = h = 0$ and $a = n - d + 3$, to give

$$
\begin{aligned}
\xi^C(G) \;\geq\; & (n - d + 3)(d+3) - 3 + (3/2)\,d^2 - 4d - 15/2 \\
=\; & n(d+2) + d^2/2 - 3d - 3/2 + n - d \\
=\; & \xi^C(V_{n,d}) + n - d.
\end{aligned}
$$

Since $n \geq d + 1 \geq d$, we have $\xi^C(G) \geq \xi^C(V_{n,d}) + n - d \geq \xi^C(V_{n,d})$, which contradicts (3.3), and Case 2, for $d \geq 5$ odd, is complete.

Now, assume that $d = 3$. Here we partition S' as $\;S' = F \cup A \cup B$, where $F = \{v_0, v_3\}$, and where A and B are defined as previously, i.e., $A = \{x \in S' \mid \deg(x) = 2\}$, $B = \{x \in S' \mid \deg(x) \geq 3\}$. Setting $|A| = a$, and $|B| = b$, we obtain

$$
2 + a + b + q + q' + h + h' + 0 = n.
\tag{3.35}
$$

Notice that $\displaystyle\sum_{x \in F} \mathrm{ec}(x)\deg(x) \geq d + d$.

Using this, (3.29), and as in (3.31), we get

$$
\begin{aligned}
\xi^C(G) \;\geq\; & a(d+3) + b(3(d+1)/2) + q((5d+7)/4) + q'((d+3)/2) - 3 \\
& + h(3(d+1)/2) + h'(3(d+1)/4) + 0 + 2d.
\end{aligned}
\tag{3.36}
$$

Minimizing as above, after the second stage, (3.35) reduces to

$$
a + b + 2q + 3h = n - 2.
$$

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Then, for the third stage, we set $b = q = h = 0$ and $a = n - 2$. Thus, (3.36) becomes

$$\begin{aligned} \xi^C(G) &\geq (n-2)(d+3) - 3 + 2d \\ &= 6n - 9 \\ &= \xi^C(V_{n,3}) + n - d, \end{aligned}$$

and as above, we get a contradiction to (3.3). Thus, Case 2, for $d = 3$, is complete.

This concludes the proof for Part A, and we have shown that for $t(G) \geq 1$,

$$\xi^C(G) \geq \xi^C(V_{n,d}).$$

3.3 Eccentric Connectivity Index in the Absence of Problem Vertices

PART B

The remaining part of the proof of the theorem is for $t(G) = 0$ (no problem vertices). The proof will parallel the proof given in Part A, but with the even and odd cases considered simultaneously. Again we must show that $\xi^C(G) \geq \xi^C(V_{n,d})$.

Suppose, to the contrary, that there exists a counterexample G, for which $t(G) = 0$, and

$$\xi^C(G) < \xi^C(V_{n,d}). \tag{3.37}$$

Of all such counterexamples, choose G to have the smallest possible order, n. Hence, any graph G' with diameter d', no problem vertices, and $n' < n$ vertices, will satisfy

$$\xi^C(G') \geq \xi^C(V_{n',d'}). \tag{3.38}$$

Let $P : v_0, v_1, \ldots, v_d$ be a diametral path in G, and define $S = V - V(P)$.

Claim **3.7** *There are no end vertices in S.*

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Proof of Claim 3.7: Suppose to the contrary, that S contains an end vertex x, and let y be the neighbour of x. Set $G' = G - x$.

Fact 3.4 *(i) The diameter of G' is d, since x is not on the diametral path P.*

(ii) $n(G') = n - 1 < n(G)$.

We now show that

$$\xi^C(G') \geq \xi^C(V_{n-1,d}). \tag{3.39}$$

If on the one hand $t(G') = 0$, then along with Fact 3.4, we conclude that G' is not a counterexample, (3.38) applies, and (3.39) follows. If on the other hand $t(G') \geq 1$, then G' satisfies the conditions of Part A, and (3.39) follows immediately.

Continuing from this point onwards, the proof of Claim 3.7 is identical to that of Claim 3.1. We arrive at a contradiction, and thus Claim 3.7 is proven.

Claim 3.7 allows us to partition S as follows:

let $A = \{x \in S \mid \deg(x) = 2\}$, $B = \{x \in S \mid \deg(x) \geq 3\}$. Setting $|A| = a$, and $|B| = b$, we obtain

$$a + b + d + 1 = n. \tag{3.40}$$

Analogous to (3.11), a simple calculation gives

$$\sum_{v \in V(P)} \mathrm{ec}(v) \deg(v) \geq \begin{cases} \frac{3}{2}d^2 & \text{for } d \text{ even} \\[2mm] \frac{3}{2}d^2 + 1/2 & \text{for } d \text{ odd.} \end{cases} \tag{3.41}$$

Combining (3.2) with $t(G) = 0$, we have that for all vertices x in A, $\mathrm{ec}(x) \geq \lceil d/2 \rceil + 1$. This inequality, in conjunction with (3.2) and (3.41), gives us

$$\xi^C(G) = \sum_{v \in V(P)} \mathrm{ec}(v) \deg(v) + \sum_{x \in A} \mathrm{ec}(x) \deg(x) + \sum_{u \in B} \mathrm{ec}(u) \deg(u)$$

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$$\geq \sum_{v \in V(P)} \mathrm{ec}(v) \deg(v) + 2\,a(\lceil d/2 \rceil + 1) + 3\,b(\lceil d/2 \rceil)$$

$$\geq \begin{cases} \frac{3}{2}d^2 + a\,(d+2) + b\,(3d/2) & \text{for } d \text{ even} \\[2em] \frac{3}{2}d^2 + 1/2 + a\,(d+3) + b\,(3\,(d+1)/2) & \text{for } d \text{ odd.} \end{cases} \qquad (3.42)$$

We will minimize (3.42) by optimizing the coefficients a and b. If $d \geq 3$, the right hand side of the inequality is minimized when a is as large as possible, so, by (3.40), set $a = n - d - 1$, and $b = 0$. Thus,

$$\xi^C(G) \;\geq\; \begin{cases} (n-d-1)(d+2) + \frac{3}{2}d^2 & \text{for } d \text{ even} \\[2em] (n-d-1)(d+3) + \frac{3}{2}d^2 + 1/2 & \text{for } d \text{ odd} \end{cases}$$

$$= \begin{cases} n(d+1) + n + \frac{3}{2}d^2 - d^2 - 2d - d - 2 & \text{for } d \text{ even} \\[2em] n(d+2) + \frac{3}{2}d^2 + n - d^2 - 3d - d - 3 + 1/2 & \text{for } d \text{ odd} \end{cases}$$

$$= \begin{cases} n(d+1) + \frac{1}{2}d^2 - 2d - 1 + n - d - 1 & \text{for } d \text{ even} \\[2em] n(d+2) + \frac{1}{2}d^2 - 3d - 3/2 + n - d - 1 & \text{for } d \text{ odd} \end{cases}$$

$$= \xi^C(V_{n,d}) + n - d - 1.$$

Finally, since $n \geq d + 1$, we have $\xi^C(G) \geq \xi^C(V_{n,d}) + n - d - 1 \geq \xi^C(V_{n,d})$, which contradicts (3.37). This contradiction completes the proof of Part B, and hence completes the proof of the theorem. $\qquad\square$

In the following chapter we continue our study of the eccentric connectivity index, and turn our attention to graphs with given order and minimum degree.[1]

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[1]We remark that soon after the publication of the result presented in this chapter, we learnt that Zhang, Zhou and Liu [80] also independently, and using different methods, obtained a similar result.

