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TEMO-TYPE REGULARITY FOR TWO GENERAL DEGREE-BASED TOPOLOGICAL INDICES

Jiajia Wang, Zhen Lin, and Shumin Zhang

Abstract. TEMO-type regularity problem is an interesting topic in chemical graph theory. In this paper, we study TEMO-type regularity problem of the general Randić index and the (a, b)-KA index, which improves the known result of Gutman [**10**].

1. Introduction

In chemical graph theory, the topological indices or molecular structure descriptors are becoming more and more the focus of attention due to the fact that chemical, physical and biological properties of molecules have good correlations with these topological indices, especially the great number of successful applications of these descriptors in structure-property or activity relationships and their increasing role in molecular discovery [**2, 14, 21**]. In particular, a large number of the degree-based topological indices have been conceived, such as the Zagreb indices [**13**], the Randić index [**19**], the harmonic index [**5**], the sum-connectivity index [**22**], the reciprocal sum-connectivity index [**4**], the Hyper-Zagreb index [**20**], the forgotten topological index [**6**], the Hyper F-index [**7**], the Y-index [**1**], the zeroth-order Randić index [**14**], the Sombor index [**9**], etc.

Let G be a simple graph with the vertex set $V(G)$ and edge set $E(G)$. Let d_i be the degree of the vertex i in G. In 1998, the general Randić index, introduced

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by Bollobás and Erdős [**3**], is defined as

$$R_\alpha(G) = \sum_{uv\in E(G)} (d_u d_v)^\alpha,$$

where α is an arbitrary real number. Clearly, $R_{-1/2}(G)$ is the Randić index. For any real number a and b, the (a,b)-KA index of a graph G is defined as

$$KA_{a,b}(G) = \sum_{uv\in E(G)} (d_u^a + d_v^a)^b,$$

which is a novel general vertex-degree-based topological index proposed by Kulli [**15**]. Obviously, this index is general form of the above vertex-degree-based topological indices, such as $KA_{1,1}$ is the first Zagreb index and $KA_{2,1/2}$ is the Sombor index. For other situations, see [**16**].

For any two vertex-disjoint graphs G_1 and G_2, we assume that u and v are two distinct vertices of G_1, and p and q are two distinct vertices of G_2. Then S is the graph obtained from G_1 and G_2 by connecting u with p and v with q. The graph T is obtained analogously, by connecting u with q and v with p, see Figure 1.

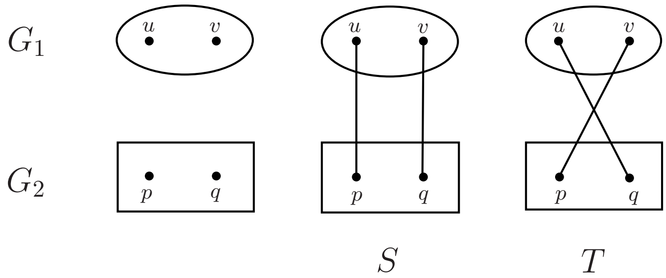

Figure 1. The structure of the graphs S and T and the labeling of their vertices.

In 1982, Polansky and Zander [**18**] studied the property of the graphs S and T, and compared the characteristic polynomials of S and T in the special case $G_1 \cong G_2$, that is $\phi(T,\lambda) \geqslant \phi(S,\lambda)$. Meanwhile, they called this a "topological effect on molecular orbitals" and used the acronym TEMO. Further, Gutman, Graovac and Polansky [**8, 11, 12, 17**] made the research express that the inequality $\phi(T,\lambda) \geqslant \phi(S,\lambda)$ implies certain regularities for the distribution of the eigenvalues of S and T and have appropriate (experimentally verifiable) consequences on the distribution of the molecular orbital energy levels. Eventually, TEMO was extensively studied, see the references in [**10**].

In 2022, Gutman [**10**] showed that a TEMO-type regularity holds for the Sombor index (SO), that is $SO(S) < SO(T)$. On this basis, we study TEMO-type regularity for the general Randić index and the (a,b)-KA index and obtain the following theorems, which extend the results of Gutman. Denote by d_u, d_v, d_p, d_q the degrees of the vertices u, v, p, q of the graphs S and T. It is obvious that if either $d_u = d_v$ or $d_p = d_q$ or both, then $R_\alpha(S) = R_\alpha(T)$ and $KA_{a,b}(S) = KA_{a,b}(T)$.

Therefore, we consider the case $d_u \neq d_v$ and $d_p \neq d_q$. Without loss of generality, we may assume that $d_u > d_v$ and $d_p > d_q$.

