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Research Article

Degree-based function index of graphs with given bipartition and small cyclomatic number

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Abstract

We investigate the degree-based function index $I_f(G) = \sum_{vw\in E(G)} f(d_G(v), d_G(w))$ of a graph G, where $E(G)$ is the set of edges of G, $d_G(v)$ and $d_G(w)$ are the degrees of vertices v and w in G, respectively, and f is a symmetric function of two variables which satisfies some conditions. We obtain sharp upper bounds on I_f for trees, unicyclic graphs and bicyclic graphs with given bipartition. Then, among trees and unicyclic graphs with given bipartition, we present graphs with the largest values of the first general Gourava index $FGO_a(G) = \sum_{vw\in E(G)}[d_G(v)d_G(w) + d_G(v) + d_G(w)]^a$ for $a \geq 1$, Bollobás-Erdős-Sarkar index $BES_{l,a}(G) = \sum_{vw\in E(G)}[(d_G(v) + l)(d_G(w) + l)]^a$ for $a \geq 1$ and $l > -1$ (with its special cases which are general reduced second Zagreb index $GRM_l(G) = \sum_{vw\in E(G)}(d_G(v) + l)(d_G(w) + l)$ for $l > -1$, and general Randić index $R_a(G) = \sum_{vw\in E(G)}[d_G(v)d_G(w)]^a$ for $a \geq 1$), general Sombor index $SO_{a,b}(G) = \sum_{vw\in E(G)}([d_G(v)]^a + [d_G(w)]^a)^b$, generalized Zagreb index $GZ_{a,b}(G) = \sum_{vw\in E(G)}([d_G(v)]^a[d_G(w)]^b + [d_G(v)]^b[d_G(w)]^a)$ and one other general index $M_{a,b}(G) = \sum_{vw\in E(G)}[d_G(v)d_G(w)]^a[d_G(v) + d_G(w)]^b$ for $a \geq 1$ and $b \geq 1$.

Keywords: tree; unicyclic graph; bicyclic graph; bipartition; function index.

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1. Introduction and preliminary results

We denote by $V(G)$ and $E(G)$ the set of vertices and edges of a graph G, respectively. The set/number of vertices adjacent to a vertex v is the neighbourhood $N_G(v)$/degree $d_G(v)$ of v in G. A vertex of degree 1 is a pendant vertex. The distance between v and w is the number of edges in a shortest path connecting v and w in G. The distance between any two furthest vertices in G is the diameter of G.

A tree, unicyclic graph and bicyclic graph is a simple connected graph with n vertices which has $n-1$, n and $n+1$ edges, respectively. In a bipartite graph, vertices can be partitioned into two partite sets V_1 and V_2, where any two vertices from the same set are non-adjacent. if $|V_1| = p$ and $|V_2| = q$, then a bipartite graph has a (p, q)-bipartition.

Indices of graphs are investigated due to their extensive applications, particularly in chemistry. Research on bond incident degree indices was carried for example in [1] and [21]. We use a real-valued symmetric function of two variables f, to study the degree-based function index

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

Let us present several general indices defined for a graph G and $a, b \in \mathbb{R}$.

If $f(d_G(v), d_G(w)) = [d_G(v)d_G(w)]^a$, we obtain the general Randić index

$$R_a(G) = \sum_{vw\in E(G)} [d_G(v)d_G(w)]^a$$

first considered by Bollobás and Erdős [4]. Note that R_1 is the second Zagreb index and R_2 is the second hyper-Zagreb index.

The general reduced second Zagreb index

$$GRM_a(G) = \sum_{vw\in E(G)} (d_G(v) + a)(d_G(w) + a)$$

was introduced in [10]. Note that GRM_0 is the second Zagreb index.

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The Bollobás-Erdős-Sarkar index

$$BES_{l,a}(G) = \sum_{vw \in E(G)} [(d_G(v) + l)(d_G(w) + l)]^a$$

which was introduced in [2] generalizes the previous two general indices. We consider it for $a \geq 1$ and $l > -1$. Note that $BES_{0,a}(G) = R_a$ and $BES_{l,1}(G) = GRM_l$.

The first general Gourava index

$$FGO_a(G) = \sum_{vw \in E(G)} [d_G(v)d_G(w) + d_G(v) + d_G(w)]^a$$

was defined in [18]. Note that FGO_1 is the first Gourava index (defined in [13]) and FGO_2 is the first hyper-Gourava index (defined in [12]).