Chapter 4

Bounds on the Eccentric Connectivity Index in Terms of Minimum Degree

4.1 Introduction

In this chapter we focus on the eccentric connectivity index for graphs with given minimum degree. In the first part of the chapter we study graphs with constant degree, viz., regular graphs. Došlić, Saheli and Vukičević [22] as well as Ilić [40] stated that it would be interesting to determine extremal regular (and, in particular, cubic) graphs with respect to the eccentric connectivity index. We completely solve this open problem for the upper bound. Thereafter a lower bound is given, which is attained by the Petersen graph. (See [60].)

The remaining part of this chapter deals with graphs of given minimum degree. We find an asymptotic upper bound on the eccentric connectivity index, for a graph of given order and minimum degree. We also construct graphs which attain this bound. (See [17].)

4.2 Regular Graphs

Let G be a k-regular graph of order n. For $k = 2$, cycle graphs are the only admissible class of graphs and hence in this case, the (unique) extremal graphs are the cycle graphs, with an index value of

$$\xi^C(C_n) = \begin{cases} n^2 & \text{for } n \text{ even} \\ n(n-1) & \text{for } n \text{ odd.} \end{cases}$$

Henceforth, we consider $k \geq 3$.

First, we investigate the upper bound. Recall the bound on average eccentricity in Theorem 1.1

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

$$\text{avec}(G) \leq \frac{9n}{4(\delta + 1)} + \frac{15}{4}.$$

It immediately follows that

$$\sum_{u \in V(G)} \text{ec}(u) \leq \frac{9n^2}{4(\delta + 1)} + \frac{15\,n}{4}.$$

When restricted to k-regular graphs, the eccentric connectivity index simplifies to

$$\xi^C(G) = \sum_{u \in V(G)} \deg(u)\,\text{ec}(u) = k \sum_{u \in V(G)} \text{ec}(u).$$

Applying Theorem 1.1, we conclude

$$\xi^C(G) \leq \frac{9\,kn^2}{4(k + 1)} + \frac{15\,kn}{4}. \tag{4.1}$$

It remains to identify regular graphs which meet this upper bound asymptotically. Given the pharmaceutical motivation for this topological model, we focus on chemical graphs.

For $k = 3$, (4.1) reduces to $\xi^C(G) \leq \dfrac{27n^2}{16} + \dfrac{45\,n}{4}.$

One class of extremal graphs in this cubic case is shown in Figure 4.1.
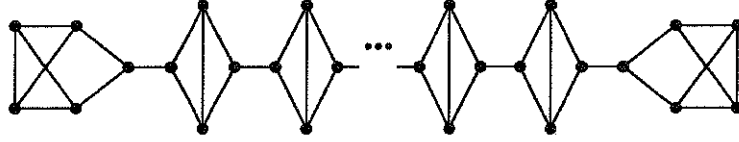

Figure 4.1: An extremal 3-regular graph, $R3_n$

The eccentric connectivity index of these graphs is

$$\xi^C(R3_n) = \begin{cases} \frac{27n^2}{16} - \frac{1}{4}(15n + 33) & \text{for } n \equiv 6 \, (\text{mod} \, 8) \\[2mm] \frac{27n^2}{16} - \frac{1}{4}(15n + 21) & \text{for } n \equiv 2 \, (\text{mod} \, 8). \end{cases}$$

Modification of the two outer blocks in Figure 4.1 will generate similar extremal graphs for $n \equiv 0, \ 4 \, (\text{mod} \, 8)$.

For $k = 4$, (4.1) becomes $\xi^C(G) \leq \dfrac{9n^2}{5} + 15\,n.$

Since maximizing the total eccentricity of a graph is closely linked to maximizing its diameter, we draw on work of Mukwembi [63] to provide an example of an extremal graph, as seen in Figure 4.2.
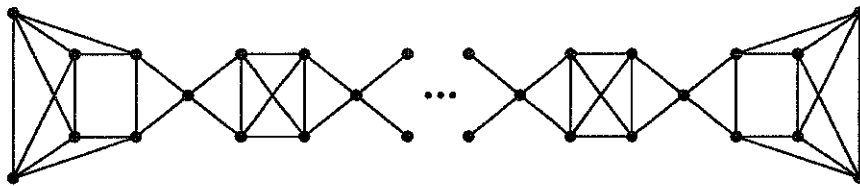

Figure 4.2: An extremal 4-regular graph, $R4_n$

This graph has
$$
\xi^C(R4_n) =
\begin{cases}
\frac{9n^2}{5} - \frac{1}{5}(38n + 112) & \text{for } n \text{ even} \\[2mm]
\frac{9n^2}{5} - \frac{1}{5}(38n + 107) & \text{for } n \text{ odd.}
\end{cases}
$$

Finally, note that these two extremal 'sausage-like' graphs can be generalized to larger k values (non-chemical graphs), for both the k even and the k odd cases.

Thus, we have proved the following theorem.

Theorem 4.1 *Let G be a k-regular graph of order n. Then, for $k \geq 3$,*

$$
\xi^C(G) \leq \frac{9 \, k \, n^2}{4(k+1)} + O(n)
$$

and the bound is sharp.

Second, we consider a lower bound. Here, we have

Theorem 4.2 *Let G be a k-regular ($k \geq 3$) connected graph of order n. Then*

$$
\xi^C(G) \geq k \, n \left[\log_{k-1}(n(k-2) + 2) - \log_{k-1} k \right].
$$

Proof. We first show that, for $r = \mathrm{rad}(G)$,

$$
r \geq \frac{\log\left(\frac{(n-1)(k-2)}{k} + 1\right)}{\log(k-1)}. \tag{4.2}
$$

Let v be a vertex with eccentricity equal to the radius, r. Then, for each $i = 0, 1, 2, \ldots, r$, let $N_i := \{x \in V \mid d(x, v) = i\}$ and $|N_i| = n_i$.

Then, $n_0 = 1$ and $n_1 = k$. Furthermore, for all $i = 1, 2, \ldots, (r - 1)$, we have

$$
n_{i+1} \leq (k - 1) \, n_i.
$$

Hence,

$$
\begin{aligned}
n &= n_0 + n_1 + n_2 + \ldots + n_r \\
&\leq 1 + k + k\,(k - 1) + k\,(k - 1)^2 + \ldots + k\,(k - 1)^{r-1} \\
&= 1 + k \cdot \frac{(k - 1)^r - 1}{k - 2}.
\end{aligned}
$$

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Thus $\quad (k-1)^r \geq \dfrac{(n-1)(k-2)}{k} + 1$, and (4.2) follows by taking logarithms and rearranging.

