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On the eccentric distance sum of graphs ☆

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ABSTRACT

The eccentric distance sum is a novel topological index that offers a vast potential for structure activity/property relationships. For a graph G, it is defined as $\xi^d(G) = \sum_{v \in V} \varepsilon(v)D(v)$, where $\varepsilon(v)$ is the eccentricity of the vertex v and $D(v) = \sum_{u \in V(G)} d(u, v)$ is the sum of all distances from the vertex v. Motivated by [G. Yu, L. Feng, A. Ilić, On the eccentric distance sum of trees and unicyclic graphs, J. Math. Anal. Appl. 375 (2011) 934–944], in this paper we characterize the extremal trees and graphs with maximal eccentric distance sum. Various lower and upper bounds for the eccentric distance sum in terms of other graph invariants including the Wiener index, the degree distance, eccentric connectivity index, independence number, connectivity, matching number, chromatic number and clique number are established. In addition, we present explicit formulae for the values of eccentric distance sum for the Cartesian product, applied to some graphs of chemical interest (like nanotubes and nanotori).

1. Introduction

Let G be a simple connected graph with the vertex set $V(G)$. For a vertex $v \in V(G)$, $deg(v)$ denotes the degree of v. For vertices $u, v \in V(G)$, the *distance* $d(u, v)$ is defined as the length of the shortest path between u and v in G and $D_G(v)$ (or $D(v)$ for short) denotes the sum of all distances from v. The *eccentricity* $\varepsilon(v)$ of a vertex v is the maximum distance from v to any other vertex. The *radius* $r(G)$ of a graph is the minimum eccentricity among the vertices of G, while the *diameter* $d(G)$ of a graph is the maximum eccentricity among the vertices of G. Let S_n and P_n be a star and a path on n vertices, respectively.

The *Wiener index* is defined as the sum of all distances between unordered pairs of vertices

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

It is considered as one of the most used topological index with high correlation with many physical and chemical indices of molecular compounds (for the recent survey on Wiener index see [8,9]).

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The parameter $DD(G)$ is called the *degree distance* of G and it was introduced by Dobrynin and Kochetova [7] and Gutman [23] as a graph-theoretical descriptor for characterizing alkanes; it can be considered as a weighted version of the Wiener index

$$DD(G) = \sum_{\{u,v\} \subseteq V(G)} \big(deg(u) + deg(v)\big) d(u, v) = \sum_{v \in V(G)} deg(v) \cdot D_G(v),$$

where the summation goes over all pairs of vertices in G. In fact, when G is a tree on n vertices, it has been demonstrated that Wiener index and degree distance are closely related by (see [19,20]) $DD(G) = 4W(G) - n(n-1)$.

Sharma, Goswami and Madan [32] introduced a distance-based molecular structure descriptor, *eccentric connectivity index* (ECI) defined as

$$\xi^c(G) = \sum_{v \in V(G)} \varepsilon(v) deg(v).$$

The index $\xi^c(G)$ was successfully used for mathematical models of biological activities of diverse nature [12,13,16,26, 30,32]. The investigation of its mathematical properties started only recently (for a survey on eccentric connectivity index see [22]). In [10,21,28,36], the extremal graphs in various class of graphs with maximal or minimal ECI are determined. In [1,2,11] the authors determined the closed formulae for the eccentric connectivity index of nanotubes and nanotori.

It is sometimes interesting to consider the sum of eccentricities of all vertices of a given graph G [6]. We call this quantity the *total eccentricity* of the graph G and denote it by

$$\zeta(G) = \sum_{v \in V(G)} \varepsilon(v).$$

Recently, a novel graph invariant for predicting biological and physical properties – *eccentric distance sum* was introduced by Gupta, Singh and Madan [16]. The authors in [16] have shown that some structure activity and quantitative structure-property studies using eccentric distance sum were better than the corresponding values obtained using the Wiener index. The eccentric distance sum of G (EDS) is defined as

$$\xi^d(G) = \sum_{v \in V(G)} \varepsilon(v) D_G(v).$$

The eccentric distance sum can be defined alternatively as

$$\xi^d(G) = \sum_{\{u,v\} \subseteq V(G)} \big(\varepsilon(v) + \varepsilon(u)\big) d(u, v).$$

In [35] the present authors investigated the eccentric distance sum of unicyclic graphs with given girth and characterized the extremal graphs with the minimal and the second minimal eccentric distance sum. Furthermore, the authors characterized the extremal trees with minimal and second minimal eccentric distance sum in the class of trees with given diameter. Inspired by papers [1,35] we continue the research on the eccentric distance sum invariant.

This paper is organized as follows. In Section 2 we introduce one graph transformation that increases the eccentric distance sum and using this result we prove that path P_n is the unique extremal tree on n vertices having maximum $\xi^d(G)$. In Section 3 we present explicit formulae for the values of eccentric distance sum for the Cartesian product, applied to some graphs of chemical interest. In Section 4 various lower and upper bounds for the eccentric distance sum in terms of other graph invariants (the Wiener index, the degree distance, eccentric connectivity index, independence number, connectivity, matching number, chromatic number and clique number) are established.

2. The maximal EDS of trees

Theorem 2.1. *Let w be a vertex of a nontrivial connected graph G. For nonnegative integers p and q, let $G(p,q)$ denote the graph obtained from G by attaching to vertex w pendant paths $P = wv_1v_2 \ldots v_p$ and $Q = wu_1u_2 \ldots u_q$ of lengths p and q, respectively. Let $G(p+q, 0) = G(p,q) - wu_1 + v_pu_1$. Let r be the eccentricity of the vertex w in G. If $r \geqslant p \geqslant q \geqslant 1$, then*

$$\xi^d\big(G(p,q)\big) < \xi^d\big(G(p+q,0)\big).$$

Proof. Let $\varepsilon'(v)$ (resp. $\varepsilon(v)$) denote the eccentricity of v in $G(p+q,0)$ (resp. $G(p,q)$). Since $\varepsilon(w) = r \geqslant p \geqslant q$, we have

$$\varepsilon'(v_i) \geqslant \varepsilon(v_i) = i + r, \quad i = 1, 2, \ldots, p,$$
$$\varepsilon'(u_j) = p + j + r, \qquad \varepsilon(u_j) = j + r, \quad j = 1, 2, \ldots, q,$$
$$\varepsilon'(w) \geqslant \varepsilon(w) = r.$$

The eccentricities of the vertices in G do not decrease, $\varepsilon'(v) \geqslant \varepsilon(v)$ for $v \in G$. Let $D = \sum_{v \in G} d(v, w)$ be the sum of distances from w to all vertices from G.

