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Terminal eccentricity indices of graphs

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Abstract

Let $V_T(G)$ be the set of pendent vertices of G and $d(u,v)$ be the distance between the vertices u and v. The terminal eccentricity of a vertex u is defined as $te_G(u) = \max\{d(u,v) \mid v \in V_T(G)\}$. In this paper we introduce new topological indices of graphs called as first and second terminal eccentricity indices and are defined as

$$TE_1(G) = \sum_{uv \in E(G)} [te_G(u) + te_G(v)] \quad \text{and} \quad TE_2(G) = \sum_{uv \in E(G)} te_G(u) te_G(v),$$

where $E(G)$ is the edge set of G. We discuss properties of terminal eccentricity indices of graphs and carry regression analysis of these indices with the chemical properties of benzenoid hydrocarbons. The terminal eccentricity indices are useful in the graphs where pendent vertices exists.

Keywords: Eccentricity of a vertex, Terminal eccenticity of a vertex, Terminal eccentricity indices.

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1. Introduction

Topological indices are mathematical boundaries of a graph which characterize its topology and are typically graph invariant. Over the years numerous topological indices are proposed and contemplated dependent on the degree, distance and other parameters of graphs. Some of them might be found in [2, 3, 4, 5, 8, 9, 10, 11]. The indices based on the terminal distances are terminal Wiener index [6] and terminal status indices [7].

Let G be a simple, connected graph with n vertices and m edges. Let $V(G)$ be the vertex set and $E(G)$ be the edge set of G. The edge joining the vertices u and v is denoted by uv. Two vertices are said to be neighbors of each other if they are adjacent. The degree of a vertex u in a graph G is the number of its neighbors and is denoted by $d_G(u)$. A vertex u is said to be terminal vertex or pendent vertex if $d_G(u) = 1$. In G, the distance between the vertices u and v is the length of the shortest path joining them and is denoted by $d_G(u,v)$. The diameter of a graph G, denoted by $diam(G)$ is the maximum distance between any pair of vertices of G.

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The eccentricity of a vertex u, denoted by $e_G(u)$ is defined as

$$e_G(u) = \max\{d_G(u,v) \mid v \in V(G)\}.$$

The eccentricity indices of graphs are defined as [1]

$$\xi_1(G) = \sum_{uv \in E(G)} [e_G(u) + e_G(v)] \quad \text{and} \quad \xi_2(G) = \sum_{uv \in E(G)} e_G(u)e_G(v).$$

Let $V_T(G) = \{v_1, v_2, \ldots, v_k\}$ be the set of all pendent vertices of G.

The terminal status of a vertex u is defined as

$$ts_G(u) = \sum_{v \in V_T(G)} d_G(u,v). \tag{1.1}$$

This distance-based molecular structure descriptor was put forward by Ramane et al. [7].

Analogous to the Eq. (1.1), we define here the terminal eccentricity of a vertex u as

$$te_G(u) = max\{d(u,v) \mid v \in V_T(G)\},$$

where $V_T(G)$ is the set of all pendent vertices of G.

The first and second status connectivity indices of a connected graph G are defined as [7]

$$TS_1(G) = \sum_{uv \in E(G)} [ts_G(u) + ts_G(v)] \tag{1.2}$$

and

$$TS_2(G) = \sum_{uv \in E(G)} ts_G(u)ts_G(v). \tag{1.3}$$

Motivated by the invariants as above, we define here first and second terminal eccentricity indices $TE_1(G)$ and $TE_2(G)$ of a connected graph G as:

$$TE_1(G) = \sum_{uv \in E(G)} [te_G(u) + te_G(v)]$$

and

$$TE_2(G) = \sum_{uv \in E(G)} te_G(u)te_G(v).$$

The vertex set of a graph given in Fig. 1 is $V(G) = \{v_1, v_2, v_3, v_4, v_5, v_6, v_7\}$ and pendent vertex set is $V_T(G) = \{v_1, v_2, v_7\}$. The terminal eccentricity of vertices of G are $te_G(v_1) = 3$, $te_G(v_2) = 3$, $te_G(v_3) = 2$, $te_G(v_4) = 2$, $te_G(v_5) = 3$, $te_G(v_6) = 3$ and $te_G(v_7) = 3$. Therefore $TE_1(G) = 35$ and $TE_2(G) = 43$.

