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Properties of Connected (n, m)–Graphs Extremal Relatively to Vertex Degree Function Index for Convex Functions

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Abstract

In this paper some structural properties of connected (n, m)-graphs which are maximum (minimum) with respect to vertex-degree function index $H_f(G)$, when f is a strictly convex (concave) function are deduced. Also, it is shown that the unique graph obtained from the star S_n by adding γ edges between a fixed pendent vertex v and γ other pendent vertices, has the maximum general zeroth-order Randić index ${}^0R_\alpha$ in the set of all n-vertex connected graphs having cyclomatic number γ when $1 \leq \gamma \leq n-2$ and $\alpha \geq 2$. A conjecture concerning connected (n, m)-graphs G having maximum ${}^0R_\alpha(G)$ for every $n-1 \leq m \leq \frac{1}{2}\binom{n-1}{2}$ and $\alpha \geq 2$ was proposed, which completes the characterization of maximal graphs in the case $\alpha < 0$.

1 Introduction and notation

Let G be a simple graph having vertex set $V(G)$ and edge set $E(G)$. For a vertex $u \in V(G)$, its degree is denoted by $d(u)$. A universal vertex in a graph of order n is a vertex v having $d(v) = n-1$. All extremal graphs considered in this paper will contain universal vertices. An (n, m)-graph is a graph having n vertices and m edges. The set of (n, m)-graphs will be denoted by $G(n, m)$. For $u \in V(G)$, $G - u$ denotes the graph deduced from G by deleting u and all edges incident with it. Similar notations are $G - e$ and $G + e$, where $e \in E(G)$ and $e \notin E(G)$, respectively.

The disjoint union of two vertex-disjoint graphs G_1 and G_2, denoted by $G_1 \cup G_2$, is the graph whose vertex and edge sets are $V(G_1) \cup V(G_2)$ and $E(G_1) \cup E(G_2)$, respectively. The union of k copies of a graph G will be denoted by kG.

For two vertex-disjoint graphs G and H, the join $G \vee H$ is obtained by joining by edges each vertex of G to all vertices of H. The join between a complete graph and a regular graph is called a multicone graph.

The n-vertex star graph is denoted by S_n or $K_{1,n-1}$, the complete graph of order n by K_n and the path and the cycle with n vertices by P_n and C_n, respectively.

The general sum-connectivity index of graphs $\chi_\alpha(G)$ was proposed by Zhou and Trinajstić [23] as

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

where α is a non-zero real number. The topological index χ_1 coincides with the first Zagreb index, which is one of the most studied topological indices. In what follows we will use the following graph invariant, introduced in [3]:

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

where $\alpha \neq 0$ and $a > 0$ are real numbers. The invariant ${}^0R_{\alpha,a}$ is a modified form of the general zeroth-order Randić index [8], which is defined as

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

where α is a non-zero real number. In particular, ${}^0R_\alpha(G) = {}^0R_{\alpha,0}(G)$ and ${}^0R_2(G) = \chi_1(G)$.

Some extremal results concerning the general zeroth-order Randić index were deduced in [4, 6, 10–13, 21]; see also the surveys [2, 4].

The cyclomatic number or the circuit rank of a graph G, denoted $\gamma(G)$ is the minimum number of edges whose deletion transforms G into an acyclic graph. For a connected (n, m)-graph the value of this parameter is $\gamma(G) = m - n + 1$.

Let $\mathbb{G}_{n,\gamma}$ be the set of all connected n-vertex graphs with cyclomatic number γ.
Let v be a fixed pendent vertex of the n-vertex star S_n, where $n \geq 3$. As in [3], for $0 \leq \gamma \leq n-2$ denote by $H_{n,\gamma}$ the graph obtained from S_n by joining by edges v with γ other pendent vertices. We have $H_{n,\gamma} \in \mathbb{G}_{n,\gamma}$ and $H_{n,0} = S_n$.

The second multiplicative Zagreb index or modified Narumi–Katayama index [6, 10] is defined as

$$\prod_2(G) = \prod_{v\in V(G)} d(v)^{d(v)} = \prod_{uv\in E(G)} d(u)d(v).$$

This index is maximum if and only if $\ln \prod_2(G) = \sum_{v\in V(G)} d(v)\ln d(v)$ is maximum.

