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General approach for obtaining extremal results on degree-based indices illustrated on the general sum-connectivity index

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Abstract

Among bipartite graphs with given order and matching number/vertex cover number/edge cover number/independence number, among multipartite graphs with given order, and among graphs with given order and chromatic number, we present the graphs having the maximum degree-based index if that index satisfies certain conditions. We show that those conditions are satisfied by the general sum-connectivity index χ_a for all or some $a \geq 0$.

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1. Introduction and preliminary results

The vertex set and edge set of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The order of a graph G is the number of vertices of G. The degree $d_G(u)$ of a vertex u in G is the number of edges incident with u.

A vertex independent set is a set of vertices of G, where no two vertices in that set are adjacent in G. A matching is a set of edges of G, where no two edges in that set have a vertex in common. The independence number/matching number of G is the cardinality of a maximum independent set/matching. An edge cover of a graph G is a set of edges, where each vertex of G is incident

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with at least one edge from that set. A vertex cover of G is a set of vertices, where each edge of G is incident with at least one vertex from that set. The cardinality of a minimum edge cover/vertex cover is the edge/vertex cover number. The smallest number of colors needed to color the vertices of a graph G such that every two adjacent vertices have different colors is the chromatic number of G.

For $k \geq 2$, a graph whose vertices can be partitioned into k sets in such a way that any two vertices in the same set are non-adjacent is called a k-partite graph. It is called complete multipartite (k-partite) graph if every two vertices from different partite sets are adjacent. We use the notation $K_{n_1,n_2,\ldots,n_k}$ for a complete k-partite graph having partite sets with cardinalities $n_1, n_2, \ldots, n_k$. A 2-partite graph is called a bipartite graph.

Let $f(x, y)$ be a real-valued symmetric function of two variables x and y. We study degree-based indices defined in the following way for a graph G:

$$I_f(G) = \sum_{uv \in E(G)} f(d_G(u), d_G(v)).$$

The function $f(x, y) = (x + y)^a$ where $a \in \mathbb{R}$ can be used to obtain the general sum-connectivity index. The general sum-connectivity index of a graph G was introduced by Zhou and Trinajstić [9]. For $a \in \mathbb{R}$, it is defined as

$$\chi_a(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^a.$$

In this paper, we consider χ_a for $a \geq 0$, therefore we mention special cases of χ_a only for positive a. For $a = \frac{1}{2}$ we get the reciprocal sum-connectivity index, for $a = 1$ we obtain the first Zagreb index, and for $a = 2$ we get the first hyper-Zagreb index. Ali, Zhong and Gutman [2] gave a survey about the general sum-connectivity index.

Indices defined by a degree-based edge-weight function were studied also by Hu et al. [4] who presented extremal results for graphs of given order and size. Zhou et al. [10] studied degree-based indices under the name bond incident degree indices and presented extremal results for graphs with given order and number of pendant vertices. Extremal results for trees were given by Ali and Dimitrov [1]. For other works on general degree-based indices, see for example [3], [5], [6] and [7].

We present our own approach in this area. Let us introduce a function having property Q.

Definition 1.1. *A symmetric function $f(x, y)$ of two variables having property Q is any function satisfying the following conditions:*

(i) $f(x, y) > 0$ *for* $x, y \geq 1$,

(ii) $f(x_1, y_1) \leq f(x_2, y_2)$ *for* $1 \leq x_1 \leq x_2$ *and* $1 \leq y_1 \leq y_2$,

(iii) $f(x, y) \leq f(x + c, y - c)$ *for* $x \geq y$, $c \geq 0$ *and* $y - c \geq 1$.

Let us give one function which has property Q.

Lemma 1.1. *The function* $f(x,y) = (x+y)^a$ *has property* Q *for* $a \geq 0$.

Proof. (i) Let $f(x,y) = (x+y)^a$. Since $x, y \geq 1$, we get $f(x,y) \geq 2^a > 0$ for $a \geq 0$.