2. Terminal eccentricity of a vertex

Observations:

1. If G has no pendent vertex, then $te_G(u) = 0$ for all $u \in V(G)$.
2. If G has exactly one pendent vertex, say v, then $te_G(v) = 0$.
3. If G has at least one pendent vertex, then $te_G(u) \geqslant 1$, where u is not a pendent vertex.
4. If G has at least two pendent vertices, then $te_G(u) \geqslant 1$, for all $u \in V(G)$.
5. There is no pendent vertex in G such that $te_G(u) = 1$, except for $G \cong K_2$, where K_n is a complete graph on n vertices.

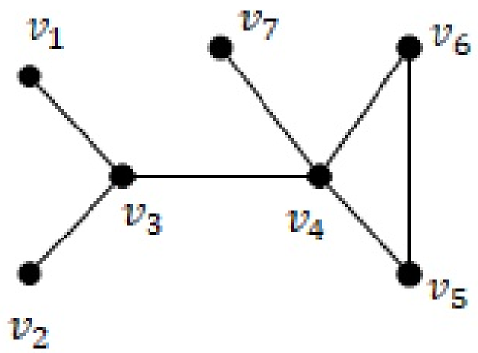

Figure 1: Graph G

Theorem 2.1. Let G be a graph on n vertices with $\mathrm{diam}(G) \leqslant 2$ and $n_t \geqslant 1$ be the number of pendent vertices of G.
(i) If u is not a pendent vertex, then

$$te_G(u) = \begin{cases} 2, & \text{if } u \text{ has no pendent neighbor} \\ 1, & \text{if } u \text{ has pendent neighbor.} \end{cases}$$

(ii) If u is a pendent vertex, then

$$te_G(u) = \begin{cases} 0, & \text{for } n_t = 1 \\ 1, & \text{for } n = 2 \\ 2, & \text{for } n \geqslant 3 \text{ and } n_t \geqslant 2. \end{cases}$$

Proof. (i) Let u be a non-pendent vertex having no pendent neighbor. Then the distance between vertex u and any pendent vertex is 2. Therefore $te_G(u) = 2$. Similarly if u is non pendent vertex having pendent neighbor, then the distance between vertex u and any pendent vertex is 1. Therefore $te_G(u) = 1$.

(ii) Let u be the pendent vertex. If $n_t = 1$ then $te_G(u) = 0$. If $n = 2$, then $G \cong K_2$. Hence for any pendent vertex u of K_2, $te_G(u) = 1$. Now let $n \geqslant 3$ and $n_t \geqslant 2$. Then distance between u and any other pendent vertex is 2. Therefore $te_G(u) = 2$. □

The graph G^+ is obtained from G by attaching one pendent vertex to each vertex of G.

Theorem 2.2. Let G be a connected graph on n vertices with vertex set $V(G)$. Then,

$$te_{G^+}(u) = \begin{cases} 2 + e_G(v), & \text{if } u \text{ is a pendent in } G^+ \text{ and } u \text{ is adjacent to } v \text{ in } G \\ 1 + e_G(u), & \text{if } u \text{ is not a pendent vertex in } G^+. \end{cases}$$

Proof. Case 1: Let u be the pendent vertex in G^+ adjacent to $v \in V(G)$ and x be the pendent vertex in G^+ adjacent to $w \in V(G)$. Then

$$\begin{aligned} te_{G^+}(u) &= d_{G^+}(u,v) + \max\{d(v,w) \mid w \in V(G)\} + d_{G^+}(w,x) \\ &= 1 + e_G(v) + 1 \\ &= 2 + e_G(v). \end{aligned}$$

Case 2: Let u be the non-pendent vertex in G^+ and x be the pendent vertex in G^+ adjacent to $w \in V(G)$. Then

$$\begin{aligned} te_{G^+}(u) &= \max\{d(u,w) \mid w \in V(G)\} + d_{G^+}(w,x) \\ &= e_G(u) + 1. \end{aligned}$$

□

3. Terminal eccentricity indices of graphs

Observations:

1. If G has no pendent vertex then $TE_1(G) = 0$ and $TE_2(G) = 0$.
2. If G has at least two pendent vertices, then $TE_1(G) \geqslant 2$ and $TE_2(G) \geqslant 1$.