The sum lordeg index is one of the Adriatic indices introduced in [16] and it is defined by

$$SL(G) = \sum_{v\in V(G)} d(v)\sqrt{\ln d(v)} = \sum_{v\in V(G):d(v)\geq 2} d(v)\sqrt{\ln d(v)}.$$

The sum exdeg index of a graph G was defined in [17–19] as

$$SEI_a(G) = \sum_{v\in V(G)} d(v)a^{d(v)},$$

where $a \neq 1$ is a positive real number.

The vertex-degree function index $H_f(G)$ was introduced in [21] as

$$H_f(G) = \sum_{v\in V(G)} f(d(v)),$$

for a function $f(x)$ defined on non-negative real numbers. In this paper we will impose to function $f(x)$ to be strictly convex (concave). All indices mentioned above are vertex-degree function indices $H_f(G)$: ${}^0R_\alpha(G)$ corresponds to $f(x) = x^\alpha$, which is strictly convex for $\alpha < 0$ or $\alpha > 1$ and strictly concave for $0 < \alpha < 1$; the logarithm of the second multiplicative Zagreb index $\prod_2(G)$ to $f(x) = x\ln x$, which is strictly convex for $x \geq 1$; the sum lordeg index to $f(x) = x\sqrt{\ln x}$, being strictly convex for $x \geq 2$ (see [20]) and the sum exdeg index to $f(x) = xa^x$, which is strictly convex for $a > 1$ and $x > 0$.

The rest of the paper is organized as follows. In Section 2, some structural properties of graphs which maximize (minimize) the vertex-degree function index $H_f(G)$, where $f(x)$ is a convex (concave) function are deduced, as well as some extremal connected (n,m)-graphs for general zeroth-order Randić index ${}^0R_\alpha$ when $n \leq m \leq n+4$ and $\alpha > 0$. In Section 3, we find extremal graphs which have the maximum ${}^0R_\alpha$ value in the set of all n-vertex connected graphs having cyclomatic number γ when $1 \leq \gamma \leq n-2$ and $\alpha \geq 2$. In the last section, a conjecture was proposed that asserts that a graph consisting of a multicone graph with some edges inducing a star added attains the maximum value of ${}^0R_\alpha$ index in the set of connected (n,m)-graphs for every $n-1 \leq m \leq \frac{1}{2}\binom{n-1}{2}$ and $\alpha \geq 2$.

2 Structure of graphs which maximize vertex–degree function index for convex functions

The property expressed by next lemma was used many times for particular convex functions to deduce properties of extremal graphs related to different topological graph indices.

Lemma 2.1. Let $x \geq y \geq 1$. If function $f(x)$ is strictly convex, then

$$f(x+1) + f(y-1) > f(x) + f(y).$$

Proof. The function $f(x)$ being strictly convex, $\varphi(x) = f(x+1) - f(x)$ is a strictly increasing function. Since $x > y-1$ it follows that $\varphi(x) > \varphi(y-1)$, or $f(x+1) - f(x) > f(y) - f(y-1)$. ■

If $f(x)$ is strictly concave, then this inequality is reversed.

Lemma 2.2. If $G \in G(n,m)$ maximizes (minimizes) $H_f(G)$ where $f(x)$ is strictly convex (concave), then G has at most one nontrivial connected component C and C has a universal vertex.

Proof. Suppose that $f(x)$ is strictly convex and let G be a graph that has maximum $H_f(G)$. If there exist two nontrivial connected components C_1 and C_2, we can obtain a new graph $G_1 \in G(n,m)$ by identifying two vertices belonging to C_1 and C_2, respectively, and adding a new isolated vertex.

