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Extremal Topological Indices for Graphs of Given Connectivity

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Abstract. In this paper, we show that in the class of graphs of order n and given (vertex or edge) connectivity equal to k (or at most equal to k), $1 \le k \le n-1$, the graph $K_k + (K_1 \cup K_{n-k-1})$ is the unique graph such that zeroth-order general Randić index, general sum-connectivity index and general Randić connectivity index are maximum and general hyper-Wiener index is minimum provided $\alpha \ge 1$. Also, for 2-connected (or 2-edge connected) graphs and $\alpha > 0$ the unique graph minimizing these indices is the n-vertex cycle C_n.

1. Introduction

Let G be a simple graph having vertex set $V(G)$ and edge set $E(G)$. For a vertex $u \in V(G)$, $d(u)$ denotes the degree of u and $N(u)$ the set of vertices adjacent with u. The distance between vertices u and v of a connected graph, denoted by $d(u,v)$, is the length of a shortest path between them. For two vertex-disjoint graphs G and H, the join $G+H$ is obtained by joining by edges each vertex of G to all vertices of H and the union $G \cup H$ has vertex set $V(G) \cup V(H)$ and edge set $E(G) \cup E(H)$.

The connectivity of a graph G, written $\kappa(G)$, is the minimum size of a vertex set S such that $G-S$ is disconnected or has only one vertex. A graph G is said to be k-connected if its connectivity is at least k. Similarly, the edge-connectivity of G, written $\kappa'(G)$, is the minimum size of a disconnecting set of edges. For every graph G we have $\kappa(G) \le \kappa'(G)$. For other notations in graph theory, we refer [23].

The Randić index $R(G)$, proposed by Randić [19] in 1975, one of the most used molecular descriptors in structure-property and structure-activity relationship studies [9, 10, 14, 18, 20, 22], was defined as

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2}.$$

The general Randić connectivity index (or general product-connectivity index), denoted by R_α, of G was defined by Bollobás and Erdös [3] as

$$R_\alpha = R_\alpha(G) = \sum_{uv \in E(G)} (d(u)d(v))^{\alpha},$$

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where α is a real number. Then $R_{-1/2}$ is the classical Randić connectivity index and for $\alpha = 1$ it is also known as second Zagreb index. For an extensive history of this index see [21].

This concept was extended to the general sum-connectivity index $\chi_\alpha(G)$ in [26], which is defined by

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d(u) + d(v))^\alpha,$$

where α is a real number. The sum-connectivity index $\chi_{-1/2}(G)$ was proposed in [25].

The zeroth-order general Randić index, denoted by ${}^0R_\alpha(G)$ was defined in [13] and [14] as

$${}^0R_\alpha(G) = \sum_{u \in V(G)} d(u)^\alpha,$$

where α is a real number. For $\alpha = 2$ this index is also known as first Zagreb index. This sum, which is just the sum of powers of vertex degrees, was much studied in mathematical literature (see [1, 4–6, 17]).

Thus, the general Randić connectivity index generalizes both the ordinary Randić connectivity index and the second Zagreb index, while the general sum-connectivity index generalizes both the ordinary sum-connectivity index and the first Zagreb index [26].

We shall also study the extremal properties in graphs of given connectivity of another general index. We introduce here this new index, called general hyper-Wiener index, denoted by $WW_\alpha(G)$ and defined for any real α by

$$WW_\alpha(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} (d(u,v)^\alpha + d(u,v)^{2\alpha}).$$

For $\alpha = 1$ this index was introduced by Randić as an extension of the Wiener index for trees [20] and defined for cyclic structures by Klein et al. [15] . Several extremal properties of the sum-connectivity and general sum-connectivity index for trees, unicyclic graphs and general graphs were given in [7, 8, 25, 26].

Gutman and Zhang [11] proved that among all n-vertex graphs with (vertex or edge) connectivity k, the graph $K_k + (K_1 \cup K_{n-k-1})$, which is the graph obtained by joining by edges k vertices of K_{n-1} to a new vertex, is the unique graph having minimum Wiener index. This property was extended to Zagreb and hyper-Wiener indices by Behtoei, Jannesari and Taeri [2] and to the first and second Zagreb indices when connectivity is at most k by Li and Zhou [16].

In this paper, we further study the extremal properties of this graph relatively to zeroth-order general Randić index, general sum-connectivity index and general Randić connectivity index provided $\alpha \geq 1$ and general hyper-Wiener index for any $\alpha \neq 0$. Also, for 2-(vertex or edge)-connected graphs of order n and $\alpha > 0$ the unique graph minimizing these indices is the n-vertex cycle C_n.