Theorem 3.1. Let G be a connected graph with $diam(G) = 2$ having n vertices and m edges. Then

$$TE_1(G) = 4m - n + 1 \quad \text{and} \quad TE_2(G) = 4m - 2n + 2.$$

Proof. The edge set $E(G)$ can be partitioned into three sets E_1, E_2 and E_3, where
$E_1 = \{uv \mid u$ and v has no pendent neighbor and $d_G(u), d_G(v) > 1\}$,

$E_2 = \{uv \mid u$ has pendent neighbor but v does not or vice-versa and $d_G(u), d_G(v) > 1\}$ and

$E_3 = \{uv \mid$ either u or v is a pendent vertex$\}$.

It is easy to check that $|E_1| = m - n + 1$, $|E_2| = n - n_t - 1$ and $|E_3| = n_t$, where n_t is the number of pendent vertices. Therefore

$$\begin{aligned} TE_1(G) &= \sum_{uv \in E(G)} [te_G(u) + te_G(v)] \\ &= \sum_{uv \in E_1} [te_G(u) + te_G(v)] + \sum_{uv \in E_2} [te_G(u) + te_G(v)] + \sum_{uv \in E_3} [te_G(u) + te_G(v)] \\ &= \sum_{uv \in E_1} [2+2] + \sum_{uv \in E_2} [1+2] + \sum_{uv \in E_3} [2+1] \\ &= 4(m - n + 1) + 3(n - n_t - 1) + 3n_t \\ &= 4m - n + 1 \end{aligned}$$

and

$$\begin{aligned} TE_2(G) &= \sum_{uv \in E(G)} te_G(u) te_G(v) \\ &= \sum_{uv \in E_1} te_G(u) te_G(v) + \sum_{uv \in E_2} te_G(u) te_G(v) + \sum_{uv \in E_3} te_G(u) te_G(v) \\ &= \sum_{uv \in E_1} (2)(2) + \sum_{uv \in E_2} (1)(2) + \sum_{uv \in E_3} (2)(1) \\ &= 4(m - n + 1) + 2(n - n_t - 1) + 2n_t \\ &= 4m - 2n + 2. \end{aligned}$$

□

Theorem 3.2. Let G be a connected graph with n vertices and m edges. Then

$$TE_1(G^+) = 3n + 2m + 2 \sum_{u \in V(G)} e_G(u) + \xi_1(G)$$

and

$$TE_2(G^+) = 2n + m + \sum_{u \in V(G)} \left(3e_G(u) + e_G(u)^2\right) + \xi_1(G) + \xi_2(G).$$

Proof. The edge set $E(G^+)$ can be partitioned into two sets E_1 and E_2, where $E_1 = \{uv \mid d_{G^+}(u) = 1 \text{ and } d_{G^+}(v) > 1\}$, and

$$E_2 = \{uv \mid d_{G^+}(u) > 1 \text{ and } d_{G^+(}v) > 1\}.$$

It is easy to check that $|E_1| = n$ and $|E_2| = m$. Therefore

$$\begin{aligned} TE_1(G) &= \sum_{uv \in E(G^+)} [te_{G^+}(u) + te_{G^+}(v)] \\ &= \sum_{uv \in E_1} [te_{G^+}(u) + te_{G^+}(v)] + \sum_{uv \in E_2} [te_{G^+}(u) + te_{G^+}(v)] \\ &= \sum_{uv \in E_1} [2 + e_G(u) + 1 + e_G(v)] + \sum_{uv \in E_2} [1 + e_G(u) + 1 + e_G(v)] \\ &= 3n + 2 \sum_{u \in V(G)} e_G(u) + 2m + \sum_{uv \in E(G)} [e_G(u) + e_G(v)] \\ &= 3n + 2m + 2 \sum_{u \in V(G)} e_G(u) + \xi_1(G) \end{aligned}$$

and

$$\begin{aligned} TE_2(G) &= \sum_{uv \in E(G^+)} te_{G^+}(u) te_{G^+}(v) \\ &= \sum_{uv \in E_1} te_{G^+}(u) te_{G^+}(v) + \sum_{uv \in E_2} te_{G^+}(u) te_{G^+}(v) \\ &= \sum_{uv \in E_1} (2 + e_G(u))(1 + e_G(v)) + \sum_{uv \in E_2} (1 + e_G(u))(1 + e_G(v)) \\ &= 2n + \sum_{u \in V(G)} \left(3e_G(u) + e_G(u)^2\right) + m + \sum_{uv \in E(G)} [e_G(u) + e_G(v)] + \sum_{uv \in E(G)} e_G(u) e_G(v) \\ &= 2n + m + \sum_{u \in V(G)} \left(3e_G(u) + e_G(u)^2\right) + \xi_1(G) + \xi_2(G). \end{aligned}$$

□

4. Regression analysis

Here we carry regression analysis of the boiling point (BP) of benzenoid hydrocarbons (given in Fig. 2) with the terminal eccentricity indices of G^+ where G is the molecular graph of the benzenoid hydrocarbon.