We obtain

$$H_f(G_1) - H_f(G) = f(p+q) + f(0) - f(p) - f(q)\,,$$

where $p, q \geq 1$ are the degrees of identified vertices. If $p \leq q$, by Lemma 2.1 we get $f(p) + f(q) < f(p-1) + f(q+1) < \ldots < f(0) + f(p+q)$, a contradiction. It follows that if G has at least one edge then G consists of a nontrivial component C and some isolated vertices. If $2 \leq |C| \leq 3$ then C contains a universal vertex. Otherwise, let v be a vertex of maximum degree $d(v) = s$ in C. If v is not a universal vertex, there exists a vertex u which is not adjacent with v. Since C is connected, there exists a path $v, \ldots, w, u$ from v to u in C. We can define a new connected graph $H \in G(n,m)$ by adding edge uv and deleting edge uw. Let $d(w) = t \leq s$. We get $H_f(H) - H_f(G) = f(s+1) + f(t-1) - f(s) - f(t) > 0$ by Lemma 2.1, a contradiction. It follows that v is a universal vertex in C. The case of concave functions can be proved analogously. ■

Corollary 2.3. In the set of connected (n,m)-graphs G having $m \geq n$, the graph which maximizes (minimizes) $H_f(G)$ where $f(x)$ is strictly convex (concave) possesses the following properties:

(1) G has a universal vertex v;

(2) G contains nor P_4 neither C_p where $p \geq 4$ as induced subgraphs;

(3) The subgraph $G - v$ consists of some isolated vertices and a nontrivial connected component C which is maximum (minimum) relatively to H_g, where $g(x) = f(x+1)$. C also contains a universal vertex and no induced subgraph isomorphic to P_4 or C_p where $p \geq 4$.

Proof. 1) As in the proof of Lemma 2.2, if G has no universal vertices, G being connected we can define a new connected (n,m)-graph G_1 such that $H_f(G_1) > H_f(G)$, a contradiction.

2) If G would contain an induced P_4: a, b, c, d, then $ac, bd \notin E(G)$. Without loss of generality we can suppose that $d(b) \geq d(c)$. By letting $G_1 = G + bd - cd$ we get that G_1 is also a connected (n,m)-graph and $H_f(G_1) - H_f(G) = f(d(b)+1) + f(d(c)-1) - f(d(b)) - f(d(c)) > 0$ by Lemma 2.1, a contradiction. The argument is similar when G has an induced C_4: a, b, c, d, a, where $ac, bd \notin E(G)$ and $d(b) \geq d(c)$. Because G has no P_4 this implies that it has no C_p where $p \geq 5$ as induced subgraph.

(3) Let v be a universal vertex of G. We have $H_f(G) = f(n-1) + H_g(G-v)$, where $g(x) = f(x+1)$ is also strictly convex and we can apply Lemma 2.2 to $G - v$, since $H_g(G-v)$ must be maximum also. The case of minimization when $f(x)$ is strictly concave follows similarly. ■

Analogous properties to those given in Corollary 2.3 were deduced for zeroth-order general Randić index ${}^0R_\alpha$, with incomplete proofs in [9]. For unicyclic, bicyclic and tricyclic graphs we obtain the following corollary:

Corollary 2.4. Let $G \in G(m,n)$ be a connected graph such that $H_f(G)$ is maximum and $f(x)$ is strictly convex. Then for:

a) $m = n$: $G = K_1 \vee (K_2 \cup (n-3)K_1)$;

b) $m = n+1$: $G = K_1 \vee (K_{1,2} \cup (n-4)K_1)$;

c) $m = n+2$: $G = K_1 \vee (K_{1,3} \cup (n-5)K_1)$ or $G = K_1 \vee (K_3 \cup (n-4)K_1)$. The first case occurs when $f(4) + 3f(2) > 3f(3) + f(1)$; when the inequality is reversed then the second graph is maximum. In case of equality both graphs are maximum. A similar result holds when convex is replaced by concave and maximum by minimum.

When $f(x) = x^\alpha$, then $H_f(G) = {}^0R_\alpha(G)$, function x^α being strictly convex for $\alpha < 0$ or $\alpha > 1$. We can deduce the following corollary treating the cases of unicyclic, bicyclic, tricyclic, quadricyclic and pentacyclic graphs of order n which maximizes ${}^0R_\alpha$ for $\alpha > 1$. Note that the case of $\alpha < 0$ was solved in [11, 13] for connected graphs in $G(n,m)$ for every $m \geq n$.