(ii) We obtain $\frac{\partial f(x,y)}{\partial x} = a(x+y)^{a-1} \geq 0$ for $x, y \geq 1$ and $a \geq 0$. Since $f(x,y)$ is symmetric, we have $\frac{\partial f(x,y)}{\partial y} \geq 0$ for $a \geq 0$. Thus $f(x_1,y_1) \leq f(x_2,y_2)$ for $1 \leq x_1 \leq x_2$ and $1 \leq y_1 \leq y_2$.

(iii) We have $f(x+c, y-c) = [(x+c)+(y-c)]^a = f(x,y)$.

Hence $f(x,y) = (x+y)^a$ has property Q for $a \geq 0$. □

Definition 1.2 is similar to Definition 1.1. The first two points are the same in both definitions, the third point is different and Definition 1.2 has a new point (iv).

Definition 1.2. *A symmetric function* $f(x,y)$ *of two variables having property* P *is any function satisfying the following conditions:*

(i) $f(x,y) > 0$ *for* $x, y \geq 1$,

(ii) $f(x_1,y_1) \leq f(x_2,y_2)$ *for* $1 \leq x_1 \leq x_2$ *and* $1 \leq y_1 \leq y_2$,

(iii) $f(x,y) \geq f(x+c, y-c)$ *for* $x \geq y$, $c \geq 0$ *and* $y - c \geq 1$,

(iv) $g(x_1,y_1) = f(x_1+c, y_1+c') - f(x_1,y_1) \geq f(x_2+c, y_2+c') - f(x_2,y_2) = g(x_2,y_2)$ *for* $1 \leq x_1 \leq x_2$, $1 \leq y_1 \leq y_2$ *and* $c, c' \geq 0$.

We show that the function $f(x,y) = (x+y)^a$ has property P if $0 \leq a \leq 1$.

Lemma 1.2. *The function* $f(x,y) = (x+y)^a$ *has property* P *for* $0 \leq a \leq 1$.

Proof. The proofs that f satisfies conditions (i), (ii) and (iii) of Definition 1.2 are the same as in the proof of Lemma 1.1. It remains to prove that f satisfies condition (iv) of Definition 1.2. We obtain

$$g(x,y) = f(x+c, y+c') - f(x,y) = (x+y+c+c')^a - (x+y)^a,$$

thus

$$\frac{\partial g(x,y)}{\partial x} = a[(x+y+c+c')^{a-1} - (x+y)^{a-1}].$$

For $0 \leq a \leq 1$, we get $(x+y+c+c')^{a-1} \leq (x+y)^{a-1}$. So $\frac{\partial g(x,y)}{\partial x} \leq 0$ for $0 \leq a \leq 1$. The function $f(x,y)$ is symmetric, thus $g(x,y)$ is also symmetric. So $\frac{\partial g(x,y)}{\partial y} \leq 0$ for $0 \leq a \leq 1$. Therefore $g(x_1,y_1) = f(x_1+c, y_1+c') - f(x_1,y_1) \geq f(x_2+c, y_2+c') - f(x_2,y_2) = g(x_2,y_2)$ for $1 \leq x_1 \leq x_2$, $1 \leq y_1 \leq y_2$ and $c, c' \geq 0$. Hence $f(x,y) = (x+y)^a$ has property P for $0 \leq a \leq 1$. □

We compare I_f of two graphs which differ only by one edge.

Lemma 1.3. *Let* $f(x,y)$ *be a function satisfying conditions (i) and (ii) of Definitions 1.1 and 1.2. Then* $I_f(G) < I_f(G + v_1v_2)$, *where* v_1, v_2 *are any two non-adjacent vertices of a connected graph* G.