2. Main Results

Theorem 2.1. *Let G be an n-vertex graph, $n \geq 3$, with vertex connectivity k, $1 \leq k \leq n-1$ and $\alpha \geq 1$. Then ${}^0R_\alpha(G)$, $\chi_\alpha(G)$ and $R_\alpha(G)$ are maximum if and only if $G \cong K_k + (K_1 \cup K_{n-k-1})$.*

Proof. Let G be an n-vertex graph with $\kappa(G) = k$ such that ${}^0R_\alpha(G)$ is maximum. Since $\alpha > 0$, by addition of new edges this index strictly increases. If $k = n-1$ then G is a complete graph K_n and we have nothing to prove. Otherwise, $k \leq n-2$, there exists a disconnecting set $S \subset V(G)$ such that $|S| = k$ and $G - S$ has at least two connected components. Since ${}^0R_\alpha(G)$ is maximum it follows that $G - S$ has two components, C_1 and C_2, which are complete subgraphs. Also $S \cup C_1$ and $S \cup C_2$ induce complete subgraphs. By setting $|C_1| = x$ we get $|C_2| = n-k-x$ and $G \cong K_k + (K_x \cup K_{n-k-x})$. In this case we have ${}^0R_\alpha(G) = k(n-1)^\alpha + \varphi(x)$, where $\varphi(x) = x(k+x-1)^\alpha + (n-k-x)(n-1-x)^\alpha$. Since $\varphi(x) = \varphi(n-k-x)$, where $1 \leq x \leq n-k-1$, φ has the axis of symmetry $x = (n-k)/2$. Its derivative equals $\varphi'(x) = (k+x-1)^{\alpha-1}(k-1+x(1+\alpha)) - (n-1-x)^{\alpha-1}(n(1+\alpha)-1-\alpha k-x(1+\alpha))$. By the symmetry of φ we can only consider the case when $x \geq (n-k)/2$. In this case $(k+x-1)^{\alpha-1} \geq (n-1-x)^{\alpha-1}$, which implies that $\varphi'(x) \geq (n-1-x)^{\alpha-1}(2x+k-n)(1+\alpha)$. We have $\varphi'((n-k)/2) = 0$ and $\varphi'(x) > 0$ for

$x > (n-k)/2$. It follows that $\varphi(x)$ is maximum only for $x = 1$ or $x = n-k-1$. In both cases the extremal graph is isomorphic to $K_k + (K_1 \cup K_{n-k-1})$.

As above, if $\chi_\alpha(G)$ is maximum, it follows that $G \cong K_k + (K_x \cup K_{n-k-x})$ and $\chi_\alpha(G) = \binom{k}{2}(2n-2)^\alpha + \binom{x}{2}2^\alpha(k+x-1)^\alpha + \binom{n-k-x}{2}2^\alpha(n-1-x)^\alpha + kx(n+k+x-2)^\alpha + k(n-k-x)(2n-2-x)^\alpha$. Since $n, 2^\alpha$ and k are constant, it is necessary to find the maximum when $1 \le x \le n-k-1$, of the functions:

$\varphi_1(x) = \binom{x}{2}(k+x-1)^\alpha + \binom{n-k-x}{2}(n-1-x)^\alpha$ and $\varphi_2(x) = x(n+k+x-2)^\alpha + (n-k-x)(2n-2-x)^\alpha$. Both functions have the axis of symmetry $x = (n-k)/2$. As for $\varphi(x)$ we get $\varphi_2'((n-k)/2) = 0$ and $\varphi_2'(x) \ge (2n-2-x)^{\alpha-1}(2x+k-n)(\alpha+1) > 0$ for $x > (n-k)/2$. Hence $\varphi_2(x)$ is maximum only for $x = 1$ or $x = n-k-1$.

Similarly, $2\varphi_1'(x) = (2x-1)(k+x-1)^\alpha + \alpha(x^2-x)(k+x-1)^{\alpha-1} - (2n-2k-2x-1)(n-x-1)^\alpha - \alpha((n-k-x)^2 - n+k+x)(n-x-1)^{\alpha-1}$. If $x \ge (n-k)/2$ we obtain $2\varphi_1'(x) \ge (n-x-1)^{\alpha-1}(2x-n+k)(2n-3+\alpha(n-k-1)) > 0$ for $x > (n-k)/2$. The same conclusion follows, $\varphi_1(x)$ is maximum only for $x = 1$ or $x = n-k-1$ and the extremal graph is the same as for ${}^0R_\alpha(G)$.