Corollary 2.5. Let $G \in G(n,m)$ be a connected graph. Then if:

a) $m = n$: for $G = K_1 \vee (K_2 \cup (n-3)K_1)$, ${}^0R_\alpha(G)$ is maximum for $\alpha > 1$ and minimum for $0 < \alpha < 1$.

b) $m = n+1$: for $G = K_1 \vee (K_{1,2} \cup (n-4)K_1)$, ${}^0R_\alpha(G)$ is maximum for $\alpha > 1$ and minimum for $0 < \alpha < 1$.

c) $m = n+2$: for $G = K_1 \vee (K_{1,3} \cup (n-5)K_1)$, ${}^0R_\alpha(G)$ is maximum for $\alpha > 2$; for $1 < \alpha < 2$ there exists another maximum graph, namely $G = K_1 \vee (K_3 \cup (n-4)K_1)$ which is minimum for $0 < \alpha < 1$ and for $\alpha = 2$ both graphs are maximum.

d) $m = n+3$: for $G = K_1 \vee (K_{1,4} \cup (n-6)K_1)$, ${}^0R_\alpha(G)$ is maximum for $\alpha > 1$ and minimum for $x_0 < \alpha < 1$, where $x_0 \approx 0.784115$ is a root of the equation $5^x - 4^x - 2\cdot 3^x + 3\cdot 2^x - 1 = 0$; for $0 < \alpha < x_0$ $G = K_1 \vee (K_{1,3} + e \cup (n-5)K_1)$ is minimum and for $\alpha = x_0$ both graphs are minimum.

e) $m = n+4$: for $G = K_1 \vee (K_{1,5} \cup (n-7)K_1)$, ${}^0R_\alpha(G)$ is maximum for $\alpha > 1$ and if $G = K_1 \vee ((K_2 \vee 2K_1) \cup (n-5)K_1)$ then ${}^0R_\alpha(G)$ is minimum for $0 < \alpha < 1$.

All extremal graphs mentioned above are unique with these properties.

Proof. Properties a) and b) follow from Corollary 2.3. Similarly, for case c) if v denotes a universal vertex, one finds that $G - v$ is $K_3 \cup (n-4)K_1$ or $K_{1,3} \cup (n-5)K_1$. By letting the corresponding graphs G_1 and G_2 we get ${}^0R_x(G_1) > {}^0R_x(G_2)$ if and only if $h(x) = 4^x - 3\cdot 3^x + 3\cdot 2^x - 1 < 0$. Using mathematical software [20] we obtain that $h(x) > 0$ for $0 < x < 1$ and for $x > 2$. Also $h(x) < 0$ for $1 < x < 2$ and $h(x) = 0$ for $x = 0, 1, 2$.

Similarly, for case d) G is $G_1 = K_1 \vee (K_{1,4} \cup (n-6)K_1)$ or $G_2 = K_1 \vee (K_{1,3} + e \cup (n-5)K_1)$. We get ${}^0R_x(G_1) > {}^0R_x(G_2)$ if and only if $\rho(x) = 5^x - 4^x - 2\cdot 3^x + 3\cdot 2^x - 1 > 0$. Equation $\rho(x) = 0$ has three roots: $x = 0, x = 1$ and $x = x_1 \approx 0.784115$ and $\rho(x) > 0$ for $0 < x < x_1$ and for $x > 1$ and $\rho(x) < 0$ for $x_1 < x < 1$. [20]

For case e) G is $G_1 = K_1 \vee (K_{1,5} \cup (n-7)K_1)$ or $G_2 = K_1 \vee ((K_2 \vee 2K_1) \cup (n-5)K_1)$ or