The general Sombor index $SO_{a,b}(G)$ is obtained from $I_f(G)$ when $f(d_G(v), d_G(w)) = ([d_G(v)]^b + [d_G(w)]^b)^a$. We have

$$SO_{a,b}(G) = \sum_{vw \in E(G)} ([d_G(v)]^b + [d_G(w)]^b)^a;$$

see [9]. Note that $SO_{a,1}(G)$ is the general sum-connectivity index introduced by Zhou and Trinajstić [20], $SO_{1,1}$ is the first Zagreb index, $SO_{2,1}$ is the first hyper-Zagreb index and $SO_{1,2}$ is the forgotten index. The generalized Zagreb index

$$GZ_{a,b}(G) = \sum_{vw \in E(G)} ([d_G(v)]^a [d_G(w)]^b + [d_G(v)]^b [d_G(w)]^a)$$

was introduced by Azari and Iranmanesh [3] and for one other general index

$$M_{a,b}(G) = \sum_{vw \in E(G)} [d_G(v)d_G(w)]^a [d_G(v) + d_G(w)]^b;$$

see [7]. Note that $M_{1,1}$ is the second Gourava index (see [13]) known also as the third redefined Zagreb index and $M_{2,2}$ is the second hyper-Gourava index (see [12]).

Trees, unicyclic and bicyclic graphs are important networks that can represent chemical structures. Among trees and unicyclic graphs with given bipartition, trees having the largest and smallest Steiner Wiener index were given in [14], trees with the smallest energy of Hosoya index were presented in [19], trees with the smallest Zagreb eccentricity indices were obtained in [16], trees with the extremal general eccentric distance sum were given in [6], trees and unicyclic graphs with the largest and smallest hyper-Wiener index were obtained in [5], and unicyclic graphs with given bipartition having the largest Wiener index were presented in [11]. Indices of trees were studied also in [8] and [15]. Indices for bicyclic graphs with given bipartition have not been studied.

Except for trees, we study unicyclic and bicyclic graphs which are bipartite. It follows that those graphs contain only even cycles.

Let us introduce Definition 1.1.

Definition 1.1. *A symmetric function $f(x, y)$ of two variables x and y having property P is any function such that*

(i) $f(x_1, y_1) < f(x_2, y_2)$ for $1 \leq x_1 \leq x_2$ and $1 \leq y_1 \leq y_2$, where $\{x_1, y_1\} \neq \{x_2, y_2\}$,

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

Lemma 1.1. *The following functions of two variables x and y have property P:*

- *$(xy + x + y)^a$ for $a \geq 1$,*
- *$(x^b + y^b)^a$, $(xy)^a(x + y)^b$ and $x^a y^b + x^b y^a$ for $a, b \geq 1$,*
- *$[(x + l)(y + l)]^a$ for $a \geq 1$, $l > -1$.*

Proof. Lemma 1.1 for the functions $(xy+x+y)^a$, $(xy)^a(x+y)^b$ and $x^a y^b + x^b y^a$, where $a, b \geq 1$, was proved in [18]. Lemma 1.1 for $(x^b + y^b)^a$, where $a, b \geq 1$, was proved in [17].

Let $f(x, y) = [(x + l)(y + l)]^a$, where $x, y \geq 1$ and $l > -1$.

(i) For $a > 0$, we get $\frac{\partial f(x,y)}{\partial x} = a[(x + l)(y + l)]^{a-1}(y + l) > 0$. Similarly, $\frac{\partial f(x,y)}{\partial y} > 0$, so the condition (i) of Definition 1.1 is satisfied.

(ii) Let
$$g(x,y) = f(x+c, y+c') - f(x,y) = [(x+l+c)(y+l+c')]^a - [(x+l)(y+l)]^a.$$
Then
$$\frac{\partial g(x,y)}{\partial x} = a[(x+l+c)(y+l+c')]^{a-1}(y+l+c') - a[(x+l)(y+l)]^{a-1}(y+l).$$
Condition (i) holds for $a > 0$, thus
$$[(x+l+c)(y+l+c')]^{a-1} > [(x+l)(y+l)]^{a-1}$$
for $a > 1$. Note that $y+l+c' \geq y+l$, so $\frac{\partial g(x,y)}{\partial x} > 0$ for $a > 1$. For $a = 1$, we get $\frac{\partial g(x,y)}{\partial x} = c' \geq 0$, therefore $\frac{\partial g(x,y)}{\partial x} \geq 0$ for $a \geq 1$. Similarly, $\frac{\partial g(x,y)}{\partial y} \geq 0$ for $a \geq 1$, so the condition (ii) of Definition 1.1 is satisfied.

Thus, the function $[(x+l)(y+l)]^a$ has property P for $a \geq 1$ and $l > -1$. □

Lemma 1.2 is used in the proofs of our theorems mostly for $s = 2$. Note that the vertex v can be adjacent to more than s non-pendant vertices in G'.