Proof. Let G' be the graph $G + v_1v_2$. For any $uv \in E(G)$, we have $d_{G'}(u) \geq d_G(u) \geq 1$ and $d_{G'}(v) \geq d_G(v) \geq 1$. The function f satisfies part (ii) of Definitions 1.1 and 1.2, therefore $f(d_{G'}(u), d_{G'}(v)) \geq f(d_G(u), d_G(v))$. Since $d_{G'}(v_1) \geq 1$, $d_{G'}(v_2) \geq 1$ and f satisfies part (i) of Definitions 1.1 and 1.2, we have $f(d_{G'}(v_1), d_{G'}(v_2)) > 0$. Thus

$$\begin{aligned} I_f(G') &= \sum_{uv \in E(G')} f(d_{G'}(u), d_{G'}(v)) \\ &= f(d_{G'}(v_1), d_{G'}(v_2)) + \sum_{uv \in E(G)} f(d_{G'}(u), d_{G'}(v)) \\ &> \sum_{uv \in E(G)} f(d_{G'}(u), d_{G'}(v)) \\ &\geq \sum_{uv \in E(G)} f(d_G(u), d_G(v)) \\ &= I_f(G). \end{aligned}$$

□

2. Bipartite graphs with given matching number/vertex cover number/edge cover number/ independence number

For the matching number ν of any graph, we have $1 \leq \nu \leq \lfloor \frac{n}{2} \rfloor$. The only connected bipartite graphs with matching number 1 are stars, therefore we investigate bipartite graphs for $2 \leq \nu \leq \lfloor \frac{n}{2} \rfloor$.

Theorem 2.1. *Let G be a bipartite graph of order n and matching number ν, where $2 \leq \nu \leq \lfloor \frac{n}{2} \rfloor$. If f has property Q, then*

$$I_f(G) \leq \nu(n-\nu)\, f(\nu, n-\nu)$$

with equality if and only if G is $K_{\nu,n-\nu}$.

Proof. Let G' be a graph with the largest I_f among graphs of order n and matching number ν. For the partite sets V_1 and V_2 of G', we can assume that $|V_1| \leq |V_2|$. We show that G' is $K_{\nu,n-\nu}$.

Assume to the contrary that G' is not $K_{\nu,n-\nu}$. We have $|V_1| \geq \nu$ (otherwise if $|V_1| < \nu$, then the matching number of G' would be less than ν). We also know that G' is not a subgraph of $K_{\nu,n-\nu}$, (if G' would be a subgraph of $K_{\nu,n-\nu}$, from Lemma 1.3, we obtain $I_f(G') < I_f(K_{\nu,n-\nu})$ since I_f increases when adding edges to a graph). So $\nu < |V_1| \leq |V_2|$.

We denote any matching in G' with ν edges by M'. For $j = 1, 2$, let V_j^ν be the subset of V_j having ν vertices incident with the edges in M'. We get $|V_j| = \nu + l_j$ where $l_j \geq 1$ (and $2\nu + l_1 + l_2 = n$). Clearly, a vertex $v_1 \in V_1 \setminus V_1^\nu$ and a vertex $v_2 \in V_2 \setminus V_2^\nu$ are not adjacent, otherwise we would have the matching $M' \cup \{v_1v_2\}$ in G' containing $\nu + 1$ edges.

We define H' which is a graph with $V(H') = V(G')$ and having all the edges between V_1^ν and V_2^ν, between V_1^ν and $V_2 \setminus V_2^\nu$, and between $V_1 \setminus V_1^\nu$ and V_2^ν. Then G' is a subgraph of H', so by Lemma 1.3, we get $I_f(G') < I_f(H')$. Note that H' has matching number at least $\nu + 1$. We get

$d_{H'}(v) = \nu + l_2$ for $v \in V_1^\nu$, $d_{H'}(v) = \nu + l_1$ for $v \in V_2^\nu$, and $d_{H'}(v) = \nu$ for $v \in V(H') \setminus (V_1^\nu \cup V_2^\nu)$. Note that $n - \nu = \nu + l_1 + l_2$. We obtain