We have the following contribution of vertices $v_1, v_2, \dots, v_p$ in EDS of $G(p,q)$

$$\sum_{i=1}^{p} (i+r)\big((1+\dots+(i-1)) + (1+\dots+(p-i)) + ((i+1)+\dots+(i+q)) + |G| \cdot i + D\big),$$

while in EDS of $G(p+q,0)$ we have at least

$$\sum_{i=1}^{p} (i+r)\big((1+\dots+(i-1)) + (1+\dots+(p-i+q)) + |G| \cdot i + D\big).$$

For the difference of contributions for $\xi^d(G(p+q,0))$ and $\xi^d(G(p,q))$, we get

$$\Delta_1 \geqslant -\frac{pq}{6}\big(2+3p+p^2+6r\big).$$

Similarly, we have the following contribution of vertices $u_1, u_2, \dots, u_q$ in EDS of $G(p,q)$

$$\sum_{j=1}^{q} (j+r)\big(1+\dots+(j-1) + 1+\dots+(q-j) + (j+1)+\dots+(j+p) + |G| \cdot j + D\big),$$

while in EDS of $G(p+q,0)$ we have at least

$$\sum_{j=1}^{q} (p+j+r)\big(1+\dots+(j+p-1) + 1+\dots+(q-j) + |G| \cdot (j+p) + D\big).$$

For the difference of contributions for $\xi^d(G(p+q,0))$ and $\xi^d(G(p,q))$ we get

$$\Delta_2 \geqslant \frac{pq}{6}\big(-5+6D+3p^2-3q+3pq+2q^2-6r+6|G|(1+p+q+r)\big).$$

We have the following contribution of vertices from G in EDS of $G(p,q)$

$$\sum_{v \in G} \varepsilon(v)\left(\sum_{u \in G} d(u,v) + \sum_{i=1}^{p}\big(d(v,w)+i\big) + \sum_{j=1}^{q}\big(d(v,w)+j\big)\right),$$

while in EDS of $G(p+q,0)$ we have at least

$$\sum_{v \in G} \varepsilon(v)\left(\sum_{u \in G} d(u,v) + \sum_{i=1}^{p}\big(d(v,w)+i\big) + \sum_{j=1}^{q}\big(d(v,w)+j+p\big)\right).$$

For the difference of contributions for $\xi^d(G(p+q,0))$ and $\xi^d(G(p,q))$ we get

$$\Delta_3 \geqslant pq \sum_{v \in G} \varepsilon(v).$$

By summing all contributions, we get

$$\begin{aligned}
&\xi^d\big(G(p+q,0)\big) - \xi^d\big(G(p,q)\big) \\
&\quad \geqslant \Delta_1 + \Delta_2 + \Delta_3 \\
&\quad \geqslant \frac{pq}{6}\left(-7+6D+2p^2-3p+3pq-3q+2q^2-12r+6|G|(1+p+q+r)+6\sum_{v \in G}\varepsilon(v)\right).
\end{aligned}$$

Obviously, we have $|G| \geqslant 2$ and $6|G|(1+p+q+r) > 7+3p+3q+12r$. Therefore, $\xi^d(G(p+q,0)) > \xi^d(G(p,q))$. □

Note that if $T \ncong P_n$, then in T there is always a vertex w of degree greater than 2, such that we can apply Theorem 2.1 on w.

Let $e = (u,v)$ be an edge of G such that $G' = G - e$ is also connected. The removal of e does not introduce shorter paths than the ones in G, and therefore $d(i,j) \leqslant d'(i,j)$ for all $i, j \in V$. Moreover, $1 = d(u,v) < d'(u,v)$ and

$$\xi^d(G) < \xi^d\big(G'\big).$$

In particular, for any spanning tree T of G, we have that

$$\xi^d(G) \leqslant \xi^d(T). \tag{1}$$

The inequality (1) shows that the maximum eccentric distance sum will be attained for a particular tree. By repeated application of Theorem 2.1, the path P_n has maximal eccentric distance sum among all n-vertex graphs.

Theorem 2.2. *Among graphs on n vertices, the complete graph K_n has minimum and the path P_n has maximum value of eccentric distance sum.*

Next we will calculate $\xi^d(P_n)$.

Lemma 2.3. *(See [27].) Let $P_n = v_0 v_1 \ldots v_{n-1}$ be a path of order n. Then*

$$D_{P_n}(v_j) = \frac{1}{2}\bigl(2j^2 - 2(n-1)j + (n-1)^2 + (n-1)\bigr)$$

for $0 \leqslant j \leqslant n-1$.

Using the following formula for the vertex eccentricities of a path,

$$\varepsilon_{P_n}(v_j) = \begin{cases} j & \text{if } \lceil \frac{n-1}{2} \rceil \leqslant j \leqslant n-1, \\ n-1-j & \text{if } 0 \leqslant j \leqslant \lceil \frac{n-1}{2} \rceil - 1, \end{cases}$$

finally, we have

$$\xi^d(P_n) = \begin{cases} \frac{25n^4}{96} - \frac{n^3}{6} - \frac{17n^2}{48} + \frac{n}{6} + \frac{3}{32} & \text{if } n \text{ is odd}, \\ \frac{25n^4}{96} - \frac{n^3}{6} - \frac{7n^2}{24} + \frac{n}{6} & \text{if } n \text{ is even}. \end{cases}$$

3. Composite graphs

In [11,18,25,34], the authors obtained the eccentric connectivity index, the first and second Zagreb index, the PI index and the Wiener-type indices of some graph operations. Motivated by these results, here we present explicit formulae for the values of the eccentric distance sum for the Cartesian product and join of graphs.

The *Cartesian product* $G_1 \square G_2 \square \cdots \square G_k$ of graphs $G_1, G_2, \ldots, G_k$ has the vertex set $V(G_1) \times V(G_2) \times \cdots \times V(G_k)$, two vertices $(u_1, u_2, \ldots, u_k)$ and $(v_1, v_2, \ldots, v_k)$ being adjacent if they differ in exactly one position, say in i-th, and $u_i v_i$ is an edge of G_i. It is well known (see [24]) that for $G = G_1 \square G_2 \square \cdots \square G_k$ and its two vertices $u = (u_1, u_2, \ldots, u_k)$ and $v = (v_1, v_2, \ldots, v_k)$ we have

$$d_G(u, v) = \sum_{i=1}^{k} d_{G_i}(u_i, v_i).$$

The following relation is easily deduced

$$\varepsilon_{G_1 \square G_2}(u_1, u_2) = \varepsilon_{G_1}(u_1) + \varepsilon_{G_2}(u_2).$$

Theorem 3.1. *For graph G and H, we have*

$$\xi^d(G \square H) = |H|^2 \cdot \xi^d(G) + |G|^2 \cdot \xi^d(H) + 2|G|\zeta(G) \cdot W(H) + 2|H|\zeta(H) \cdot W(G),$$

where $|G|$ and $|H|$ denote the number of vertices of G and H, respectively.