THEOREM 1.1. *Let G_1 and G_2 be arbitrary vertex-disjoint graphs and u, v, p, q their vertices as indicated in Figure 1. If $\alpha \neq 0$, $d_u > d_v$ and $d_p > d_q$, then*

$$R_\alpha(S) > R_\alpha(T).$$

THEOREM 1.2. *Let G_1 and G_2 be arbitrary vertex-disjoint graphs and u, v, p, q their vertices as indicated in Figure 1. If $d_u > d_v$ and $d_p > d_q$, then*
(i) *If $a \neq 0$ and $b \in (-\infty, 0) \cup (1, +\infty)$, then $KA_{a,b}(S) > KA_{a,b}(T)$.*
(ii) *If $a \neq 0$ and $b \in (0, 1)$, then $KA_{a,b}(S) < KA_{a,b}(T)$.*
Note that the degree of the vertex u in the graph G_1 is $d_u - 1$, etc.

2. Proofs of Theorems

LEMMA 2.1. *Let $F(x, y, z, w) = (x + z)^b + (y + w)^b - (y + z)^b - (x + w)^b$ be a quaternion function with regard to x, y, z, w and $(x - y)(z - w) > 0$, and $x, y, z, w \in (1, (n - 1)^a), n \in \mathbb{N}^+$ for $a > 0$, or $x, y, z, w \in ((n - 1)^a, 1), n \in \mathbb{N}^+$ for $a < 0$. Then we have*
(i) *If $b \in (-\infty, 0) \cup (1, +\infty)$, then $F(x, y, z, w)_{\min} > 0$.*
(ii) *If $b \in (0, 1)$, then $F(x, y, z, w)_{max} < 0$.*

PROOF. By taking partial derivative for x, y, z, w, respectively, we have

$$\frac{\partial F}{\partial x} = b(x + z)^{b-1} - b(x + w)^{b-1},$$

$$\frac{\partial F}{\partial z} = b(x + z)^{b-1} - b(y + z)^{b-1},$$

$$\frac{\partial F}{\partial y} = b(y + w)^{b-1} - b(y + z)^{b-1},$$

$$\frac{\partial F}{\partial w} = b(y + w)^{b-1} - b(x + w)^{b-1}.$$

Now we use the method of linear programming to prove eight cases:

- $x > y$, $z > w$, $b \in (-\infty, 0) \cup (1, +\infty)$, $a > 0$ and $x, y, z, w \in (1, (n - 1)^a), n \in \mathbb{N}^+$.
- $x < y$, $z < w$, $b \in (-\infty, 0) \cup (1, +\infty)$, $a > 0$ and $x, y, z, w \in (1, (n - 1)^a), n \in \mathbb{N}^+$.
- $x > y$, $z > w$, $b \in (-\infty, 0) \cup (1, +\infty)$, $a < 0$ and $x, y, z, w \in ((n - 1)^a, 1), n \in \mathbb{N}^+$.
- $x < y$, $z < w$, $b \in (-\infty, 0) \cup (1, +\infty)$, $a < 0$ and $x, y, z, w \in ((n - 1)^a, 1), n \in \mathbb{N}^+$.
- $x > y$, $z > w$, $b \in (0, 1)$, $a > 0$ and $x, y, z, w \in (1, (n - 1)^a), n \in \mathbb{N}^+$.
- $x < y$, $z < w$, $b \in (0, 1)$, $a > 0$ and $x, y, z, w \in (1, (n - 1)^a), n \in \mathbb{N}^+$.
- $x > y$, $z > w$, $b \in (0, 1)$, $a < 0$ and $x, y, z, w \in ((n - 1)^a, 1), n \in \mathbb{N}^+$.
- $x < y$, $z < w$, $b \in (0, 1)$, $a < 0$ and $x, y, z, w \in ((n - 1)^a, 1), n \in \mathbb{N}^+$.

However, we only discuss the following case, and the other seven cases prove almost the same.

If $x > y$, $z > w$, $b \in (-\infty, 0) \cup (1, +\infty)$, $a > 0$ and $x, y, z, w \in (1, (n-1)^a), n \in \mathbb{N}^+$, then

$$\frac{\partial F}{\partial x} = b(x+z)^{b-1} - b(x+w)^{b-1} > 0,$$
$$\frac{\partial F}{\partial z} = b(x+z)^{b-1} - b(y+z)^{b-1} > 0,$$
$$\frac{\partial F}{\partial y} = b(y+w)^{b-1} - b(y+z)^{b-1} < 0,$$
$$\frac{\partial F}{\partial w} = b(y+w)^{b-1} - b(x+w)^{b-1} < 0.$$

First, we take z and w as constant parameters and use linear programming to minimize the function $f(x, y) = (x+z)^b + (y+w)^b - (y+z)^b - (x+w)^b$, subject to

$$\begin{cases} 1 \leqslant x \leqslant (n-1)^a \\ 1 \leqslant y \leqslant (n-1)^a \\ x > y \end{cases}$$

then, the feasible region is shown in Figure 2.