It remains to see what happens if $R_\alpha(G)$ is maximum. In this case also $G \cong K_k + (K_x \cup K_{n-k-x})$ and $R_\alpha(G) = \binom{k}{2}(n-1)^{2\alpha} + \binom{x}{2}(k+x-1)^{2\alpha} + \binom{n-k-x}{2}(n-x-1)^{2\alpha} + kx(n-1)^\alpha(k+x-1)^\alpha + k(n-1)^\alpha(n-k-x)(n-x-1)^\alpha$. The sum of the last two terms equals $k(n-1)^\alpha\varphi(x)$ and we have seen that this function is maximum if and only if $x = 1$ or $x = n-k-1$. To finish, it is necessary to find the maximum of $\psi(x) = \binom{x}{2}(k+x-1)^{2\alpha} + \binom{n-k-x}{2}(n-x-1)^{2\alpha}$. This function is exactly $\varphi_1(x)$ with α replaced by 2α. It follows that for $x > (n-k)/2$ we have $2\psi'(x) > (n-x-1)^{2\alpha-1}(2x+k-n)(2n-3+2\alpha(n-k-1)) > 0$ and the extremal graph is the same. □

Theorem 2.2. *Let G be an n-vertex graph, $n \ge 3$, with vertex connectivity k, $1 \le k \le n-1$. Then $WW_\alpha(G)$ is minimum for $\alpha > 0$ and maximum for $\alpha < 0$ if and only if $G \cong K_k + (K_1 \cup K_{n-k-1})$.*

Proof. We will prove that $\sum_{\{u,v\}\subseteq V(G)} d(u,v)^\alpha$ is minimum for $\alpha > 0$ and maximum for $\alpha < 0$ only for $K_k + (K_1 \cup K_{n-k-1})$. Since by addition of edges this sum strictly decreases for $\alpha > 0$ and strictly increases for $\alpha < 0$, it follows, as above, that every extremal graph G is isomorphic to $K_k + (K_x \cup K_{n-k-x})$. All distances in this graph are 1 or 2, the distance $d(u,v) = 2$ if and only if $u \in C_1$ and $v \in C_2$. It follows that

$$\sum_{\{u,v\}\subseteq V(G)} d(u,v)^\alpha = \binom{n}{2} + x(n-k-x)(2^\alpha - 1).$$

We have $2^\alpha - 1 > 0$ for $\alpha > 0$ and the reverse inequality holds for $\alpha < 0$. Consequently, $x(n-k-x)$ must be minimum, which implies $x = 1$ or $x = n-k-1$. □

Corollary 2.3. *Let G be an n-vertex graph, $n \ge 3$, with edge connectivity k, $1 \le k \le n-1$ and $\alpha \ge 1$. Then ${}^0R_\alpha(G)$, $\chi_\alpha(G)$ and $R_\alpha(G)$ are maximum if and only if $G \cong K_k + (K_1 \cup K_{n-k-1})$.*

Proof. Suppose that $\kappa(G) = p \le k = \kappa'(G)$. Since $H = K_k + (K_1 \cup K_{n-k-1})$ consists of a vertex adjacent to exactly k vertices of K_{n-1}, it follows that ${}^0R_\alpha(H)$, $\chi_\alpha(H)$ and $R_\alpha(H)$ are strictly increasing as functions of k. We get that the values of these indices in the set of graphs G of order equal to n and $\kappa(G) = p \le k$, by Theorem 2.1, are bounded above by the values of these indices for $K_k + (K_1 \cup K_{n-k-1})$. Since this graph has edge-connectivity equal to k, the proof is complete. □

Note that in the statements of Theorem 2.1 and Corollary 2.3 we can replace (vertex or edge) connectivity k by (vertex or edge) connectivity less than or equal to k.

Corollary 2.4. *Let G be an n-vertex graph, $n \ge 3$, with edge connectivity k, $1 \le k \le n-1$. Then $WW_\alpha(G)$ is minimum for $\alpha > 0$ and maximum for $\alpha < 0$ if and only if $G \cong K_k + (K_1 \cup K_{n-k-1})$.*

Proof. The proof can be done as above, since expression $x(n-k-x)(2^\alpha - 1)$ is decreasing in k for $\alpha > 0$ and increasing for $\alpha < 0$.
□

Corollary 2.5. *Let G be an n-vertex graph, $n \ge 3$, with (vertex or edge) connectivity k, $2 \le k \le n-1$. Then ${}^0R_{-1}(G)$ is minimum if and only if $G \cong K_k + (K_1 \cup K_{n-k-1})$.*