$G_3 = K_1 \vee (K_{1,4} + e \cup (n-7)K_1)$. It is necessary to compare functions $\varphi_1(x) = 6^x + 5 \cdot 2^x$, $\varphi_2(x) = 2 \cdot 4^x + 2 \cdot 3^x + 2$ and $\varphi_3(x) = 5^x + 2 \cdot 3^x + 2 \cdot 2^x + 1$. Using the same method we get that $\varphi_1(x) > \varphi_2(x)$ and $\varphi_1(x) > \varphi_3(x)$ for any $x > 1$ and $\varphi_2(x) < \varphi_1(x)$ and $\varphi_2(x) < \varphi_3(x)$ for $0 < x < 1$. ■

3 Graphs with given cyclomatic number and maximum general zeroth–order Randić index

We need the following auxiliary result:

Lemma 3.1. If $G \in G(n,m)$ such that $1 \leq m \leq n-1$, $a \geq 1$ and $\alpha \geq 2$, then

$$^0R_{\alpha,a}(G) \leq (n-m-1)a^\alpha + m(a+1)^\alpha + (m+a)^\alpha$$

with equality if and only if $G = S_{m+1} \cup (n-m-1)K_1$ when $\alpha > 2$, and when $\alpha = 2$, the equality holds if and only if $G = S_{m+1} \cup (n-m-1)K_1$ for $m \neq 3$, and $G = S_4 \cup (n-4)K_1$ or $K_3 \cup (n-3)K_1$ for $m = 3$.

Proof. The proof is the same as the proof of Lemma 2 of [3] by replacing $n+1$ by a and setting in corresponding Lemma 1 $s = a$ instead of $s = n+1$. ■

The following theorem gives the maximum value of the index $^0R_\alpha(G)$ in the set $\mathbb{G}_{n,\gamma}$ for every $1 \leq \gamma \leq n-2$ and $\alpha \geq 2$.

Theorem 3.2. If $n \geq 3$, $1 \leq \gamma \leq n-2$, $\alpha \geq 2$ and G is a connected n-vertex graph with cyclomatic number γ, then

$$^0R_\alpha(G) \leq (n-1)^\alpha + (\gamma+1)^\alpha + \gamma 2^\alpha + n - \gamma - 2,$$

with equality if and only if $G = H_{n,\gamma} = K_1 \vee (K_{1,\gamma} \cup (n-\gamma-2)K_1)$ when $\alpha > 2$. If $\alpha = 2$, the equality holds when $G = H_{n,\gamma}$ for $\gamma \neq 3$ and $G = H_{n,3}$ or $K_1 \vee (K_3 \cup (n-4)K_1)$ for $\gamma = 3$.

Proof. Let $G \in \mathbb{G}_{n,\gamma}$ such that $^0R_\alpha(G)$ is maximum. By Corollary 2.3 there exists a universal vertex $v \in V(G)$. We can write:

$$^0R_\alpha(G) = (n-1)^\alpha + {}^0R_{\alpha,1}(G-v).$$

$G - v$ has $n' = n-1$ vertices and $m' = m - n + 1 = \gamma(G)$ edges. Since by hypothesis we have $1 \leq \gamma(G) \leq n-2$ it follows that $1 \leq m' \leq n'-1$ and we can apply Lemma 3.1 for $G - v$, since $^0R_{\alpha,1}(G-v)$ must be maximum also. ■

Note that if we replace the condition $\alpha \geq 2$ by $\alpha > 1$ the property stated by Theorem 3 may not hold. For example, for $n \geq 8$ and $m = 6$ we have

$$^0R_\alpha(K_1 \vee (K_4 \cup (n-5)K_1) >^0R_\alpha(K_1 \vee (K_{1,6} \cup (n-8)K_1))$$

for $1 < \alpha < \alpha_0 \approx 1.19281$, where α_0 is a root of the equation $7^x + 6 \cdot 2^x - 4 \cdot 4^x - 3 = 0$ [20].

Similar results for general sum-connectivity index χ_α were deduced in [3] for $\alpha \geq 2$ and in [15] for $1 < \alpha < 2$.

4 Concluding remarks

The problem of maximizing $^0R_\alpha(G)$, where G is a connected (n,m)-graph for $m \geq n-1$ and $\alpha < 0$ was completely solved in [11, 13]. The same problem will be discussed further for $\alpha \geq 2$.