Next, since $\mathrm{ec}(u) \geq r$ for all $u \in V(G)$, we have

$$
\begin{aligned}
\xi^C(G) \;&=\; \sum_{v \in V(G)} \deg(v)\,\mathrm{ec}(v) \\
&\geq\; k\,n\,r.
\end{aligned}
$$

Applying (4.2) we conclude

$$
\begin{aligned}
\xi^C(G) \;&\geq\; k\,n\,\frac{\log\!\left(\frac{(n-1)(k-2)}{k}+1\right)}{\log(k-1)} \\
&=\; k\,n\,\left[\log_{k-1}(n(k-2)+2) - \log_{k-1} k\right],
\end{aligned}
$$

as desired. $\hfill\square$

For cubic graphs, the above theorem reduces to:

Corollary 4.3 *Let G be a connected cubic graph of order n. Then*

$$
\xi^C(G) \geq 3\,n\,\left[\log_2(n+2) - \log_2 3\right].
$$

Since our derivation of this lower bound parallels the Moore bound, to search for extremal graphs we look to those which attain the Moore bound. In fact, the Petersen graph is a cubic graph which attains equality in the corollary. Also, the 7-regular Hoffman-Singleton graph almost attains equality in Theorem 4.2. Note that both these extremal graphs have a diameter of two.

However, when the diameter is greater than or equal to 3, the bound in Corollary 4.3 is not best possible, since there are no (non-trivial) graphs with diameter greater than or equal to 3 which can attain the Moore bound [58].

4.3 Minimum Degree

Turning from graphs of given regular degree, we now consider graphs with given minimum degree. We will derive an upper bound on the ECI in terms of order and minimum degree.

We begin these investigations by considering the well-known Wiener index, which calculates the total distance between all pairs of vertices in a graph. Indeed, the *Wiener index*, $W(G)$, of G is defined as

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

Several authors ([11, 14, 46]) independently showed that the average (mean) distance of a connected graph of order n and minimum degree δ is at most $\frac{n}{\delta+1}+O(1)$.

Upon multiplication by $\binom{n}{2}$, this immediately implies the following bound on the Wiener index

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

In this section we derive a similar upper bound for the ECI, in terms of order and minimum degree. The leading coefficient will be 4/9, which is close to the 1/2 value in the Wiener index.

Here we again need Theorem 1.1, which states that the average eccentricity of a connected graph of order n and minimum degree δ is at most $\frac{9n}{4(\delta+1)} + \frac{15}{4}$.

Observe that now the sum is over the vertices of G, rather than the unordered pairs $\{u, v\} \subseteq V(G)$. Multiplying by n to find total eccentricity, and noting that for all vertices $v \in V$, $\deg(v) \leq \Delta$, we have (see [81])

Proposition 4.1 *Let G be a connected graph of order n, minimum degree δ and maximum degree Δ. Then*

$$\xi^C(G) \leq \frac{9\Delta}{4(\delta+1)}n^2 + \frac{15\Delta n}{4}.$$

This Proposition gives a very good bound on the eccentric connectivity index for smaller values of Δ. However it is not sharp for larger values of Δ, where

$$\Delta \geq \frac{16}{81}n + O(1).$$

Finally, recall our Corollary 2.3, which showed that for G of order n,

$$\xi^C(G) \leq \frac{4}{27}n^3 + O(n^2).$$

The main result in this section gives a stronger bound to Proposition 4.1 for large Δ; and it strengthens, for given $\delta > 2$, Corollary 2.3.

Theorem 4.4 *Let G be a connected graph of order n and minimum degree δ. Then*

$$\xi^C(G) \leq \frac{4}{9(\delta+1)}n^3 + O(n^2).$$

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

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

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

For each vertex $v \in S$, 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 $M = \cup_{v \in S} M[v]$. See Figure 4.3. Then

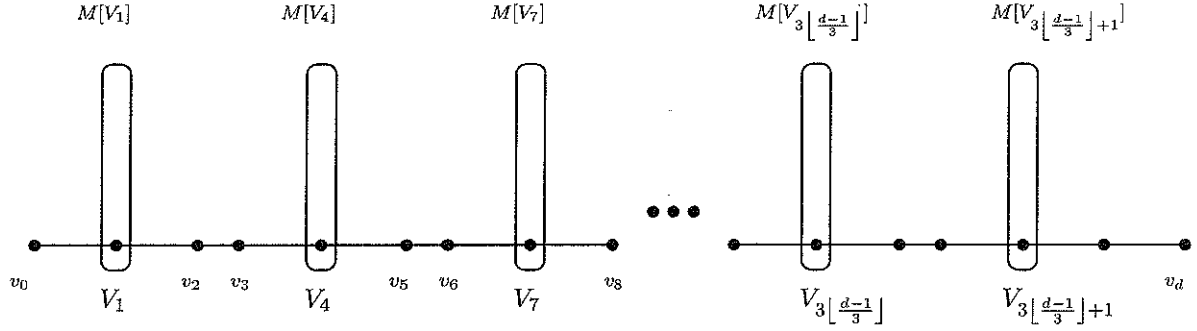$$|M| = (\delta+1)\left(\left\lfloor \frac{d-1}{3} \right\rfloor + 1 \right).$$

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Figure 4.3: Diametral path with neighbourhoods M[v]

Claim 4.1 $\sum_{x \in M} ec(x) \deg_G(x) \leq d(\delta + 1) \left(2n - \left\lfloor \frac{d-1}{3} \right\rfloor - 1 \right)$.

Proof of Claim 4.1: We need to consider 'alternating' subsets of M. Let $S_1 \subset S$ be the set $S_1 = \{ v_{3i+1} \in S \mid i = 0, 2, 4, \ldots \}$. Let $S_2 = S - S_1$. The subsets $M[v] \subset M$ are all disjoint, and so in particular, for each $u, v \in S_1$, $u \neq v$, we have $M[u] \cap M[v] = \emptyset$. Writing the elements of S_1 as $S_1 = \{ w_1, w_2, \ldots, w_{|S_1|} \}$, we have

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

Furthermore, for $u, v \in S_1$, $u \neq v$ the *neigbourhoods* of $M[u]$ and $M[v]$ are also disjoint. For each $w_j \in S_1$, relabel $M[w_j] = \{ w_j, u_1^j, \ldots, u_\delta^j \}$, where $u_1^j, \ldots, u_\delta^j$ are neighbours of w_j. Then, for each $t = 1, 2, \ldots, \delta$,

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

Summing these $\delta + 1$ inequalities, we obtain

$$(\delta + 1)n \geq \sum_{x \in M[S_1]} \deg_G(x) + (\delta + 1)|S_1|. \tag{4.3}$$

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Analogously, over the set S_2,

$$(\delta + 1)n \geq \sum_{x \in M[S_2]} \deg_G(x) + (\delta + 1)|S_2|. \tag{4.4}$$

Combining (4.3) and (4.4), and $ec(x) \leq d$, gives

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

and Claim 4.1 is proven.

Now let $A = V - M$.

Claim 4.2 If $x \in A$, then

$$ec(x)\deg_G(x) \leq d\left[n - (\delta + 1)\left\lfloor \frac{d-1}{3} \right\rfloor + \delta - 1\right].$$

Proof of Claim 4.2: Note that $x \in A$ can only be adjacent to at most $(\delta + 1) + \delta = 2\delta + 1$ vertices in M, otherwise there would be a shorter $v_0 - v_d$ path through x, contradicting the fact that P is a shortest path. Thus, using the definition of the set A,

$$\deg_G(x) \leq (|A| - 1) + 2\delta + 1 = n - (\delta + 1)\left\lfloor \frac{d-1}{3} \right\rfloor + \delta - 1.$$

The claim then follows from the fact that $ec(x) \leq d$.