Proof. For graphs G and H, we have

$$\begin{aligned}
\xi^d(G \square H) &= \sum_{(u_1,v_1),(u_2,v_2) \in V(G \square H)} \bigl(\varepsilon_{G \square H}(u_1, v_1) + \varepsilon_{G \square H}(u_2, v_2)\bigr) d_{G \square H}\bigl((u_1, v_1), (u_2, v_2)\bigr) \\
&= \sum_{u_1, u_2 \in G,\ v_1, v_2 \in H} \bigl(\varepsilon_G(u_1) + \varepsilon_H(v_1) + \varepsilon_G(u_2) + \varepsilon_H(v_2)\bigr)\bigl(d_G(u_1, u_2) + d_H(v_1, v_2)\bigr) \\
&= \sum_{u_1, u_2 \in G} \sum_{v_1, v_2 \in H} \bigl(\varepsilon_G(u_1) + \varepsilon_G(u_2)\bigr) d_G(u_1, u_2) + \sum_{u_1, u_2 \in G} \sum_{v_1, v_2 \in H} \bigl(\varepsilon_H(v_1) + \varepsilon_H(v_2)\bigr) d_H(v_1, v_2)
\end{aligned}$$

$$+\sum_{u_1,u_2\in G}\sum_{v_1,v_2\in H}\big(\varepsilon_G(u_1)+\varepsilon_G(u_2)\big)d_H(v_1,v_2)+\sum_{u_1,u_2\in G}\sum_{v_1,v_2\in H}\big(\varepsilon_H(v_1)+\varepsilon_H(v_2)\big)d_G(u_1,u_2)$$
$$=|H|^2\cdot\xi^d(G)+|G|^2\cdot\xi^d(H)+2|G|\zeta(G)\cdot W(H)+2|H|\zeta(H)\cdot W(G).$$

This completes the proof. □

It can be checked that (see [6,18])

$$W(P_n)=\frac{1}{6}n(n-1)(n+1),$$
$$W(C_n)=\begin{cases}\frac{n^3}{8} & \text{if } n \text{ is even},\\ \frac{n(n^2-1)}{8} & \text{if } n \text{ is odd},\end{cases}$$
$$\zeta(P_n)=\left\lfloor\frac{3}{4}n^2-\frac{1}{2}n\right\rfloor=\begin{cases}\frac{3}{4}n^2-\frac{1}{2}n & \text{if } n \text{ is even},\\ \frac{3}{4}n^2-\frac{1}{2}n-\frac{1}{4} & \text{if } n \text{ is odd},\end{cases}$$
$$\zeta(C_n)=n\left\lfloor\frac{1}{2}n\right\rfloor=\begin{cases}\frac{1}{2}n^2 & \text{if } n \text{ is even},\\ \frac{1}{2}n(n-1) & \text{if } n \text{ is odd}.\end{cases}$$

Since for a vertex u in C_n, $\varepsilon(u)=\lfloor\frac{n}{2}\rfloor$, we have

$$\xi^d(C_n)=\left\lfloor\frac{n}{2}\right\rfloor 2W(C_n)=n\left\lfloor\frac{n}{2}\right\rfloor\left\lfloor\frac{n^2}{4}\right\rfloor=\begin{cases}\frac{1}{8}n^4 & \text{if } n \text{ is even},\\ \frac{1}{8}n(n-1)(n^2-1) & \text{if } n \text{ is odd}.\end{cases}$$

For the rectangular grid $P_n \square P_m$, from Theorem 3.1, it follows

$$\xi^d(P_n\square P_m)=\begin{cases}\frac{1}{96}mn(32m-24m^2+(32-56m-32m^2+25m^3)n\\ \quad-(24+32m-48m^2)n^2+25mn^3) & \text{if } n,m \text{ are even},\\ \frac{1}{96}n(8m+32m^2-24m^3+(9+32m-62m^2-32m^3+25m^4)n\\ \quad-(32m+32m^2-48m^3)n^2+25m^2n^3) & \text{if } n \text{ is even}, m \text{ is odd},\\ \frac{1}{96}m(8n+32n^2-24n^3+(9+32n-62n^2-32n^3+25n^4)m\\ \quad-(32n+32n^2-48n^3)m^2+25n^2m^3) & \text{if } n \text{ is odd}, m \text{ is even},\\ \frac{1}{96}(9m^2+(16m+32m^2-32m^3)n+(9+32m-68m^2\\ \quad-32m^3+25m^4)n^2-(32m+32m^2-48m^3)n^3+25m^2n^4) & \text{if } n,m \text{ are odd}.\end{cases}$$

A C_4 nanotorus is a Cartesian product of two cycles $C_n \square C_m$, and it follows

$$\xi^d(C_n\square C_m)=\begin{cases}\frac{1}{8}m^2n^2(m+n)^2 & \text{if } n,m \text{ are even},\\ \frac{1}{8}mn^2(1-m-m^2+m^3-(1+m-2m^2)n+mn^2) & \text{if } n \text{ is even}, m \text{ is odd},\\ \frac{1}{8}nm^2(1-n-n^2+n^3-(1+n-2n^2)m+nm^2) & \text{if } n \text{ is odd}, m \text{ is even},\\ \frac{1}{8}mn(2m-m^2+(2-2m-2m^2+m^3)n-(1+2m-2m^2)n^2+mn^3) & \text{if } n,m \text{ are odd}.\end{cases}$$

A C_4 nanotube is a Cartesian product of path and cycle $P_n \square C_m$, and it follows

$$\xi^d(P_n\square C_m)=\begin{cases}\frac{1}{96}m^2n(16-16m-(28+12m-12m^2)n-(16-34m)n^2+25n^3) & \text{if } n,m \text{ are even},\\ \frac{1}{96}mn(32m-16m^2+(24-40m-24m^2+12m^3)n\\ \quad-(18+32m-34m^2)n^2+25mn^3) & \text{if } n \text{ is even}, m \text{ is odd},\\ \frac{1}{96}m^2(9+(16-22m)n-(34+12m-12m^2)n^2\\ \quad-(16-34m)n^3+25n^4) & \text{if } n \text{ is odd}, m \text{ is even},\\ \frac{1}{96}m(9m+(6+32m-22m^2)n+(24-46m-24m^2+12m^3)n^2\\ \quad-(18+32m-34m^2)n^3+25mn^4) & \text{if } n,m \text{ are odd}.\end{cases}$$

Let G and H be two graphs with $|G|$ and $|H|$ vertices, and $\|G\|$ and $\|H\|$ edges, respectively. The *join* $G\vee H$ of graphs G and H with disjoint vertex sets $V(G)$ and $V(H)$ and edge sets $E(G)$ and $E(H)$ is the graph union $G\cup H$ together with all the edges joining $V(G)$ and $V(H)$.