$$\begin{aligned}
&I_f(K_{\nu,n-\nu}) - I_f(H') \\
&= \sum_{uv \in E(K_{\nu,n-\nu})} f(d_{K_{\nu,n-\nu}}(u), d_{K_{\nu,n-\nu}}(v)) - \sum_{uv \in E(H')} f(d_{H'}(u), d_{H'}(v)) \\
&= \nu(n-\nu)\, f(\nu, n-\nu) - \nu\nu f(\nu + l_1, \nu + l_2) - \nu l_1 f(\nu, \nu + l_1) - \nu l_2\, f(\nu, \nu + l_2) \\
&= \nu^2[f(\nu, \nu + l_1 + l_2) - f(\nu + l_1, \nu + l_2)] + \nu l_1[f(\nu, \nu + l_1 + l_2) - f(\nu, \nu + l_1)] \\
&\quad + \nu l_2[f(\nu, \nu + l_1 + l_2) - f(\nu, \nu + l_2)].
\end{aligned}$$

Since the function f satisfies Definition 1.1 (ii), we get

$$f(\nu, \nu + l_1 + l_2) \geq f(\nu, \nu + l_1) \text{ and } f(\nu, \nu + l_1 + l_2) \geq f(\nu, \nu + l_2).$$

The function f has property Q, thus from part (iii) of Definition 1.1, we obtain

$$f(\nu, \nu + l_1 + l_2) \geq f(\nu + l_1, \nu + l_2).$$

Thus $I_f(K_{\nu,n-\nu}) - I_f(H') \geq 0$. We get $I_f(G') < I_f(H') \leq I_f(K_{\nu,n-\nu})$. which means that G' does not have the largest I_f. We have a contradiction. Hence G' is $K_{\nu,n-\nu}$ and

$$I_f(K_{\nu,n-\nu}) = \nu(n-\nu)\, f(\nu, n-\nu).$$

□

We denote the independence number by α, the vertex cover number by β and the edge cover number by β'. From [8], we know that for any graph with n vertices,

$$\alpha + \beta = n.$$

If G does not contain isolated vertices, we have

$$\nu + \beta' = n.$$

If G is a bipartite graph without isolated vertices, then

$$\alpha = \beta', \text{ so } \nu = \beta;$$

see [8]. Thus, by Theorem 2.1, we get Corollary 2.1.

Corollary 2.1. *Let G be a bipartite graph of order n and vertex cover number β, where $2 \leq \beta \leq \lfloor \frac{n}{2} \rfloor$. If f has property Q, then*

$$I_f(G) \leq \beta(n-\beta)\, f(\beta, n-\beta)$$

with equality if and only if G is $K_{\beta,n-\beta}$.

In Theorem 2.1, $2 \leq \nu \leq \lfloor \frac{n}{2} \rfloor$, thus

$$\left\lceil \frac{n}{2} \right\rceil \leq \beta' \leq n-2.$$

Since $\nu + \beta' = n$, Theorem 2.1 states that if G is a bipartite graph with n vertices and matching number $n - \beta'$, then

$$I_f(G) \leq (n-\beta)\beta\, f(n-\beta, \beta)$$

Therefore, we get Corollary 2.2.

Corollary 2.2. *Let G be a bipartite graph of order n and edge cover number/independence number β', where $\lceil \frac{n}{2} \rceil \leq \beta' \leq n-2$. If f has property Q, then*

$$I_f(G) \leq \beta'(n-\beta')\, f(\beta', n-\beta')$$

with equality if and only if G is $K_{\beta', n-\beta'}$.

From Lemma 1.1, we know that the function $f(x,y) = (x+y)^a$ has property Q. Thus, using Lemma 1.1 and Theorem 2.1, we obtain Corollary 2.3 for the matching number. From Lemma 1.1 and Corollary 2.1, we get Corollary 2.3 for the vertex cover number.

Corollary 2.3. *Among bipartite graphs with n vertices and matching number/vertex cover number ν, where $2 \leq \nu \leq \lfloor \frac{n}{2} \rfloor$, $K_{\nu, n-\nu}$ is the unique graph with the maximum χ_a for $a \geq 0$.*

From Lemma 1.1 and Corollary 2.2, we get Corollary 2.4.