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From Claim 4.2, we get

$$\sum_{x \in A} \text{ec}(x) \deg_G(x) \leq |A| \, d \left(n - (\delta+1) \left\lfloor \frac{d-1}{3} \right\rfloor + \delta - 1 \right)$$

$$= d \left(n - (\delta+1) \left[\left\lfloor \frac{d-1}{3} \right\rfloor + 1 \right] \right) \left(n - (\delta+1) \left\lfloor \frac{d-1}{3} \right\rfloor + \delta - 1 \right)$$

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

$$-d(\delta+1)(\delta-1).$$

Combining this and Claim 4.1, we obtain

$$\xi^C(G) = \sum_{x \in A} \text{ec}(x) \deg_G(x) + \sum_{x \in M} \text{ec}(x) \deg_G(x)$$

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

$$+ d(\delta+1) \left(2n - \left\lfloor \frac{d-1}{3} \right\rfloor - 1 \right)$$

$$\leq d \left[n - (\delta+1) \left(\frac{d}{3} - 1 \right) \right]^2 - 2d \left[n - (\delta+1) \left(\frac{d-1}{3} \right) \right] - d(\delta+1)(\delta-1)$$

$$+ d(\delta+1) \left[2n - \left(\frac{d}{3} - 1 \right) - 1 \right]$$

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

Applying $d < \frac{3n}{\delta+1}$ from Theorem 1.2 to the term in curly brackets, we have

$$2d\delta \left(n - \frac{d}{3}(\delta+1) \right) + d(\delta+1)(2n + \frac{4}{3} - \frac{d}{3}) < 2d(\delta+1)n + 2d(\delta+1)(n+1)$$

$$< 2 \left(\frac{3n}{\delta+1} \right)(\delta+1)n$$

$$+2 \left(\frac{3n}{\delta+1} \right)(\delta+1)(n+1)$$

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$$= 12n^2 + 6n.$$

It follows that

$$\xi^C(G) \le d\left(n - \frac{d}{3}(\delta + 1)\right)^2 + 12n^2 + 6n.$$

This is maximized for $d = \frac{n}{\delta+1}$ to get

$$\xi^C(G) \le \frac{4n^3}{9(\delta + 1)} + 12n^2 + 6n,$$

and the bound in the theorem follows.

To see that for a fixed δ, the bound is asymptotically sharp, consider the graph G with diameter $\frac{n}{\delta+1}$ constructed as follows. For n a multiple of $3(\delta+1)$, let $k = \frac{n}{3(\delta+1)}$ and let H be the graph with vertex set $V(H) = V_0 \cup V_1 \cup \cdots \cup V_{3k-1}$, where

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

and two distinct vertices $v \in V_i$, $v' \in V_j$ are joined by an edge if and only if $|j - i| \le 1$. Let G be the graph obtained from H by taking the complete graph $K_{n-|V(H)|}$ and joining each vertex of $K_{n-|V(H)|}$ to the vertex of V_{3k-1}. That is, G is formed by joining $K_{n-|V(H)|}$ to the end vertex of H. See Figure 4.4.

A simple calculation shows that $\xi^C(G) = \frac{4n^3}{9(\delta + 1)} + O(n^2)$, and the proof is complete. $\qquad\square$
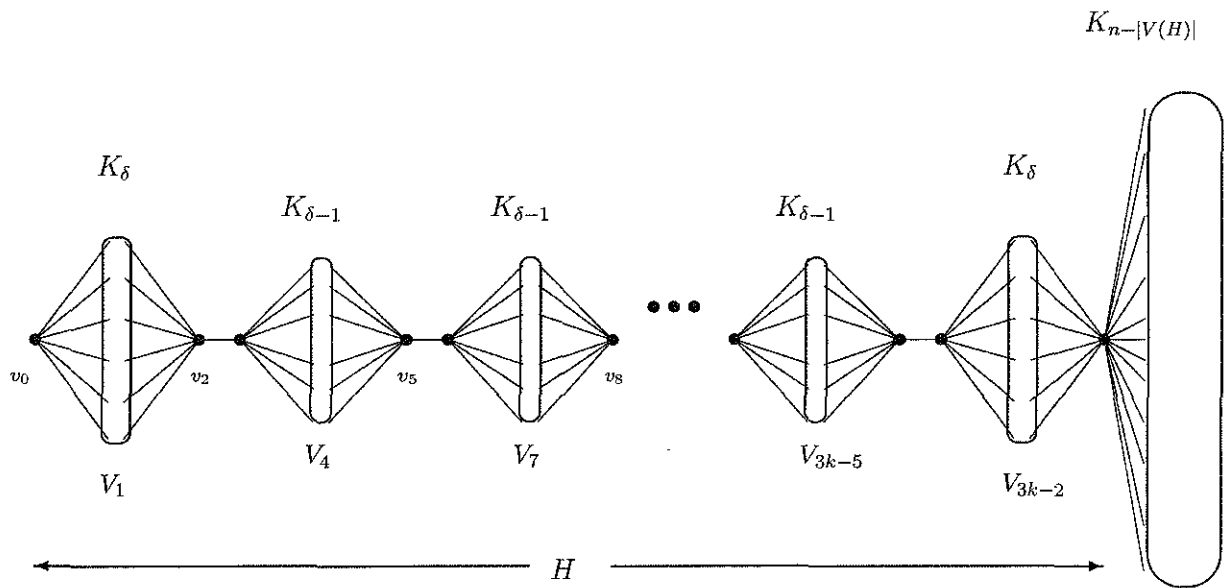
Figure 4.4: Extremal Graph for Theorem 4.4

Thus, in this chapter we have given upper and lower bounds on the ECI for regular graphs, and provided extremal graphs for the upper bound. Thereafter, we derived an asymptotic upper bound on the index in terms of order and minimum degree, which was similar to the corresponding bound on the Wiener index. In the following chapter, we will again consider the Wiener index and its relationship to the eccentric connectivity index.

Chapter 5

The Wiener Index and the Eccentric Connectivity Index

5.1 Introduction

In this chapter we investigate the Wiener index, and determine upper bounds on this well-studied topological index, in terms of the eccentric connectivity index.

Recall that the *Wiener index*, $W(G)$, of G is defined as

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

while the *eccentric connectivity index*, $\xi^C(G)$, of G is

$$\xi^C(G) = \sum_{v \in V} \mathrm{ec}_G(v) \deg_G(v).$$

We begin by investigating the relationship between the eccentric connectivity index of a graph and of its spanning trees. Then we derive a sharp upper bound on the Wiener index of a tree, in terms of its eccentric connectivity index. Thereafter, applying our spanning tree relationship, a corollary determines an upper bound on the Wiener index of a graph, in terms of its eccentric connectivity index. (See [17].)