For $v \in V(G)$, we have

$$\varepsilon_{G\vee H}(v) = \begin{cases} 1 & \text{if } deg_G(v) = |G|-1, \\ 2 & \text{if } deg_G(v) < |G|-1, \end{cases}$$

$$D_{G\vee H}(v) = \begin{cases} |G|-1+|H| & \text{if } deg_G(v) = |G|-1, \\ deg_G(v) + 2(|G|-1-deg_G(v)) + |H| & \text{if } deg_G(v) < |G|-1. \end{cases}$$

Let

$$A_G = \{v \mid v \in G,\ deg_G(v) = |G|-1\}, \qquad B_G = \{v \mid v \in G,\ deg_G(v) < |G|-1\},$$
$$A_H = \{v \mid v \in H,\ deg_H(v) = |H|-1\}, \qquad B_H = \{v \mid v \in H,\ deg_H(v) < |H|-1\}.$$

Theorem 3.2. *For graphs G and H with parameters described above, we have*

$$\xi^d(G \vee H) = 4\big(|G|^2 + |H|^2 + |G||H| - |G| - |H| - \|G\| - \|H\|\big) - \big(|G|+|H|-1\big)\big(|A_G|+|A_H|\big).$$

Proof. For graphs G and H, we have

$$\begin{aligned}
\xi^d(G \vee H) &= \sum_{v\in A_G} \varepsilon_{G\vee H}(v)D_{G\vee H}(v) + \sum_{v\in B_G} \varepsilon_{G\vee H}(v)D_{G\vee H}(v) + \sum_{v\in A_H} \varepsilon_{G\vee H}(v)D_{G\vee H}(v) + \sum_{v\in B_H} \varepsilon_{G\vee H}(v)D_{G\vee H}(v) \\
&= |A_G|\big(|G|-1+|H|\big) + 2\sum_{v\in B_G}\big(deg_G(v) + 2\big(|G|-1-deg_G(v)\big) + |H|\big) + |A_H|\big(|H|-1+|G|\big) \\
&\quad + 2\sum_{v\in B_H}\big(deg_H(v) + 2\big(|H|-1-deg_H(v)\big) + |G|\big) \\
&= |A_G|\big(|G|-1+|H|\big) + 2\big(2|G|+|H|-2\big)|B_G| - 2\sum_{v\in B_G} deg_G(v) + |A_H|\big(|H|-1+|G|\big) \\
&\quad + 2\big(2|H|+|G|-2\big)|B_H| - 2\sum_{v\in B_H} deg_H(v) \\
&= |A_G|\big(|G|-1+|H|\big) + 2\big(2|G|+|H|-2\big)\big(|G|-|A_G|\big) - 2\left(2\|G\| - \sum_{v\in A_G} deg_G(v)\right) \\
&\quad + |A_H|\big(|H|-1+|G|\big) + 2\big(2|H|+|G|-2\big)\big(|H|-|A_H|\big) - 2\left(2\|H\| - \sum_{v\in A_H} deg_H(v)\right) \\
&= |A_G|\big(-|G|-|H|+1\big) + |G|\big(4|G|+2|H|-4\big) - 4\|G\| + |A_H|\big(-|G|-|H|+1\big) \\
&\quad + |H|\big(4|H|+2|G|-4\big) - 4\|H\| \\
&= 4\big(|G|^2 + |H|^2 + |G||H| - |G| - |H| - \|G\| - \|H\|\big) - \big(|G|+|H|-1\big)\big(|A_G|+|A_H|\big),
\end{aligned}$$

and this completes the proof. □

4. Relations with other parameters

The graphs satisfying $r(G) = d(G)$ are called *self-centered graphs* [5].

Theorem 4.1. *Let G be a connected graph with radius $r(G)$ and diameter $d(G)$. Then*

$$2W(G)\cdot r(G) \leqslant \xi^d(G) \leqslant 2W(G)\cdot d(G),$$

with equality if and only if G is a self-centered graph.

Proof. Using simple inequality $r(G) \leqslant \varepsilon(v) \leqslant d(G)$ and $\sum_{v\in V} D(v) = 2W(G)$, the result follows. □

Let $K_n - ke$ be the graph formed by deleting k, where $k = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$, independent edges from the complete graph K_n.

Theorem 4.2. *Let G be a connected graph on $n \geqslant 3$ vertices. Then*

$$\xi^d(G) \leqslant 2n \cdot W(G) - DD(G),$$

with equality if and only if $G \cong K_n - ke$, for $k = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor$, or $G \cong P_4$.

Proof. Let $d_i(v)$ be the number of vertices at distance i from the vertex v. It can be easily seen that $\varepsilon(v) \leqslant n - deg(v)$. The equality is achieved for $\varepsilon(v) = 1$ and $deg(v) = n-1$, or $\varepsilon(v) \geqslant 2$ and $d_2(v) = d_3(v) = \cdots = d_{\varepsilon(v)}(v) = 1$. Next, we get

$$\begin{aligned}\xi^d(G) &\leqslant \sum_{v\in V(G)} \big(n - deg(v)\big) D_G(v) \\ &= n \sum_{v\in V(G)} D_G(v) - \sum_{v\in V(G)} deg(v) D_G(v) \\ &= 2n \cdot W(G) - DD(G).\end{aligned}$$

Suppose that equality holds in the above inequality. If $\varepsilon(u) = 1$ for some $u \in V(G)$, then $deg(v) = n-1$ and $\varepsilon(v) \leqslant 2$ for all $v \neq u$. If $\varepsilon(v) = 1$ for all $v \in V(G)$, then $G \cong K_n$. Suppose that $\varepsilon(v) = 2$ for some $v \in V(G)$. Then, there exists a vertex $w \in V(G)$, such that $d(v,w) = 2$. Since $d_2(v) = d_2(w) = 1$, the vertex v is unique for fixed v, and it follows that $deg(v) = deg(w) = n-2$. This implies that $G \cong K_n - ke$, for $k = 1, 2, \ldots, \lfloor \frac{n-1}{2} \rfloor$.