Proof. In this case $\alpha = -1$ and we obtain $\varphi'(x) = (k-1)((k+x-1)^{-2} - (n-1-x)^{-2}) < 0$ for $x > (n-k)/2$. It follows that minimum of ${}^0R_{-1}(G)$ is reached only for $x = 1$ or $x = n-k-1$. For edge connectivity note that $\frac{1}{k} + k(\frac{1}{n-1} - \frac{1}{n-2}) + \frac{n-1}{n-2}$ is strictly decreasing in k. For $k = 1$ the graph $G_x = K_k + (K_x \cup K_{n-k-x})$ has ${}^0R_{-1}(G_x) = 2 + \frac{1}{n-1}$ for every $1 \leq x \leq n-k-1$. □

If $\alpha > 0$ and G is a connected graph minimizing ${}^0R_\alpha(G), \chi_\alpha(G)$ and $R_\alpha(G)$, then G must be minimally connected, i. e., G must be a tree. For $\alpha > 0$ in [12] it was proved that among trees with $n \geq 5$ vertices, the path P_n has minimum general Randić index and in [26] it was shown that the same property holds for general sum-connectivity index for trees with $n \geq 4$ vertices.

In order to see what happens for 2-connected graphs we need some definitions related to Whitney's characterization of 2-connected graphs [23, 24]. An ear of a graph G is a maximal path whose internal vertices (if any) have degree 2 in G and an ear decomposition of G is a decomposition $P_0, \ldots, P_k$ such that P_0 is a cycle and P_i for $i \geq 1$ is an ear of $P_0 \cup \ldots \cup P_i$. Similarly, a closed ear in G is a cycle C such that all vertices of C except one have degree 2 in G. A closed-ear decomposition of G is a decomposition $P_0, \ldots, P_k$ such that P_0 is a cycle and P_i for $i \geq 1$ is either an ear or a closed ear in $P_0 \cup \ldots \cup P_i$. A graph is 2-connected if and only if it has an ear decomposition and it is 2-edge-connected if and only if it has a closed-ear decomposition.

Theorem 2.6. *Let G be a 2-(connected or edge-connected) graph with $n \geq 3$ vertices. Then for $\alpha > 0$, ${}^0R_\alpha(G), \chi_\alpha(G)$ and $R_\alpha(G)$ are minimum if and only if $G \cong C_n$.*

Proof. We shall prove the theorem only for 2-connected graphs and general sum-connectivity index, because in the remaining cases the proof is similar. The proof is by induction. The unique 2-connected graph of order $n = 3$ is C_3. Suppose that $n \geq 4$ and for any graph G of order $m < n$ we have $\chi_\alpha(G) \geq m4^\alpha$ and equality holds if and only if $G \cong C_m$. Let H be a 2-connected graph of order n which is not a cycle, such that $\chi_\alpha(H)$ is minimum. It has an ear decomposition $P_0, \ldots, P_k$ with $k \geq 1$. P_k cannot be an edge, since by deleting this edge the resulting graph is still 2-connected and has a smaller value of χ_α. Denote by $r \geq 1$ the number of inner vertices of P_k and by u and v the common vertices of P_k with $P_0 \cup \ldots \cup P_{k-1}$. Let H' denote the subgraph of H of order $n - r$ deduced by deleting the inner vertices of P_k. Let $N_{H'}(u) \backslash \{v\} = \{u_1, \ldots, u_s\}$ and $N_{H'}(v) \backslash \{u\} = \{v_1, \ldots, v_t\}$, where $s, t \geq 2$ if $uv \notin E(H)$ and $s, t \geq 1$ otherwise. We have $\chi_\alpha(H) = \chi_\alpha(H') + (d_H(u)+2)^\alpha + (d_H(v)+2)^\alpha + (r-1)4^\alpha + \sum_{i=1}^{s}[(d_H(u)+d_H(u_i))^\alpha - (d_H(u)+d_H(u_i)-1)^\alpha] + \sum_{i=1}^{t}[(d_H(v)+d_H(v_i))^\alpha - (d_H(v)+d_H(v_i)-1)^\alpha]$. If $uv \in E(H)$, then we must add $(d_H(u)+d_H(v))^\alpha - (d_H(u)+d_H(v)-2)^\alpha > 0$. By the induction hypothesis, we have $\chi_\alpha(H) > (n-1)4^\alpha + (d_H(u)+2)^\alpha + (d_H(v)+2)^\alpha \geq (n-1)4^\alpha + 2 \cdot 5^\alpha > n4^\alpha = \chi_\alpha(C_n)$, a contradiction. □

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