Using the data given in Table 1, the linear regression models for the boiling point (BP) are

$$BP = 166.8(\pm 29.49) + 0.4543(\pm 0.0399) TE_1(G^+)$$

Table 1: The values of boiling point, $\mathsf{TE}_1(\mathsf{G}^+)$ and $\mathsf{TE}_2(\mathsf{G}^+)$ of benzenoid hydrocarbons.

Benzenoid hydrocarbon	Boiling point (BP) in ^{0}C	$\mathsf{TE}_1(\mathsf{G}^+)$	$\mathsf{TE}_2(\mathsf{G}^+)$
1	218	226	616
2	338	346	1275
3	340	414	1452
4	431	620	2520
5	425	628	2578
6	429	558	2016
7	440	654	2800
8	496	696	2826
9	493	638	2336
10	497	638	2336
11	547	772	3100
12	542	718	2651
13	535	808	3460
14	536	906	4382
15	531	866	3974
16	519	906	4382
17	590	798	2976
18	592	876	3775
19	596	988	4717
20	594	988	4718
21	595	854	3494

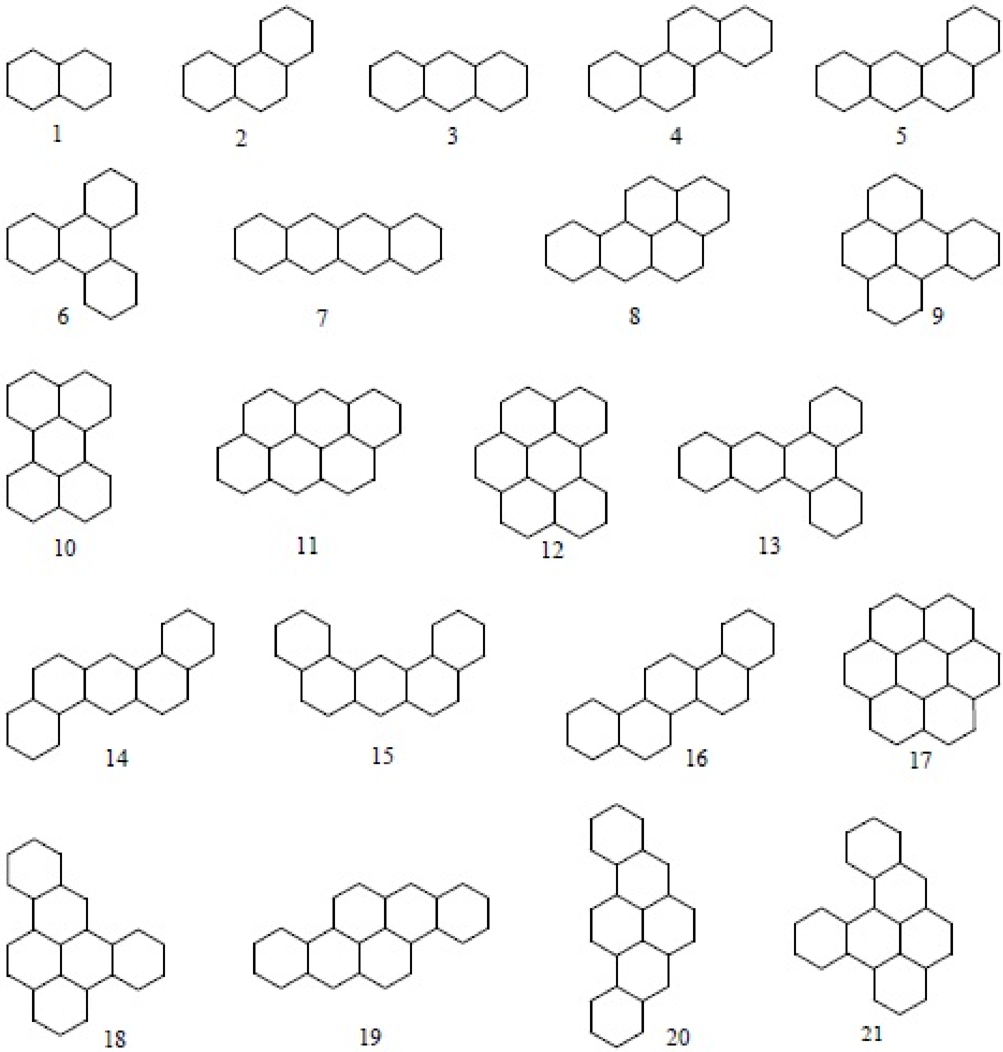

Figure 2: Benzenoid hydrocarbons

and

$$\mathsf{BP} = 265.7(\pm 34.32) + 0.0754(\pm 0.0108)\mathsf{TE}_2(\mathsf{G}^+).$$

