Discrete Applied Mathematics 175 (2014) 55–61

Contents lists available at ScienceDirect

Discrete Applied Mathematics

journal homepage: www.elsevier.com/locate/dam

On eccentric distance sum and minimum degree

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ARTICLE INFO

Article history:
Received 20 January 2014
Received in revised form 10 May 2014
Accepted 15 May 2014
Available online 2 June 2014

Keywords:
Eccentric distance sum
Minimum degree

ABSTRACT

Let G be a connected graph of order n and minimum degree $\delta \geq 2$. The eccentric distance sum $\xi^d(G)$ of G is defined as $\sum_{v\in V(G)} \mathrm{ec}_G(v)D_G(v)$, where $\mathrm{ec}_G(v)$ is the eccentricity of vertex v in G and $D_G(v)$ is the sum of all distances from v to other vertices of G. We prove the upper bound

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

Our bound is, for a fixed δ, asymptotically sharp and it extends a result of Ilić, Yu and Feng (2011), and that of Zhang and Li (2011).

1. Introduction

Much recent research in pharmaceutical drug design has focused on identifying properties of chemicals directly from their molecular structure. A key tool in this analysis is the use of topological indices, i.e., invariants of graphs that represent the chemical compound under study. Many topological indices have been defined and used, but only a limited number have been found to successfully predict activity. The first of these topological indices [8], introduced in 1947, is the well-studied Wiener index which is defined as the sum of all distances in the graph. In this paper we are concerned with a distance-based topological index of connected graphs called the *eccentric distance sum*.

Let G be a connected graph of order n with vertex set $V = V(G)$. The *eccentricity*, $\mathrm{ec}_G(v)$, of a vertex v in G is defined as the maximum of the distances between v and all other vertices of G. The *distance* or *status*, $D_G(v)$, of a vertex v of G is the sum $\sum_{x\in V} d_G(v, x)$, where $d_G(v, x)$ is the distance between vertices v and x in G. Formally, the *eccentric distance sum*, $\xi^d(G)$, of G is defined as

$$\xi^d(G) = \sum_{v\in V} \mathrm{ec}_G(v)D_G(v),$$

or equivalently

$$\xi^d(G) = \sum_{\{u,v\}\subseteq V} [\mathrm{ec}_G(u) + \mathrm{ec}_G(v)]d_G(u, v).$$

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[1] This work will be part of the first author's Ph.D. thesis.

[2] This material is based upon work supported financially by the National Research Foundation no. UID 74298.

http://dx.doi.org/10.1016/j.dam.2014.05.019

The eccentric distance sum was conceptualised, in 2002, by Gupta, Singh and Madan [3] who revealed that this invariant, just like the Wiener index, is a very good predictor of anti-HIV activity of dihydroseselin analogues and that it can provide valuable leads for the development of safe and potent therapeutic agents of diverse nature. Further comparisons between the two indices, Wiener index and the eccentric distance sum, were undertaken showing that the latter is more superior in the prediction of physical properties.

As such the investigations of the mathematical properties of these indices become a necessity. Several authors studied the Wiener index, for instance, Beezer, Riegsecker and Smith [1], Dankelmann and Entringer [2] and Kouider and Winkler [7] proved independently that the average distance, a variant of the Wiener index, 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 bound is equivalent to the bound,

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

On the other hand, the investigations on the mathematical properties of the eccentric distance sum was started recently and a fair number of bounds on the index for graphs, or graph classes, in terms of other graph parameters such as order, diameter, the Wiener index, the degree distance, eccentric connectivity index, independence number, connectivity, matching number, chromatic number and the clique number have been reported [4,6,9,10]. Various explicit formulae for the eccentric distance sum of graphs of chemical interest, such as the C_4 nanotorus, i.e., a Cartesian product of two cycles, the rectangular grid, the C_4 nanotube, i.e., a Cartesian product of the path and the cycle, and for the join of two graphs, were also presented in [6].