Corollary 2.4. *Among bipartite graphs with n vertices and edge cover number/independence number β', where $\lceil \frac{n}{2} \rceil \leq \beta' \leq n-2$, $K_{\beta', n-\beta'}$ is the unique graph with the maximum χ_a for $a \geq 0$.*

3. Multipartite graphs with given order and graphs with given chromatic number

Let us consider the index I_f for a function f which has property P.

Theorem 3.1. *Let G be any k-partite graph with n vertices where $2 \leq k \leq n$. If f has property P, then*

$$I_f(G) \leq I_f(K_{n_1, n_2, \ldots, n_k}).$$

with equality if and only if G is $K_{n_1, n_2, \ldots, n_k}$, where $|n_i - n_j| \leq 1$, $1 \leq i < j \leq k$ and $n_1 + n_2 + \cdots + n_k = n$.

Proof. Let G' be any k-partite graph of order n having the maximum I_f index. The function f has property P, thus f satisfies Definition 1.2 (i) and (ii), so by Lemma 1.3, I_f increases when adding edges to a graph. Thus any two vertices of G' from distinct partite sets are adjacent. So G' is $K_{n_1, n_2, \ldots, n_k}$, where $n_1, n_2, \ldots, n_k$ are some positive integers. Let us prove that $|n_i - n_j| \leq 1$, where $1 \leq i < j \leq k$.

Assume to the contrary that $|n_i - n_j| \geq 2$ for some i, j, where $1 \leq i < j \leq k$. We can assume that $n_1 \geq n_2 + 2$ (and $n_2 \geq 1$). Let us investigate $I_f(G') - I_f(G'')$ for $G' = K_{n_1, n_2, \ldots, n_k}$ and $G'' = K_{n_1 - 1, n_2 + 1, \ldots, n_k}$.

For $i = 1, 2, \dots, k$, let V_i' and V_i'' be the i-th partite set of G' and G'', respectively. For any vertex $v' \in V_1'$ and any $w' \in V_2'$, we obtain $d_{G'}(v') = n - n_1$ and $d_{G'}(w') = n - n_2$. For any vertex $v'' \in V_1''$ and any $w'' \in V_2''$, we obtain $d_{G''}(v'') = n - (n_1 - 1)$ and $d_{G''}(w'') = n - (n_2 + 1)$. For any other vertex z, we have $d_{G'}(z) = d_{G''}(z)$. Therefore, we obtain

$$
\begin{aligned}
& I_f(G'') - I_f(G') \\
&= \sum_{v'' \in V_1'', w'' \in V_2''} f(d_{G''}(v''), d_{G''}(w'')) - \sum_{v' \in V_1', w' \in V_2'} f(d_{G'}(v'), d_{G'}(w')) \\
&\quad + \sum_{v'' \in V_1'', z'' \in V_3'' \cup \ldots \cup V_k''} f(d_{G''}(v''), d_{G''}(z'')) + \sum_{w'' \in V_2'', z'' \in V_3'' \cup \ldots \cup V_k''} f(d_{G''}(w''), d_{G''}(z'')) \\
&\quad - \sum_{v' \in V_1', z' \in V_3' \cup \ldots \cup V_k'} f(d_{G'}(v'), d_{G'}(z')) - \sum_{w' \in V_2', z' \in V_3' \cup \ldots \cup V_k'} f(d_{G'}(w'), d_{G'}(z')) \\
&= (n_1 - 1)(n_2 + 1) f(n - n_1 + 1, n - n_2 - 1) - n_1 n_2 f(n - n_1, n - n_2) \\
&\quad + (n_1 - 1) \sum_{i=3}^{k} n_i\, f(n - n_1 + 1, n - n_i) + (n_2 + 1) \sum_{i=3}^{k} n_i\, f(n - n_2 - 1, n - n_i) \\
&\quad - n_1 \sum_{i=3}^{k} n_i\, f(n - n_1, n - n_i) - n_2 \sum_{i=3}^{k} n_i\, f(n - n_2, n - n_i) \\
&= n_1 n_2 [f(n - n_1 + 1, n - n_2 - 1) - f(n - n_1, n - n_2)] \\
&\quad + (n_1 - n_2 - 1) f(n - n_1 + 1, n - n_2 - 1) \\
&\quad + (n_1 - n_2 - 2) \sum_{i=3}^{k} n_i [f(n - n_1 + 1, n - n_i) - f(n - n_1, n - n_i)] \\
&\quad + (n_2 + 1) \sum_{i=3}^{k} n_i [f(n - n_1 + 1, n - n_i) - f(n - n_1, n - n_i)] \\
&\quad - (n_2 + 1) \sum_{i=3}^{k} n_i [f(n - n_2, n - n_i) - f(n - n_2 - 1, n - n_i)] \\
&\quad + \sum_{i=3}^{k} n_i [f(n - n_2, n - n_i) - f(n - n_1, n - n_i)].
\end{aligned}
$$