In the other case, $\varepsilon(u) \geqslant 2$ for all $u \in V(G)$. If $\varepsilon(v) = 2$ for all $v \in V$, then $deg(v) = n-2$ for all $v \in V(G)$, implying that $G \cong K_n - \frac{n}{2}e$ (with even n). If $\varepsilon(v) \geqslant 3$ for some vertex v, then the diameter of G is equal to 3 (otherwise, the center vertex would have at least two neighbors at distance two), and $G \cong P_4$.

It can be easily seen that the upper bound for $\xi^d(G)$ is attained for $G \cong K_n - ke$, $k = 0, 1, \ldots, \lfloor \frac{n}{2} \rfloor$, or $G \cong P_4$. □

Let G be a connected graph on $n \geqslant 3$ vertices and minimum degree δ. Then from the proof of Theorem 4.2, we have

$$\xi^d(G) \leqslant \sum_{v\in V(G)} \big(n - deg(v)\big) D_G(v) \leqslant 2(n-\delta) W(G),$$

with equality if and only if $G \cong K_n$ or $G \cong K_n - \frac{n}{2}e$ for even n.

Theorem 4.3. *Let G be a connected graph on $n \geqslant 3$ vertices. Then $\xi^c(G) \leqslant \xi^d(G)$ with equality if and only if $G \cong K_n$.*

Proof. The result follows using simple relation $D_G(v) \geqslant deg(v)$, with equality if and only if $\varepsilon(v) = 1$ and $deg(v) = n-1$. □

Lemma 4.4. *(See [14].) Let G be a connected graph on $n \geqslant 3$ vertices and m edges. For any $v \in V(G)$, we have*

$$n - 1 \leqslant D_G(v) \leqslant \frac{1}{2}(n-1)(n+2) - m,$$

these bounds can be achieved for each m, $n - 1 \leqslant m \leqslant \binom{n}{2}$.

Theorem 4.5. *Let G be a connected graph on $n \geqslant 3$ vertices and m edges. Then*

$$(n-1)\zeta(G) \leqslant \xi^d(G) \leqslant \left(\frac{1}{2}(n-1)(n+2) - m\right) \cdot \zeta(G).$$

The lower bound holds if and only if $G \cong K_n$, while the upper bound can be achieved for each m, $n - 1 \leqslant m \leqslant \binom{n}{2}$.

Proof. The lower bound can be derived using a simple inequality $D_G(v) \geqslant n-1$. For the upper bound, using Lemma 4.4 it follows

$$\begin{aligned}\xi^d(G) &= \sum_{v\in V(G)} \varepsilon(v) D_G(v) \\ &\leqslant \left(\frac{1}{2}(n-1)(n+2) - m\right) \sum_{v\in V(G)} \varepsilon(v) \\ &= \left(\frac{1}{2}(n-1)(n+2) - m\right) \zeta(G).\end{aligned}$$

This implies the result. □

A subset S of $V(G)$ is called an *independent set* of G if no two vertices in S are adjacent in G. The *independence number* of G, denoted by $\alpha(G)$, is the size of a maximum independent set of G.

Since adding edges decreases the eccentric distance sum of G, from Theorem 3.2 we have

Theorem 4.6. *Let G be a connected graph of order n with the independence number α. Then*

$$\xi^d(G) \geqslant n^2 + (\alpha - 1)n + 2\alpha^2 - 3\alpha,$$

with equality if and only if $G \cong \overline{K_\alpha} \vee K_{n-\alpha}$.

For $k \geqslant 1$, a graph G is k-connected if either G is a complete graph K_{k+1}, or G has at least $k+2$ vertices and contains no $(k-1)$-vertex cut. The maximal value of k for which a connected graph G is k-connected is the connectivity of G, denoted by $\kappa(G)$. If G is disconnected, we define $\kappa(G) = 0$. If G is a graph of order n, then (1) $\kappa(G) \leqslant \kappa'(G) \leqslant n-1$; (2) $\kappa(G) = n-1$, $\kappa'(G) = n-1$ and $G \cong K_n$ are equivalent [17].

Theorem 4.7. *Let G be a connected graph of order n with the vertex connectivity k. Then*

$$\xi^d(G) \geqslant n^2 + (k+1)n - (k+1)^2 - 1,$$

with equality if and only if $G \cong K_k \vee (K_1 \cup K_{n-k-1})$.

Proof. Let G^* be a graph having the minimum EDS among all connected graphs of order n with connectivity k. Then there exists a vertex cut $C^* \subset V(G^*)$ with $|C^*| = k$, such that $G^* - C^* = G_1 \cup G_2 \cup \cdots \cup G_t$, where $G_1, G_2, \ldots, G_t$ are $t \geqslant 2$ connected components of $G^* - C^*$. Since adding edges will decrease EDS, we have $t = 2$, graphs G_1, G_2 and C^* are complete, and any vertex of G_1 and G_2 is adjacent to any vertex in C^*. Let $n_i = |G_i|$ for $i = 1, 2$ and $n_1 \leqslant n_2$. Then $G^* \cong K_k \vee (K_{n_1} \cup K_{n_2})$ and $n_1 + n_2 = n - k$. Therefore

$$\begin{aligned}
\xi^d(G^*) &= \sum_{v \in V(K_k)} \varepsilon_{G^*}(v) D_{G^*}(v) + \sum_{v \in V(K_{n_1})} \varepsilon_{G^*}(v) D_{G^*}(v) + \sum_{v \in V(K_{n_2})} \varepsilon_{G^*}(v) D_{G^*}(v) \\
&= k(k - 1 + n_1 + n_2) + n_1 \cdot 2(k + 2n_2 + n_1 - 1) + n_2 \cdot 2(k + 2n_1 + n_2 - 1) \\
&= k(k-1) + (3k-1)(n_1 + n_2) + 4n_1 n_2 + n_1^2 + n_2^2 \\
&= k(k-1) + (3k-1)(n-k) + 2n_1 n_2 + (n-k)^2 \\
&\geqslant k(k-1) + (3k-1)(n-k) + 2(n-k-1) + (n-k)^2 \\
&= n^2 + (k+1)n - k^2 - 2k - 2,
\end{aligned}$$

and the last equality holds if and only if $n_1 = 1$ and $n_2 = n - k - 1$. □

A matching M of the graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. The *matching number* of the graph G, denoted by $\beta(G)$, is the number of edges in a maximum matching. For a connected graph G with $n \geqslant 2$ vertices, $\beta(G) = 1$ if and only if $G \cong S_n$ or $G \cong K_3$, where S_n is the star with n vertices. Thus, we consider graphs with matching number at least 2. If $\beta(G) = \frac{n}{2}$, the graph has a perfect matching. Feng and Ilić [15] investigated the Zagreb, Harary and hyper-Wiener indices of graphs with given matching number. By modifying their method, we can get the following result.