In light of the comparisons between the eccentric distance sum and the Wiener index, it is natural to ask how an upper bound on the eccentric distance sum in terms of order and minimum degree differs from that of the Wiener index given in (1). In [5], it was proved that $\xi^d(G) \leq n(n-1)(n-\delta)^2$ for a connected graph G of order n and minimum degree δ. From this, and (1), it is easy to see, using the inequality $\xi^d(G) \leq 2\,\mathrm{diam}(G)W(G)$, where $\mathrm{diam}(G)$ is the diameter of G, that

$$\xi^d(G) \leq \frac{n^3(n-\delta)}{\delta+1} + O(n^3).$$

Unfortunately, these two bounds on the eccentric distance sum in terms of order and minimum degree are not sharp for all values of δ. The bounds are only attained when $\delta = n-1$, i.e., for complete graphs. The purpose of this paper is to find a sharp upper bound on the eccentric distance sum in terms of order and minimum degree.

The notation that we use is as follows. The minimum degree is denoted by δ. In this paper, the minimum degree is fixed. The distance between a vertex u in G and a subset $S \subseteq V$ is defined as $\min_{v\in S} d_G(u,v)$ and is denoted by $d(u,S)$. If K is a subgraph of G we write $K \leq G$. For a vertex v, $N(v)$ denotes the set of all neighbours of v whilst $N[v] = N(v) \cup \{v\}$. For a subset $S \subseteq V$, $G[S]$ denotes the induced subgraph of G by S and $N[S]$ denotes the set $\cup_{u\in S} N[u]$. We will also abuse notation and write $\xi_G^d(S)$ for the quantity $\sum_{\{u,v\}\subseteq S}[\mathrm{ec}_G(u) + \mathrm{ec}_G(v)]d_G(u,v)$ and call this the eccentric distance sum of vertices in S in G. A 2-*packing* of G is a subset $A \subseteq V$ with $d_G(u,v) > 2$ for all $u, v \in A$. The kth *power* of G, denoted by G^k, is the graph with vertex set $V(G)$, in which two distinct vertices u and v are adjacent if $d_G(u,v) \leq k$. The *diameter* of G, i.e., the largest value of the eccentricities of vertices of G, is denoted by d. The path on n vertices will be denoted by P_n.

We state here a result that will be used later in the paper.

Proposition 1.1 (*[6,10]*). *Let G be a connected graph of order n. Then*

$$\xi^d(G) \leq \xi^d(P_n) = \frac{5^2}{2^5\cdot 3}n^4 + O(n^3). \quad \square$$

2. Results

We first present a technical lemma that proves an upper bound on the eccentric distance sum of any tree T of order $n+b$ obtained by taking some tree H of order n and attaching b pendent vertices to H.

Lemma 2.1. *Let T be a tree of order $n+b$ obtained from a tree H of order n and diameter d by attaching b pendent vertices to H. Then*

$$\xi^d(T) \leq \xi^d(H) + d^2b[2n-d+b] + O(b^2)\cdot O(n) + O(b)\cdot O(n^2) + O(n^3).$$

Proof. Denote the set of b pendent vertices attached to H to obtain T by B, i.e., $B = V(T) - V(H)$, so that $b = |B|$. Then

$$\begin{aligned}\xi^d(T) &= \sum_{\{x,y\}\subseteq V(T)} (\mathrm{ec}_T(x) + \mathrm{ec}_T(y))d_T(x,y)\\ &= \sum_{\{x,y\}\subseteq V(H)} (\mathrm{ec}_T(x) + \mathrm{ec}_T(y))d_T(x,y) + \sum_{(x,y)\in B\times V(H)} (\mathrm{ec}_T(x) + \mathrm{ec}_T(y))d_T(x,y)\\ &\quad + \sum_{\{x,y\}\subseteq B} (\mathrm{ec}_T(x) + \mathrm{ec}_T(y))d_T(x,y).\end{aligned} \tag{2}$$