We will need Claim 1.1, which gave a relationship between the radius and diameter of a graph. *For every graph G, $\mathrm{rad}(G) \geq \lceil \frac{1}{2} \mathrm{diam}(G) \rceil \geq \frac{1}{2} \mathrm{diam}(G)$.*

Furthermore, we saw in Theorem 2.7 that the volcano graph gives the lowest ECI for trees of fixed order and diameter. Precisely, we have

Theorem 5.1 *Let T be a tree of order n and diameter d. Then*

$$\xi^C(T) \geq \xi^C(V_{n,d}) = \begin{cases} n(d+1) + \frac{1}{2}d^2 - 2d - 1 & \text{if } d \text{ is even,} \\ n(d+2) + \frac{1}{2}d^2 - 3d - \frac{3}{2} & \text{if } d \text{ is odd.} \end{cases}$$

Finally, it is well known that for every graph, a radius-preserving spanning tree can be found by applying a breadth-first search, starting from any central vertex of the graph.

5.2 An Upper Bound for the Wiener Index in Terms of the Eccentric Connectivity Index

It is folklore that for any connected graph G, every spanning tree T of G satisfies the inequality

$$W(G) \leq W(T). \tag{5.1}$$

In contrast to (5.1), there are graphs (e.g., K_5, Petersen) with a spanning tree T for which $\xi^C(G) \not\leq \xi^C(T)$.

In [29], Entringer, Kleitman and Székely showed that it is always possible to find a spanning tree whose Wiener index is not much larger than that of G. They proved that if G is a connected graph, then there exists a spanning tree T of G such that $W(T) \leq 2W(G)$. Here we derive the corresponding property for the ECI.

Theorem 5.2 *Let G be a connected graph. Then there exists a spanning tree T of G for which*

$$\xi^C(T) \leq 2\xi^C(G).$$

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Proof. Let T be a radius-preserving spanning tree of G, and applying Claim 1.1, we have that for every vertex $v \in V$,

$$\mathrm{ec}_G(v) \geq \mathrm{rad}(G) = \mathrm{rad}(T) \geq \frac{1}{2}\,\mathrm{diam}(T) \geq \frac{1}{2}\,\mathrm{ec}_T(v).$$

Hence $\mathrm{ec}_T(v) \leq 2\,\mathrm{ec}_G(v)$ for every vertex v of G. This, in conjunction with the fact that $\deg_T(v) \leq \deg_G(v)$ for every vertex v of G, yields

$$
\begin{aligned}
\xi^C(T) &= \sum_{v \in V} \mathrm{ec}_T(v)\deg_T(v) \\
&\leq \sum_{v \in V} 2\,\mathrm{ec}_G(v)\deg_G(v) \\
&= 2\,\xi^C(G),
\end{aligned}
$$

as desired. $\qquad\qquad\square$

We now present upper bounds on the Wiener index in terms of the eccentric connectivity index, for trees, and then for general graphs.

Theorem 5.3 *Let T be a tree of order $n \geq 3$. Then*

$$W(T) \leq \frac{1}{3}\,n\,\xi^C(T) - n + 1.$$

Moreover, equality in the bound is attained by the star graph.

Proof. We prove the result by induction on the order n of T. For $n = 3$, T is the path of order 3, and the result can easily be verified. Consider $n > 3$, and assume that the result holds for any tree of order less than n. Denote the diameter of T by d and let x be a vertex with eccentricity d. Then x is an end vertex. Let T' be the tree of order $n - 1$ obtained by removing x from T. By our induction hypothesis we have

$$W(T') \leq \frac{1}{3}(n-1)\xi^C(T') - (n-1) + 1 = \frac{1}{3}(n-1)\xi^C(T') - n + 2. \qquad (5.2)$$

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Let v be the neighbour of x in T. Note that on one hand

$$
\begin{aligned}
\xi^C(T) - \xi^C(T') &\geq \mathrm{ec}_T(x) + \mathrm{ec}_T(v) \\
&= 2d - 1,
\end{aligned}
$$

and so

$$
\xi^C(T') \leq \xi^C(T) - 2d + 1. \tag{5.3}
$$

On the other hand, if all the vertices of T are as far as possible from x, we have

$$
\begin{aligned}
\sum_{u \in V} d(x, u) &\leq 0 + 1 + 2 + \cdots + d - 1 + d(n - (d-1) - 1) \\
&= dn - \frac{d^2}{2} - \frac{d}{2},
\end{aligned}
$$

so that

$$
\begin{aligned}
W(T) &= W(T') + \sum_{u \in V} d(x, u) \\
&\leq W(T') + dn - \frac{d^2}{2} - \frac{d}{2}.
\end{aligned}
$$

This, in conjunction with (5.2) and (5.3), gives

$$
\begin{aligned}
W(T) &\leq W(T') + dn - \frac{d^2}{2} - \frac{d}{2} \\
&\leq \frac{1}{3}(n-1)\xi^C(T') - n + 2 + dn - \frac{d^2}{2} - \frac{d}{2} \\
&\leq \frac{1}{3}(n-1)[\xi^C(T) - 2d + 1] - n + 2 + dn - \frac{d^2}{2} - \frac{d}{2} \\
&= \frac{1}{3}n\,\xi^C(T) - n + 1 + \left\{ \frac{1}{3}n(d+1) - \frac{d^2}{2} + \frac{d}{6} + \frac{2}{3} - \frac{\xi^C(T)}{3} \right\}.
\end{aligned}
$$

To complete the proof, it is adequate to show that the term in curly brackets is at most zero. By Theorem 5.1, we have

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$$\frac{1}{3}n(d+1) - \frac{d^2}{2} + \frac{d}{6} + \frac{2}{3} - \frac{\xi^C(T)}{3} \leq \frac{1}{3}n(d+1) - \frac{d^2}{2} + \frac{d}{6} + \frac{2}{3}$$

$$-\frac{1}{3}\begin{cases} n(d+1) + \frac{1}{2}d^2 - 2d - 1 & \text{if } d \text{ is even,} \\ n(d+2) + \frac{1}{2}d^2 - 3d - \frac{3}{2} & \text{if } d \text{ is odd,} \end{cases}$$

$$= \begin{cases} -\frac{1}{6}(4d^2 - 5d - 6) & \text{if } d \text{ is even,} \\ -\frac{1}{6}(4d^2 - 7d - 7 + 2n) & \text{if } d \text{ is odd,} \end{cases}$$

$$\leq 0,$$

for all $d \geq 2$, as desired. □

Corollary 5.4 *Let G be a connected graph of order $n \geq 3$. Then*

$$W(G) \leq \frac{2}{3}n\,\xi^C(G) - n + 1.$$

Proof. Let T be a radius-preserving spanning tree of G. By (5.1), $W(G) \leq W(T)$. Applying Theorem 5.3, we have $W(G) \leq W(T) \leq \frac{1}{3}n\,\xi^C(T) - n + 1$. Then using Theorem 5.2, we find $W(G) \leq \frac{2}{3}n\,\xi^C(G) - n + 1$, as desired. □

We remark here that the bound proved in Corollary 5.4 is close to best possible. To see this, consider the star graph S_n of order n. Straightforward calculations show that

$$\lim_{n \to \infty} \frac{W(S_n)}{\frac{2}{3}n\,\xi^C(S_n) - n + 1} = \frac{1}{2}.$$

This completes our studies into the eccentric connectivity index. In the following chapter we will consider a slightly older distance-based TI, the degree distance.

Chapter 6

Degree Distance

6.1 Introduction

In this chapter we turn our attention to another, much studied, topological index, the degree distance, also known as the Schultz index.