Theorem 4.8. *Let G be a connected graph of order n with the matching number β, $2 \leqslant \beta \leqslant \lfloor \frac{n}{2} \rfloor$. Let $b = \frac{1}{20}(9 + 5n + \sqrt{(9+5n)^2 + 40(1-5n)})$. Then the following statements hold*:

(1) *if $\beta = \lfloor \frac{n}{2} \rfloor$, then $\xi^d(G) \geqslant n(n-1)$, with equality if and only if $G \cong K_n$*;
(2) *if $b < \beta \leqslant \lfloor \frac{n}{2} \rfloor - 1$, then $\xi^d(G) \geqslant 4n^2 - 9n - 8\beta^2 + 12\beta + 1$ with equality if and only if $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$*;
(3) *if $\beta = b$, then $\xi^d(G) \geqslant 4n^2 - 9n - 8\beta^2 + 12\beta + 1 = 4n^2 - 5n\beta - 4n + 2\beta^2 + 3\beta$ with equality if and only if $G \cong K_1 \vee (K_{2\beta-1} \cup \overline{K_{n-2\beta}})$, or $G \cong K_\beta \vee \overline{K_{n-\beta}}$*;
(4) *if $2 \leqslant \beta < b$, then $\xi^d(G) \geqslant 4n^2 - 5n\beta - 4n + 2\beta^2 + 3\beta$ with equality if and only if $G \cong K_\beta \vee \overline{K_{n-\beta}}$.*

Let $T_{n,k}$ be the *Turán graph* which is a complete k-partite graph on n vertices whose partite sets differ in size by at most one. This famous graph appears in many extremal graph theory problems [4,29,33].

Theorem 4.9. *Let G be a connected graph of order n with chromatic number χ. Assume that $n = \chi s + r$ with $0 \leqslant r < \chi$. Then*

$$\xi^d(G) \geqslant 2\big(n^2 + (n + r - \chi)s - n\big),$$

with equality if and only if $G \cong T_{n,\chi}$.

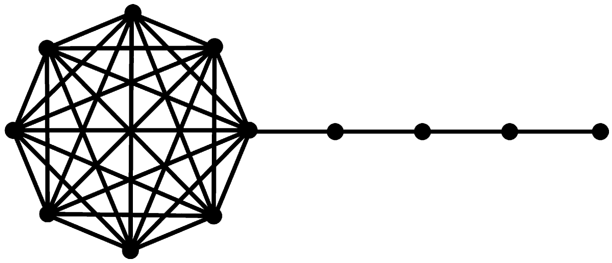

Fig. 1. The kite $K(12, 8)$.

Proof. Let G^* be a χ-chromatic graph with minimal EDS. Since adding new edges in a graph decreases EDS, G^* must be of the form $\overline{K_{n_1}} \vee \cdots \vee \overline{K_{n_\chi}}$. For any $v \in V(K_{n_i})$, it holds $\varepsilon(v) = 2$ and $D(v) = n + n_i - 2$. Therefore, we have

$$\xi^d(G^*) = \sum_{i=1}^{\chi} 2n_i(n + n_i - 2) = 2n(n-2) + 2\sum_{i=1}^{\chi} n_i^2.$$

Assume that $n_1 \leqslant n_2 \leqslant \cdots \leqslant n_\chi$. If $2 \leqslant n_i < n_j$, let

$$G' = \overline{K_{n_1}} \vee \cdots \vee \overline{K_{n_i+1}} \vee \cdots \vee \overline{K_{n_j-1}} \vee \cdots \vee \overline{K_{n_\chi}}.$$

Then we have

$$\begin{aligned} \xi^d(G^*) - \xi^d(G') &= 2n_i^2 + 2n_j^2 - 2(n_i+1)^2 - 2(n_j-1)^2 \\ &= 4(n_j - n_i - 1) \geqslant 0. \end{aligned}$$

Therefore, $T_{n,\chi}$ has the minimal EDS. By simple calculations, we get

$$\xi^d(T_{n,\chi}) = 2n(n-2) + 2\big((s+1)^2 r + s^2(\chi - r)\big) = \big(n^2 + (n + r - \chi)s - n\big),$$

which completes the proof. □

The *clique number* of a graph G is the size of a maximal complete subgraph of G and it is denoted as $\omega(G)$.

The *kite* $K(n,k)$ is obtained from a complete graph K_k and a path P_{n-k+1}, by joining one of the end vertices of P_{n-k+1} to one vertex of K_k (see Fig. 1). An asymptotically sharp upper bound for the eccentric connectivity index is derived independently in [10,28], with the extremal graph $K(n, \lfloor n/3 \rfloor)$. Furthermore, it is shown that the eccentric connectivity index grows no faster than a cubic polynomial in the number of vertices.

By similar transformation as described in Theorem 2.1, we can prove that

Theorem 4.10. *Let G be a connected graph of order n with clique number ω. Then*

$$\xi^d(G) \leqslant \xi^d\big(K(n,\omega)\big),$$

with equality if and only if $G \cong K(n,\omega)$.

Finally, we calculate the exact value of $\xi^d(K(n,\omega))$, which is

$$\xi^d\big(K(n,\omega)\big) = \begin{cases} \frac{1}{96}(112\omega - 292\omega^2 + 236\omega^3 - 59\omega^4 - 208n + 608\omega n - 552\omega^2 n \\ \quad + 152\omega^3 n - 220n^2 + 300\omega n^2 - 102\omega^2 n^2 + 16n^3 - 16\omega n^3 + 25n^4) & \text{if } n - \omega \text{ is even}, \\ \frac{1}{96}(9 + 100\omega - 286\omega^2 + 236\omega^3 - 59\omega^4 - 208n + 608\omega n - 552\omega^2 n \\ \quad + 152\omega^3 n - 226n^2 + 300\omega n^2 - 102\omega^2 n^2 + 16n^3 - 16\omega n^3 + 25n^4) & \text{if } n - \omega \text{ is odd}. \end{cases}$$

To get the result, let u be the vertex with degree $deg(u) = \omega$.