For every $n \geq 3$ and $1 \leq k \leq n-1$, we shall consider multicone graphs $G_{n,k} = K_k \vee (n-k)K_1$. We have $G_{n,1} = S_n$, $G_{n,n-1} = K_n$, $G_{n,k}$ has k vertices of degree $n-1$ and $n-k$ vertices of degree k and it has $\binom{k}{2} + k(n-k) = nk - k(k+1)/2$ edges. Now for every $0 \leq p \leq n-k-1$ we define graph $G_{n,k,p}$, which consists of $G_{n,k}$ and p new edges joining one vertex of degree k of $G_{n,k}$ with other p vertices of degree k of this graph. Consequently, $G_{n,k,p} = K_k \vee (K_{1,p} \cup (n-k-p-1)K_1)$ having k vertices of degree $n-1$, p vertices of degree $k+1$, $n-k-p-1$ vertices of degree k and one vertex of degree $k+p$. It is obtained from a multicone graph by adding some edges inducing a star.

In [1] the problem of maximizing $^0R_2(G)$ for (n,m)-graphs G which are not necessarily connected was considered. In order to present this approach, we shall define first a class of graphs denoted C_n^m depending on n and m as follows [1]: Let a, b be unique integers such that $m = \binom{a}{2} + b$, where $0 \leq b < a$ and $a \geq 1$. C_n^m consists of a clique with vertex set $\{1, \ldots, a\}$, vertex $a+1$ which is adjacent with b vertices of the clique and $n-a-1$ isolated vertices. One result of [1] asserts that for every $0 \leq m \leq \frac{1}{2}\binom{n}{2} - n$, the graph which realizes the maximum of $^0R_2(G)$ is the complement of the graph $C_n^{\binom{n}{2}-m}$. For $m \geq \frac{1}{2}\binom{n}{2} + n$ the extremal graph is C_n^m.

Let G be a connected (n,m)-graph. If $^0R_2(G)$ is maximum, then G has a universal vertex x and $^0R_2(G) = (n-1)^2 + \sum_{v \in V(G-x)}(d(v)+1)^2 = (n-1)^2 + 4|E(G-x)| + |V(G-x)| + {}^0R_2(G-x) = (n-1)^2 + 4(m-n+1) + n - 1 + {}^0R_2(G-x)$. It follows that $^0R_2(G-x)$ is maximum as well. $G-x$ has $m' = m-n+1$ edges and $n' = n-1$ vertices. We get that if $m-n+1 \leq \frac{1}{2}\binom{n-1}{2}-n+1$, or $m \leq \frac{1}{2}\binom{n-1}{2}$, then ${}^0R_2(G-x)$ is maximum for the complement of the graph $C_{n-1}^{\binom{n-1}{2}-m+n-1}$. We deduce that the maximal graph is the join between K_1 and the complement of $C_{n-1}^{\binom{n-1}{2}-m+n-1}$. It is not difficult to see that this graph is $G_{n,n-c-1,c-d}$, where $\binom{n-1}{2}-m+n-1=\binom{c}{2}+d$, $0 \leq d < c$ and $c \geq 1$. Since for $1 \leq \gamma \leq n-2$ we get $H_{n,\gamma}=G_{n,1,\gamma}$ for which Theorem 3.2 holds, it is plausible that the following conjecture be true:

Conjecture 4.1. If $G \in G(n,m)$ is a connected graph with $n \geq 6$, $n-1 \leq m \leq \frac{1}{2}\binom{n-1}{2}$ and $m = nk - \binom{k+1}{2} + p$, where $1 \leq k \leq n-1$ and $0 \leq p \leq n-k-1$, then for $\alpha \geq 2$ we have

$$ {}^0R_\alpha(G) \leq {}^0R_\alpha(G_{n,k,p}) = k(n-1)^\alpha + p(k+1)^\alpha + (n-k-p-1)k^\alpha + (k+p)^\alpha. $$

This statement holds for $\alpha = 2$ and for $\alpha \geq 2$ and $n \leq m \leq 2n-3$. It is interesting to note that for $\alpha < 0$ the extremal graph is $K_1 \vee C_{n-1}^{m-n+1}$ [11, 13].

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