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

$$D'(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} [\deg(u) + \deg(v)]\, d(u, v)$$

$$= \sum_{\{u,v\} \subseteq V(G)} [\deg(u) + \deg(v)]\, d(u, v).$$

Note that the degree distance can equivalently be expressed (see, for example, [41]) as $\quad D'(G) = \sum_{v \in V} D'(v),$

where $D'(v) = \deg(v)\, D(v)$ is the degree distance of a vertex v, and

$D(v) = \sum_{w \in V} d(v, w)$ is called the *status*, or total distance of v.

The purpose of this chapter is to prove a bound proposed by Tomescu [76] in 1999, viz.,

Conjecture 6.1 *For a connected graph G of order n,* $D'(G) \leq \frac{1}{27} n^4 + O(n^3).$

This conjecture was almost solved by Dankelmann et al. [16]. Here we give an

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improvement on their proof, and thus definitively resolve the Tomescu conjecture. (See [61].)

6.2 An Upper Bound

We begin by finding a bound on the degree distance, in terms of order and diameter.

Theorem 6.2 *Let G be a connected graph of order n and diameter d. Then*

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

and this bound tight.

Proof. Recall that $D'(G) = \sum_{v \in V} D'(v)$. We partition the vertex set V of G as follows. Let $P : u_0, u_1, \ldots, u_d$ be a diametral path of G. For ease of notation, we will also refer to P as the set of vertices on this path. Let C be a maximum set of disjoint pairs of vertices from $V - P$ which lie at a distance at least 3, viz., if $\{a, b\} \in C$, then $d(a, b) \geq 3$. If $\{a, b\} \in C$, we will say that a and b are *partners*. Finally, let M be the remaining set of vertices of G, i.e., $M = V - P - \{x \mid x \in \{a, b\} \in C\}$. Let $|M| = m$, $|C| = c$. This implies that

$$n = (d + 1) + 2c + m. \tag{6.1}$$

Fact 6.1 *Let $\{a, b\} \in C$. Then, $\deg(a) + \deg(b) \leq n - d + 3$.*

To establish this fact, observe that $N[a] \cap N[b] = \emptyset$, since $d(a, b) \geq 3$. Also, each of these two vertices can be adjacent to at most 3 (consecutive) vertices on P. So, $n \geq \deg(a) + \deg(b) + 2 + (d + 1) - 6$, and the fact is proven.

Claim 6.1 $\sum_{u \in P} D'(u) = O(n^3)$.

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Proof of Claim 6.1: We partition P as $P = V_0 \cup V_1 \cup V_2$, where V_0, V_1 and V_2 are defined as follows:

$$V_0 = \{u_0, u_3, u_6, \ldots\},$$

$$V_1 = \{u_1, u_4, u_7, \ldots\},$$

$$V_2 = \{u_2, u_5, u_8, \ldots\}.$$

Let $x, y \in V_i$, for some $i = 0, 1, 2$. Since the distance between x and y along P is at least 3, and P is a diametral path, we have that $N[x] \cap N[y] = \emptyset$. Thus $\sum_{x \in V_i} \deg(x) \leq n - |V_i|$, for each $i = 0, 1, 2$. Now, since for $u \in V(G)$, $D(u) \leq (n-1)d \leq (n-1)^2$, we have

$$
\begin{aligned}
\sum_{v \in P} D'(v) &= \sum_{v \in P} \deg(v) D(v) \\
&= \sum_{v \in V_0} \deg(v) D(v) + \sum_{v \in V_1} \deg(v) D(v) + \sum_{v \in V_2} \deg(v) D(v) \\
&\leq (n-1)^2 \left(\sum_{v \in V_0} \deg(v) + \sum_{v \in V_1} \deg(v) + \sum_{v \in V_2} \deg(v) \right) \\
&\leq (n-1)^2 \left(n - |V_0| + n - |V_1| + n - |V_2| \right) \\
&= (n-1)^2 (3n - d - 1) \\
&= O(n^3).
\end{aligned}
$$

and thus Claim 6.1 is proven.

The remainder of the proof presents a simplified version of the work done in [16].

We now consider two cases.

CASE 1 $m \leq 1$

For $x \in M$, $D(x) \leq (n-1)^2$, so $D'(x) \leq (n-1)^3$. Since $m \leq 1$, we conclude that

$$\sum_{x \in M} D'(x) = O(n^3). \tag{6.2}$$

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Next, we show that for all $\{a, b\} \in \mathcal{C}$,

$$D'(a) + D'(b) \leq \frac{1}{2} n \, d \, (n - d) + O(n^2). \tag{6.3}$$

Vertex a has $\deg(a)$ vertices at distance 1; and since no vertex can be further than d from vertex a, the sum of the distances from a to the remaining vertices of G is at most $2 + 3 + \ldots + (d - 1) + [n - (\deg(a) + d - 1)](d)$. Then,

$$
\begin{aligned}
D(a) &\leq \deg(a) + 2 + 3 + \ldots + (d - 1) + [n - (\deg(a) + d - 1)]d \\
&= d \left(n - \frac{1}{2} d - \deg(a) \right) + O(n),
\end{aligned}
$$

which implies $D'(a) \leq \deg(a) \left[d \left(n - \frac{1}{2} d - \deg(a) \right) \right] + O(n^2)$.

Similarly, $D'(b) \leq \deg(b) \left[d \left(n - \frac{1}{2} d - \deg(b) \right) \right] + O(n^2)$.

Hence,

$$D'(a) + D'(b) \leq \deg(a)[d(n - \frac{1}{2} d - \deg(a))] + \deg(b)[d(n - \frac{1}{2} d - \deg(b))] + O(n^2).$$

Now, define the real-valued function $f(n, d, \deg(a), \deg(b))$ as the expression on the right hand side of the above inequality, without the $O(n^2)$ term. We will maximize f, taking into consideration the inequality constraint of Fact 6.1. Fixing n and d, f becomes as large as possible when $\deg(a) = \deg(b) = \frac{1}{2}(n - d + 3)$. This gives

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

and (6.3) is shown.

Note from (6.1) that $c = 1/2 \, (n - d - 1 - m)$, and since $m \leq 1$ here, this simplifies to $c = 1/2 \, (n - d) + O(1)$. Thus, summing (6.3) over all pairs in $\mathcal{C}$, we have

$$\sum_{\{a,b\} \in \mathcal{C}} (D'(a) + D'(b)) \leq c \left(\frac{1}{2} n \, d \, (n - d) + O(n^2) \right)$$

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$$= \frac{1}{4} n \, d \, (n-d)^2 + O(n^3). \tag{6.4}$$

Thus, summing over the three sets, and using Claim 6.1 for the diametral path, (6.2) and (6.4), we have the following upper bound on the degree distance of G

$$D'(G) = \sum_{\{a,b\} \in \mathcal{C}} (D'(a) + D'(b)) + \sum_{x \in M} D'(x) + \sum_{u \in P} D'(u)$$

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

and the theorem is proven for Case 1.

CASE 2 $m \geq 2$

Now the pairs of vertices in $\mathcal{C}$ will need to be partitioned further.

Fix a vertex $x \in M$. For each pair $\{a, b\} \in \mathcal{C}$, choose the vertex closer to x; if $d(a, x) = d(b, x)$ arbitrarily choose one of the vertices. Let A be the set of all these vertices closer to x, and B to 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 6.2 For all $u, v \in A \cup M, \quad d(u, v) \leq 8$.