For the vertex u, we have $\varepsilon(u) = n - \omega$ and

$$D(u) = (\omega - 1) + 1 + 2 + \cdots + (n - \omega) = \omega - 1 + \frac{1}{2}(n - \omega + 1)(n - \omega).$$

For $v \in K_\omega$, we have $\varepsilon(v) = n - \omega + 1$ and

$$D(v) = \omega - 2 + 1 + 2 + \cdots + (n - \omega + 1) = \omega - 2 + \frac{1}{2}(n - \omega + 1)(n - \omega + 2).$$

For $v_j \in P_{n-\omega} = v_0 v_1 \ldots v_{n-\omega-1}$ (where the vertex v_0 is adjacent to u), we have

$$\varepsilon(v_j) = \begin{cases} j+2 & \text{if } \lceil \frac{n-\omega-1}{2} \rceil - 1 \leqslant j \leqslant n-\omega-1, \\ n-\omega-1-j & \text{if } 0 \leqslant j \leqslant \lceil \frac{n-\omega-1}{2} \rceil - 2, \end{cases}$$

and

$$\begin{aligned} D(v_j) &= \frac{1}{2}\big(2j^2 - 2(n-\omega-1)j + (n-\omega-1)^2 + (n-\omega-1)\big) + j + 1 + (j+2)(\omega-1) \\ &= \frac{1}{2}\big(-2 + 2j + 2j^2 + 5\omega + 4j\omega + \omega^2 - n - 2jn - 2\omega n + n^2\big). \end{aligned}$$

If $n-\omega$ is even,

$$\begin{aligned} \sum_{j=0}^{\frac{n-\omega}{2}-2} \varepsilon(v_j) D(v_j) &= \sum_{j=0}^{\frac{n-\omega}{2}-2} (n-\omega-1-j)\left(\frac{1}{2}\big(-2 + 2j + 2j^2 + 5\omega + 4j\omega + \omega^2 - n - 2jn - 2\omega n + n^2\big)\right) \\ &= \frac{1}{192}(\omega - n)(2 + \omega - n)\big(-80 - 70\omega + 9\omega^2 + 10n - 34\omega n + 25n^2\big), \end{aligned}$$

$$\begin{aligned} &\sum_{\frac{n-\omega}{2}-1}^{n-\omega-1} \varepsilon(v_j) D(v_j) \\ &\quad = \sum_{\frac{n-\omega}{2}-1}^{n-\omega-1} (j+2)\left(\frac{1}{2}\big(-2 + 2j + 2j^2 + 5\omega + 4j\omega + \omega^2 - n - 2jn - 2\omega n + n^2\big)\right) \\ &\quad = \frac{1}{192}(2 - \omega + n)\big(-96 + 192\omega - 130\omega^2 + 31\omega^3 - 96n + 108\omega n - 37\omega^2 n + 22n^2 - 19\omega n^2 + 25n^3\big). \end{aligned}$$

If $n-\omega$ is odd,

$$\begin{aligned} &\sum_{j=0}^{\frac{n-\omega-1}{2}-2} \varepsilon(v_j) D(v_j) \\ &\quad = \sum_{j=0}^{\frac{n-\omega-1}{2}-2} (n-\omega-1-j)\left(\frac{1}{2}\big(-2 + 2j + 2j^2 + 5\omega + 4j\omega + \omega^2 - n - 2jn - 2\omega n + n^2\big)\right) \\ &\quad = \frac{1}{192}(3 + \omega - n)\big(-1 - 57\omega + 49\omega^2 + 9\omega^3 + 49n - 26\omega n - 43\omega^2 n - 23n^2 + 59\omega n^2 - 25n^3\big), \end{aligned}$$

$$\begin{aligned} \sum_{j=\frac{n-\omega-1}{2}-1}^{n-\omega-1} \varepsilon(v_j) D(v_j) &= \sum_{j=\frac{n-\omega-1}{2}-1}^{n-\omega-1} (j+2)\left(\frac{1}{2}\big(-2 + 2j + 2j^2 + 5\omega + 4j\omega + \omega^2 - n - 2jn - 2\omega n + n^2\big)\right) \\ &= \frac{1}{192}(3 - \omega + n)(-1 + \omega - n)\big(57 - 80\omega + 31\omega^2 + 16n - 6\omega n - 25n^2\big). \end{aligned}$$

Finally, we have

$$\begin{aligned} \xi^d\big(K(n,\omega)\big) &= (\omega-1)(n-\omega+1)\left(\omega - 2 + \frac{1}{2}(n-\omega+1)(n-\omega+2)\right) \\ &\quad + (n-\omega)\left(\omega - 1 + \frac{1}{2}(n-\omega+1)(n-\omega)\right) + \sum_{j=0}^{n-\omega-1} \varepsilon(v_j) D(v_j), \end{aligned}$$

and this implies the formula.

5. Concluding remarks

In this paper we introduced one graph transformation that increases the eccentric distance sum and proved that path P_n is the unique extremal trees with n vertices having maximum eccentric distance sum. Various lower and upper bounds for the eccentric distance sum in terms of other graph invariants are established. Furthermore, we presented explicit formulae for the values of eccentric distance sum for the Cartesian product, applied to some graphs of chemical interest.

There are still many interesting open questions for the further study. It would be interesting to compute the values of $\xi^d(G)$ for various classes of graphs, and to introduce the ordering of trees and unicyclic graphs with respect to eccentric distance sum. In the following, we present three derivative indices of the eccentric distance sum and research of those indices seems the most natural course of the future work.

The *adjacent eccentric distance sum index* is defined in [31] as

$$\xi^{sv}(G) = \sum_{v \in V(G)} \frac{\varepsilon(v) \cdot D(v)}{deg(v)}.$$

The *augmented and super augmented eccentric connectivity indices* [3,12] are novel modifications of the eccentric connectivity index with augmented discriminating power,

$$\xi^{ac}(G) = \sum_{v \in V(G)} \frac{M(v)}{\varepsilon(v)} \quad \text{and} \quad \xi^{sac}(G) = \sum_{v \in V(G)} \frac{M(v)}{\varepsilon^2(v)},$$

where $M(v)$ is the product of degrees of all neighboring vertices of v. These indices were found to exhibit high sensitivity towards the presence and relative position of heteroatoms.