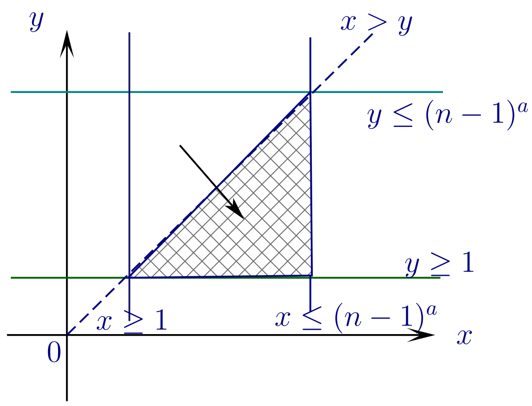

Figure 2. The feasible region of $f(x, y)$.

Therefore, we get that when $x \to y$, $f(x, y)$ tend to take the minimum value, i.e.

$$g(z, w) = f(x, y)_{min} = \lim_{x \to y} f(x, y).$$

Next, find the minimum of $g(z, w)$, subject to

$$\begin{cases} 1 \leqslant z \leqslant (n-1)^a \\ 1 \leqslant w \leqslant (n-1)^a \\ z > w \end{cases}$$

then, the feasible region is shown in Figure 3. Hence, we get that when $z \to w$, $g(z,w)$ tend to take the minimum value, i.e.,

$$F(x,y,z,w)_{min} = g(z,w)_{min} = \lim_{z\to w} g(z,w) = \lim_{z\to w}\lim_{x\to y} f(x,y,z,w) = 0.$$

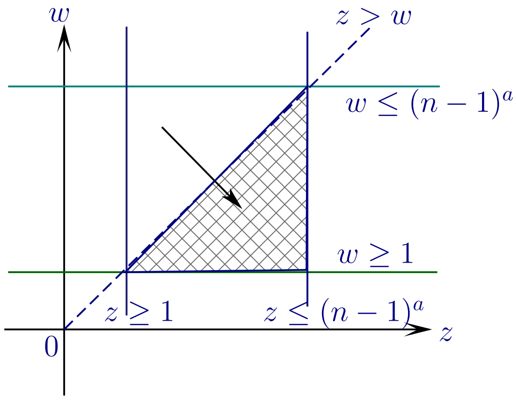

Figure 3. The feasible region of $g(z,w)$.

Combining the above arguments, we have $F(x,y,z,w)_{\min} > 0$. This completes the proof. □

The proof of Theorem 1.1 By hypothesis, we have

$$\begin{aligned} R_\alpha(S) - R_\alpha(T) &= (d_u d_p)^\alpha + (d_v d_q)^\alpha - (d_v d_p)^\alpha - (d_u d_q)^\alpha \\ &= (d_u^\alpha - d_v^\alpha)(d_p^\alpha - d_q^\alpha) \\ &> 0 \end{aligned}$$

Thus $R_\alpha(S) > R_\alpha(T)$. This completes the proof. □

The proof of Theorem 1.2 Let

$$KA_{a,b}(S) = (d_u^a + d_p^a)^b + (d_v^a + d_q^a)^b + KA'_{a,b},$$

$$KA_{a,b}(T) = (d_u^a + d_q^a)^b + (d_v^a + d_p^a)^b + KA'_{a,b},$$

where $KA'_{a,b}$ is sum of terms $(d_u^a + d_v^a)^b$ over other edges of S or T.

Thus,

$$KA_{a,b}(S) - KA_{a,b}(T) = (d_u^a + d_p^a)^b + (d_v^a + d_q^a)^b - (d_u^a + d_q^a)^b - (d_v^a + d_p^a)^b.$$

If $a = 0$ or $b = 0, 1$, then $KA_{a,b}(S) - KA_{a,b}(T) = 0$. We only consider that $b \in \mathbb{R} \setminus \{0,1\}$ and $a \in \mathbb{R} \setminus \{0\}$. By Lemma 2.1, we have the proof. □

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Jiajia Wang, School of Mathematics and Statistics, Qinghai Normal University, Xining, 810008, China
Email address: jiajialxy@163.com

Zhen Lin, School of Mathematics and Statistics, The State Key Laboratory of Tibetan Intelligent Information Processing and Application, Qinghai Normal University, Xining, 810008, China
Email address: lnlinzhen@163.com

Shumin Zhang, School of Mathematics and Statistics, The State Key Laboratory of Tibetan Intelligent Information Processing and Application, Qinghai Normal University, Xining, 810008, China
Email address: zhangshumin@qhnu.edu.cn