The function f has property P, thus from part (iii) of Definition 1.2, we obtain

$$f(n - n_1 + 1, n - n_2 - 1) \geq f(n - n_1, n - n_2).$$

Since the function f satisfies Definition 1.2 (i), we get

$$f(n - n_1 + 1, n - n_2 - 1) > 0.$$

The function f satisfies Definition 1.2 (ii), thus

$$f(n - n_1 + 1, n - n_i) \geq f(n - n_1, n - n_i) \text{ and } f(n - n_2, n - n_i) \geq f(n - n_1, n - n_i).$$

The function f has property P, so from part (iv) of Definition 1.2, we have

$$f(n-n_1+1, n-n_i) - f(n-n_1, n-n_i) \geq f(n-n_2, n-n_i) - f(n-n_2-1, n-n_i)$$

Thus $I_f(G'') - I_f(G') > 0$, so $I_f(G'') > I_f(G')$, which means that G' does not have the largest I_f. We have a contradiction. Hence, $|n_i - n_j| \leq 1$. □

We use Theorem 3.1 to get a sharp upper bound for graphs with given chromatic number.

Theorem 3.2. *Let G be any graph with n vertices and chromatic number γ where $2 \leq \gamma \leq n$. If f has property P, then*

$$I_f(G) \leq I_f(K_{n_1,n_2,\dots,n_\gamma})$$

with equality if and only if G is $K_{n_1,n_2,\dots,n_\gamma}$, where $|n_i - n_j| \leq 1$, $1 \leq i < j \leq \gamma$ and $n_1 + n_2 + \dots + n_\gamma = n$.

Proof. Let G' be any graph of order n and chromatic number γ having the maximum I_f index. The graph G' contains no edges connecting the vertices in the same color class, thus G' is a γ-partite graph. Hence, by Theorem 3.1, G' is $K_{n_1,n_2,\dots,n_\gamma}$, where $|n_i - n_j| \leq 1$ and $1 \leq i < j \leq \gamma$. □

From Lemma 1.2, we know that the function $f(x, y) = (x + y)^a$ has property P for $0 \leq a \leq 1$. Thus, using Lemma 1.2 and Theorem 3.1, we obtain the following corollary.

Corollary 3.1. *Among k-partite graphs with n vertices where $2 \leq k \leq n$, $K_{n_1,n_2,\dots,n_k}$ where $n_1 + n_2 + \dots + n_k = n$ and $|n_i - n_j| \leq 1$ for $1 \leq i < j \leq k$, are the graphs with the maximum χ_a for $0 \leq a \leq 1$.*

From Lemma 1.2 and Theorem 3.2, we obtain Corollary 3.2.

Corollary 3.2. *Among graphs with n vertices and chromatic number γ where $2 \leq \gamma \leq n$, $K_{n_1,n_2,\dots,n_\gamma}$ where $n_1 + n_2 + \dots + n_\gamma = n$ and $|n_i - n_j| \leq 1$ for $1 \leq i < j \leq \gamma$, are the graphs with the maximum χ_a for $0 \leq a \leq 1$.*

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