References

[1] A.R. Ashrafi, M. Saheli, M. Ghorbani, The eccentric connectivity index of nanotubes and nanotori, J. Comput. Appl. Math., doi:10.1016/j.cam.2010.03.001, in press.
[2] A.R. Ashrafi, T. Došlić, M. Saheli, The eccentric connectivity index of TUC4C8(R) nanotubes, MATCH Commun. Math. Comput. Chem. 65 (2011) 221–230.
[3] S. Bajaj, S.S. Sambi, S. Gupta, A.K. Madan, Model for prediction of anti-HIV activity of 2-pyridinone derivatives using novel topological descriptor, QSAR Comb. Sci. 25 (2006) 813–823.
[4] B. Bollobás, Turán's theorem and maximal degrees, J. Combin. Theory Ser. B 75 (1999) 160–164.
[5] F. Buckley, Self-centered graphs, Ann. New York Acad. Sci. 576 (1989) 71–78.
[6] P. Dankelmann, W. Goddard, C.S. Swart, The average eccentricity of a graph and its subgraphs, Util. Math. 65 (2004) 41–51.
[7] A. Dobrynin, A.A. Kochetova, Degree distance of a graph: A degree analogue of the Wiener index, J. Chem. Inf. Comput. Sci. 34 (1994) 1082–1086.
[8] A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, Acta Appl. Math. 66 (2001) 211–249.
[9] A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, Acta Appl. Math. 72 (2002) 247–294.
[10] T. Došlić, M. Saheli, D. Vukičević, Eccentric connectivity index: Extremal graphs and values, Iran. J. Math. Chem. 1 (2010), in press.
[11] T. Došlić, M. Saheli, Eccentric connectivity index of composite graphs, manuscript, 2009.
[12] H. Dureja, S. Gupta, A.K. Madan, Predicting anti-HIV-1 activity of 6-arylbenzonitriles: Computational approach using superaugmented eccentric connectivity topochemical indices, J. Mol. Graph. Model. 26 (2008) 1020–1029.
[13] S. Gupta, M. Singh, A.K. Madan, Application of graph theory: Relationship of eccentric connectivity index and Wiener's index with anti-inflammatory activity, J. Math. Anal. Appl. 266 (2002) 259–268.
[14] R.C. Entringer, D.E. Jackson, D.A. Snyder, Distance in graphs, Czechoslovak Math. J. 26 (101) (1976) 283–296.
[15] L. Feng, A. Ilić, Zagreb, Harary and hyper-Wiener indices of graphs with given matching number, Appl. Math. Lett. 23 (2010) 943–948.
[16] S. Gupta, M. Singh, A.K. Madan, Eccentric distance sum: A novel graph invariant for predicting biological and physical properties, J. Math. Anal. Appl. 275 (2002) 386–401.
[17] F. Harary, The maximum connectivity of a graph, Proc. Natl. Acad. Sci. USA 48 (1962) 1142–1146.
[18] S. Hossein-Zadeh, A. Hamzeh, A.R. Ashrafi, Wiener-type invariants of some graph operations, Filomat 23 (3) (2009) 103–113.
[19] H. Hua, Wiener and Schultz molecular topological indices of graphs with specified cut edges, MATCH Commun. Math. Comput. Chem. 61 (2009) 643–651.
[20] A. Ilić, S. Klavžar, D. Stevanović, Calculating the degree distance of partial hamming graphs, MATCH Commun. Math. Comput. Chem. 63 (2010) 411–424.
[21] A. Ilić, I. Gutman, Eccentric connectivity index of chemical trees, MATCH Commun. Math. Comput. Chem. 65 (2011) 731–744.
[22] A. Ilić, Eccentric connectivity index, in: I. Gutman, B. Furtula (Eds.), Novel Molecular Structure Descriptors – Theory and Applications II, in: Math. Chem. Monogr., vol. 9, University of Kragujevac, 2010.
[23] I. Gutman, Selected properties of the Schultz molecular topological index, J. Chem. Inf. Comput. Sci. 34 (1994) 1087–1089.
[24] W. Imrich, S. Klavžar, Product Graphs: Structure and Recognition, John Wiley & Sons, New York, 2000.
[25] M.H. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi, The first and second Zagreb indices of some graph operations, Discrete Appl. Math. 157 (2009) 804–811.
[26] V. Kumar, S. Sardana, A.K. Madan, Predicting anti-HIV activity of 2, 3-diaryl-1, 3 thiazolidin-4-ones: Computational approach using reformed eccentric connectivity index, J. Mol. Model. 10 (2004) 399–407.
[27] H. Liu, X.F. Pan, On the Wiener index of trees with fixed diameter, MATCH Commun. Math. Comput. Chem. 60 (2008) 85–94.
[28] M.J. Morgan, S. Mukwembi, H.C. Swart, On the eccentric connectivity index of a graph, Discrete Math., doi:10.1016/j.disc.2009.12.013, in press.
[29] V. Nikiforov, Spectral saturation: inverting the spectral Turán theorem, Electron. J. Combin. 15 (2009) #R33.
[30] S. Sardana, A.K. Madan, Predicting anti-HIV activity of TIBO derivatives: a computational approach using a novel topological descriptor, J. Mol. Model. 8 (2002) 258–265.
[31] S. Sardana, A.K. Madan, Relationship of Wiener's index and adjacent eccentric distance sum index with nitroxide free radicals and their precursors as modifiers against oxidative damage, J. Mol. Struct. (Theochem) 624 (2003) 53–59.
[32] V. Sharma, R. Goswami, A.K. Madan, Eccentric connectivity index: A novel highly discriminating topological descriptor for structure property and structure activity studies, J. Chem. Inf. Comput. Sci. 37 (1997) 273–282.
[33] P. Turán, On an extremal problem in graph theory, Mat. Fiz. Lapok 48 (1941) 436–452.
[34] H. Yousefi-Azari, B. Manoochehrian, A.R. Ashrafi, The PI index of product graphs, Appl. Math. Lett. 21 (2008) 624–627.
[35] G. Yu, L. Feng, A. Ilić, On the eccentric distance sum of trees and unicyclic graphs, J. Math. Anal. Appl. 375 (2011) 934–944.
[36] B. Zhou, Z. Du, On eccentric connectivity index, MATCH Commun. Math. Comput. Chem. 63 (2010) 181–198.