Proof of Claim 6.2: Since $\mathcal{C}$ is a maximum set of pairs of vertices of distance at least 3, any two vertices of M must be at a distance of at most 2. Second, we show that for each $a \in A$, $d(a, x) \leq 4$. 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 the definition of A, b must also be at a distance of at least 5 from x. Now, consider another vertex $x' \in M - \{x\}$. Since $d(x, x') \leq 2$, the triangle inequality gives $5 \leq d(b, x) \leq d(b, x') + d(x', x) \leq d(b, x') + 2$ which implies that $d(b, x') \geq 3$. We

have thus identified two pairs, $\{a, x\}$ and $\{b, x'\}$, neither of which lie in C because they contain vertices from M, but both of which consist of vertices which lie at a distance of at least 3. Thus, the single pair $\{a, b\}$ in C, could be replaced with the two pairs $\{a, x\}$ and $\{b, x'\}$. This contradicts the maximality of C, and hence we have shown that $d(a, x) \leq 4$, for each $a \in A$. Third, for $u, v \in A$, we have that $d(u, x) \leq 4$ and $d(x, v) \leq 4$, so it follows that $d(u, v) \leq 8$, thus completing the proof of the claim.

Claim 6.3 *For all* $x \in M$, $\quad D'(x) \leq (n - d - c) \, d \left(n - \frac{1}{2} d - c - c_1 - m \right) + O(n^2)$.

Proof of Claim 6.3: By Claim 6.2, all $c + m$ vertices in $A \cup M$ lie within a distance of 8 from each vertex $x \in M$. This implies that the c_1 vertices in B_1 lie within a distance of 9+8 from x. Since no vertex can be further than d from vertex x, the total distance of x has the following bound

$$
\begin{aligned}
D(x) \;\leq\;& 8(c + m) + 17(c_1) + 18 + 19 + \ldots + (d - 1) \\
& + \left[n - (c + m + c_1 + (d - 18)) \right] d \\
=\;& d \left(n - \frac{1}{2} d - c - c_1 - m \right) + O(n).
\end{aligned}
$$

In order to find a bound for the degree of x, we use a counting argument similar to the one used in Fact 6.1. Observe that x can have at most 3 (consecutive) neighbours on P. By the definitions of A and B, x can be adjacent to at most c vertices in A, and no vertices in B. So, $n \geq \deg(x) + 1 + (d + 1) - 3 + c$, giving $\deg(x) \leq n - d - c + O(1)$. Hence $D'(x) \leq (n - d - c) \, [d \, (n - \frac{1}{2} d - c - c_1 - m)] + O(n^2)$, and this completes the proof of Claim 6.3.

Next, in order to bound the degree distance of the pairs in C, we must consider two subcases. We first consider the subset $A_1 \cup B_1$.

SUBCASE 2.1

Claim **6.4** *Let* $\{a, b\} \in \mathcal{C}$. *If* $d(a, b) \leq 9$, *then*

$$D'(a) + D'(b) \leq d(n - d)(n - \tfrac{1}{2}d - c - m - c_1) + O(n^2).$$

Proof of Claim 6.4: By Claim 6.2, any two vertices in $A \cup M$ lie within a distance of 8 from each other. Also, for each vertex in B_1, its partner in $A_1 \subseteq A$ lies within a distance of 9. Thus there is a maximum distance of 8+9 between vertices of B_1 and M; furthermore, two vertices in B_1 can be joined by a path of length not more than 9+8+9. Hence, any two vertices in $A \cup M \cup B_1$ lie within a distance of 26 of each other.

Consider a vertex $w \in A_1 \cup B_1$. Since no vertex can be further than d from w, we have the following upper bound on the status of w.

$$
\begin{aligned}
D(w) &\leq 26(c + m + c_1) + 27 + 28 + \ldots + (d - 1) + [n - (c + m + c_1 + (d - 27))]d \\
&= d\left(n - \frac{1}{2}d - c - m - c_1\right) + O(n).
\end{aligned}
$$

Applying Fact 6.1 for a pair of vertices in this first subcase, the degree distance becomes

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

and this completes the proof of the claim for this subcase.

The other subcase considers pairs $\{a, b\}$ of vertices in $\mathcal{C}$ which do not lie in $A_1 \cup B_1$. That is, pairs $\{a, b\}$ with $a \in A - A_1$ and $b \in B - B_1$.

SUBCASE 2.2

Claim **6.5** *Let* $\{a, b\} \in \mathcal{C}$. *If* $d(a, b) \geq 10$, *then*

$$D'(a) + D'(b) \leq d\left((c + m)[n - \tfrac{1}{2}d - c - m] - c_1(c + m) + c[n - \tfrac{1}{2}d - c]\right) + O(n^2).$$

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Proof of Claim 6.5: Now we must calculate an upper bound on the degree distance for the vertices in $A - A_1$, and $B - B_1$, separately.

For $a \in A - A_1$, we parallel the proof of Claim 6.3. By Claim 6.2, all $c + m$ vertices in $A \cup M$ lie within a distance of 8 from a. This implies that the c_1 vertices in B_1 lie within a distance of 9+8 from a. Since no vertex can be further than d from vertex a, we have

$$
\begin{aligned}
D(a) & \leq 8(c+m) + 17(c_1) + 18 + 19 + \ldots + (d-1) + [n - (c + m + c_1 + (d - 18))]d \\
& = d\left(n - \frac{1}{2}d - c - c_1 - m\right) + O(n).
\end{aligned}
$$

We find a bound for the degree of a. Since by the definition of C, a vertex must lie at a distance of at least 3 from its partner, a cannot be adjacent to both another vertex in $A \cup B$ as well as the partner of this vertex. Hence, vertex a has at most $c - 1$ neighbours in $A \cup B$. Further, it is adjacent to at most 3 (consecutive) vertices on P and has at most m neighbours in M. So, $\deg(a) \leq c - 1 + 3 + m$.

It follows that

$$
D'(a) \leq (c+m)[d\left(n - \frac{1}{2}d - c - c_1 - m\right)] + O(n^2).
$$

For $b \in B - B_1$, we parallel the proof from Case 1. Vertex b has $\deg(b)$ vertices at distance 1; and since no vertex can be further than d from vertex b, we have,

$$
\begin{aligned}
D(b) & \leq \deg(b) + 2 + 3 + \ldots + (d-1) + [n - (\deg(b) + d - 1)]d \\
& = d\left(n - \frac{1}{2}d - \deg(b)\right) + O(n),
\end{aligned}
$$

and we have the following bound on the degree distance of b

$$
D'(b) \leq \deg(b)\,[d\left(n - \frac{1}{2}d - \deg(b)\right)] + O(n^2).
$$

We define the real-valued function $f(x) = x\,[d\,(n - \frac{1}{2}d - x)]$.

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This quadratic function is increasing for $x \leq \frac{1}{2}\left[n - \frac{1}{2}d\right]$. Note that we now have

$D'(b) \leq f(\deg(b)) + O(n^2)$.