The scatter plots between the boiling point and terminal eccentricity indices of G^+ of the molecular graphs of benzenoid htdrocarbons are shown in Figs. 3 and 4. Correlation coefficient between BP and $\mathsf{TE}_1(\mathsf{G}^+)$ is $\mathsf{R} = 0.9338$, where as correlation coefficient between BP and $\mathsf{TE}_2(\mathsf{G}^+)$ is $\mathsf{R} = 0.8473$. This shows that the linear model obtained between the values of boiling points and $\mathsf{TE}_1(\mathsf{G}^+)$ of benzenoid hydrocarbons is good one.

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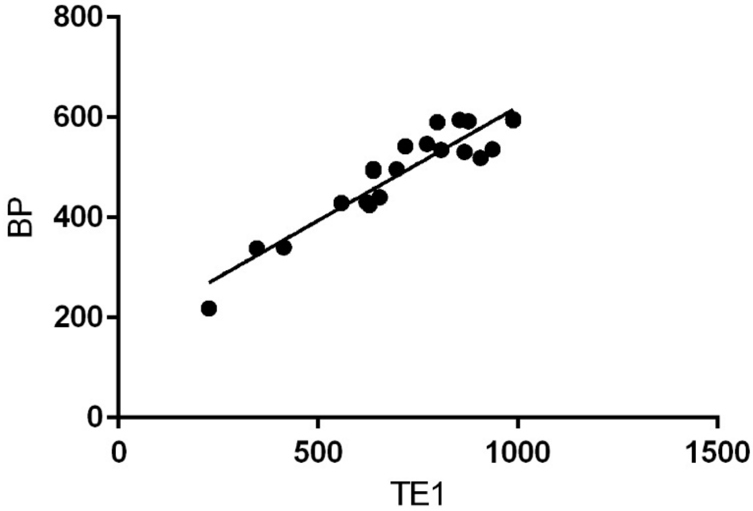

Figure 3: Scatter plot between BP and $\mathsf{TE}_1(\mathsf{G}^+)$

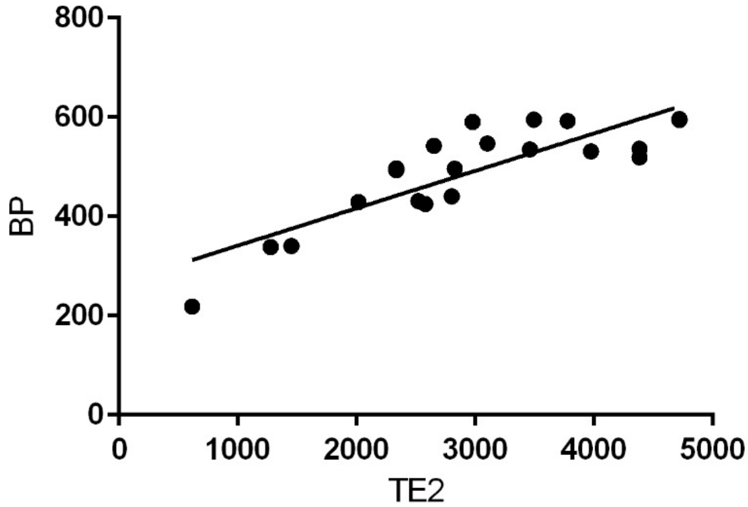

Figure 4: Scatter plot between BP and $\mathsf{TE}_2(\mathsf{G}^+)$

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