Bounding the degree of b, we note that b can be adjacent to at most $c-1$ vertices in $A \cup B$, and has at most 3 (consecutive) neighbours on P. Also, by Claim 6.2 and our assumption that $d(a,b) \geq 10$, vertex b cannot be adjacent to any vertices in M. So, $\deg(b) \leq c + 2$.

If $\deg(b) = c + 2$, then $f(\deg(b)) = f(c+2)$.

Otherwise, $\deg(b) \leq c+1$. Observe that by (6.1), and $m \geq 2$,

$$\frac{1}{2}\left[n - \frac{1}{2}d\right] = c + \frac{1}{2}m + \frac{1}{4}d + \frac{1}{2} \geq c + 1.$$

Hence, $\deg(b) \leq (c+1) \leq \frac{1}{2}\left[n - \frac{1}{2}d\right]$, and so $f(\deg(b)) \leq f(c+1)$.

Therefore,

$$D'(b) \leq f(\deg(b)) + O(n^2) \leq \max\{f(c+2), f(c+1)\} + O(n^2) = c\left[d\left(n - \frac{1}{2}d - c\right)\right] + O(n^2).$$

Finally, summing the bounds for the degree distances of a and b, we have

$$D'(a) + D'(b) \leq (c+m)\left[d\left(n - \frac{1}{2}d - c - c_1 - m\right)\right] + c\left[d\left(n - \frac{1}{2}d - c\right)\right] + O(n^2),$$

which, upon simplification, proves the claim for the second subcase.

Thus, summing Claims 6.4 and 6.5, Claim 6.3, and using Claim 6.1 for the diametral path, we have the following upper bound on the degree distance of G

$$
\begin{aligned}
D'(G) &= \sum_{\{a,b\}\in C}(D'(a) + D'(b)) + \sum_{x\in M}D'(x) + \sum_{u\in P}D'(u) \\
&\leq c_1\left[d\,(n-d)\,\left(n - \frac{1}{2}d - c - m - c_1\right)\right] \\
&\quad + (c-c_1)\,d\left((c+m)\left[n - \frac{1}{2}d - c - m\right] - c_1\,(c+m) + c\left[n - \frac{1}{2}d - c\right]\right) \\
&\quad + m\left[(n-d-c)\,d\left(n - \frac{1}{2}d - c - c_1 - m\right)\right] + O(n^3).
\end{aligned}
$$

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In order to maximize this expression, we note that $(c - c_1) \geq 0$ and, by (6.1), $(n - \frac{1}{2}d - c - m) \geq 0$, so we initially add an extra non-negative term:

$$D'(G) \leq c_1 \left[d(n-d)(n - \frac{1}{2}d - c - m - c_1) \right]$$

$$+ (c - c_1)d \left((c + m + 1)[n - \frac{1}{2}d - c - m] - c_1(c + m) + c[n - \frac{1}{2}d - c] \right)$$

$$+ m \left[(n - d - c)d(n - \frac{1}{2}d - c - c_1 - m) \right] + O(n^3).$$

Call $f(n, d, c, c_1)$ the above expression, without the asymptotic error term. That is, $D'(G) \leq f(n, d, c, c_1) + O(n^3)$.

First, we maximize f over c_1, holding the other 3 variables fixed. Differentiating with respect to c_1, and then substituting for the value of m from (6.1) in the first two terms, we find:

$$\frac{df}{dc_1} = d \left(-2c_1(c + 1) - 2c(n - d - 3c/2 - 1) - m(n - d - c) \right) < 0.$$

Hence, f is decreasing for $c_1 \leq c$, and we set $c_1 = 0$. Thus,

$$D'(G) \leq f(n, d, c, 0) + O(n^3)$$

$$= (c) \, d \left((c + m + 1)[n - \frac{1}{2}d - c - m] + c[n - \frac{1}{2}d - c] \right)$$

$$+ m \left[(n - d - c)d(n - \frac{1}{2}d - c - m) \right] + O(n^3).$$

Factoring out the lower order terms, this simplifies to

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

Second, maximizing the above expression (without the $O(n^3)$ term) over c, the maximum occurs at $c = \frac{1}{2}(n - d)$. Substituting this value, the bound simplifies to

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

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This completes Case 2, and therefore the upper bound in the theorem is proven.

An extremal graph, as given in [16], has a barbell shape. It consists of two complete graphs, H_1 and H_2 of orders $\lceil \frac{n-d+1}{2} \rceil$ and $\lfloor \frac{n-d+1}{2} \rfloor$, respectively; along with a path P of order $(d-1)$. The graph, $G_{n,d}$, is formed by joining one end of P to every vertex in H_1, and the other end of P to every vertex of H_2.

To show that the bound is tight, we calculate the degree distance of $G_{n,d}$. Let v be one of the $(n-d+1)$ vertices in $H_1 \cup H_2$. Then $\deg(v) = (n-d+1)/2$ and $D(v) \geq d(d-1)/2 + [\frac{1}{2}(n-d+1)](d) = \frac{1}{2}nd + O(n)$. Hence,

$$
\begin{aligned}
D'(G_{n,d}) &= \sum_{u \in V} \deg(u)D(u) \\
&\geq \sum_{v \in H_1 \cup H_2} \deg(v)D(v) \\
&\geq (n-d+1)\Big[\frac{(n-d+1)}{2}(\frac{1}{2}nd + O(n))\Big] \\
&= \frac{1}{4}(n-d)^2 nd + O(n^3).
\end{aligned}
$$

which, combined with the upper bound in Theorem 6.2, gives $D'(G_{n,d}) = \frac{1}{4}nd(n-d)^2 + O(n^3)$, and the proof is complete. □

Corollary 6.3 *Let G be a connected graph of order n. Then*

$$ D'(G) \leq \frac{1}{27}n^4 + O(n^3), $$

and the bound is best possible.

A simple maximization of the bound in Theorem 6.2 in terms of diameter d, yields the maximum at $d = n/3$. Substituting this value proves the bound in the corollary. Again, $G_{n,n/3}$ meets this upper bound. □

Thus, the conjecture of Tomescu has been confirmed.

Chapter 7

Conclusion

In this thesis we have explored mathematical relationships of some topological indices, which are graph invariants with many practical applications in chemistry, pharmacology and even industry. In particular, we investigated three distance-based indices: the eccentric connectivity index, the Wiener index and the Schultz index.

In Chapters 2 and 3 we considered the eccentric connectivity index. We showed that the star graph gives the minimum value of the index, for a graph of specified order. An asymptotically sharp upper bound was also derived. Then we proved that for trees of given order, the upper bound is met by the path. In the case of trees for which both order and diameter are prescribed, tight upper and lower bounds on the ECI were found. It was established in Chapter 3 that the sharp lower bound for trees also holds for graphs in general, for given order and diameter.

In Chapter 4 we considered an open question posed by Došlić, Saheli and Vukičević, as well as Ilić, concerning extremal graphs for the ECI in the case of regular, and more specifically, cubic graphs. In addressing this problem, we identified a tight upper bound on the ECI, and a lower bound on the index was also given. In this chapter we also derived an upper bound on the index in terms of order and minimum degree.

In Chapter 5, spanning trees were used to find an upper bound on the Wiener index, in terms of the ECI, for a graph of prescribed order.

Finally, we turned to the Schultz index and found an asymptotically tight upper bound for a graph of given order, thus resolving a conjecture of 1999 by Tomescu.

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