Lemma 1.2. *Let $p, q \geq 2$. Let G' be a connected graph having a (p,q)-bipartition containing two vertices u and v such that u is adjacent to exactly $s \geq 1$ non-pendant vertices, all of those s vertices are adjacent also to v, $d_{G'}(u) \geq s+1$ and $d_{G'}(v) \geq s+1$. If f has property P, then there exists a connected graph G'' with the same number of edges having a (p,q)-bipartition such that $I_f(G') < I_f(G'')$.*

Proof. Let us denote the non-pendant neighbours of u in G' by $w_1, w_2, \ldots, w_s$, and the pendant neighbours of u in G' by $u_1, u_2, \ldots, u_t$. So $d_{G'}(u) = s+t$, where $s, t \geq 1$. The vertex v is also adjacent to $w_1, w_2, \ldots, w_s$ in G', and v has r other neighbours $v_1, v_2, \ldots, v_r$, where $r \geq 1$. So $d_{G'}(v) = s+r$. Let $V(G'') = V(G')$ and
$$E(G'') = \{vu_1, vu_2, \ldots, vu_t\} \cup E(G') \setminus \{uu_1, uu_2, \ldots, uu_t\}.$$
Clearly, G' and G'' contain the same number of edges. Since u and v are in the same partite set, G'' has a (p,q)-bipartition. We get $d_{G''}(u) = s$, $d_{G''}(v) = s+r+t$ and $d_{G'}(x) = d_{G''}(x)$ for $x \in V(G') \setminus \{u, v\}$. We have $d_{G'}(u_i) = d_{G''}(u_i) = 1$ for $i = 1, 2, \ldots, t$. Then
$$\begin{aligned}
I_f(G') - I_f(G'') &= \sum_{i=1}^{t}[f(d_{G'}(u), d_{G'}(u_i)) - f(d_{G''}(v), d_{G''}(u_i))] + \sum_{i=1}^{r}[f(d_{G'}(v), d_{G'}(v_i)) - f(d_{G''}(v), d_{G''}(v_i))] \\
&\quad + \sum_{i=1}^{s}[f(d_{G'}(u), d_{G'}(w_i)) - f(d_{G''}(u), d_{G''}(w_i))] + \sum_{i=1}^{s}[f(d_{G'}(v), d_{G'}(w_i)) - f(d_{G''}(v), d_{G''}(w_i))] \\
&= t[f(s+t,1) - f(s+r+t,1)] + \sum_{i=1}^{r}[f(s+r, d_{G'}(v_i)) - f(s+r+t, d_{G'}(v_i))] \\
&\quad + \sum_{i=1}^{s}[f(s+t, d_{G'}(w_i)) - f(s, d_{G'}(w_i)) + f(s+r, d_{G'}(w_i)) - f(s+r+t, d_{G'}(w_i))].
\end{aligned}$$
Since the function f has property P, by Definition 1.1 (i), we get
$$f(s+t,1) < f(s+r+t,1) \ \text{ and } \ f(s+r, d_{G'}(v_i)) < f(s+r+t, d_{G'}(v_i)).$$
By Definition 1.1 (ii), we have
$$f(s+t, d_{G'}(w_i)) - f(s, d_{G'}(w_i)) \leq f(s+r+t, d_{G'}(w_i)) - f(s+r, d_{G'}(w_i)).$$
So $I_f(G') - I_f(G'') < 0$, hence $I_f(G') < I_f(G'')$. □

In Lemma 1.2,

- if G' is a tree, then $s = 1$,
- if G' is a unicyclic graph, then $1 \leq s \leq 2$,
- if G' is a bicyclic graph, then $1 \leq s \leq 3$.

For $s = 1$, we present a corollary of Lemma 1.2.

Corollary 1.1. *Let $p, q \geq 2$. Let G' be a connected graph having a (p,q)-bipartition containing two non-pendant vertices u and v such that u is adjacent to exactly one non-pendant vertex and that vertex is adjacent also to v. If f has property P, then there exists a connected graph G'' with the same number of edges having a (p,q)-bipartition such that $I_f(G') < I_f(G'')$.*

Remark 1.1. *The graphs G' and G'' stated in Lemma 1.2 and Corollary 1.1 are connected with the same number of edges. Thus if G' is a tree / unicyclic graph / bicyclic graph, then G'' is a tree / unicyclic graph / bicyclic graph.*

2. Main results

First, we consider trees. The unique tree having a $(p,1)$-bipartition is the star S_{p+1}. For $p \geq q \geq 2$, the double star $S_{p-1,q-1}$ presented in Figure 2.1 is a tree containing two non-pendant vertices, where one non-pendant vertex is adjacent to $p-1$ pendant vertices and the other non-pendant vertex is adjacent to $q-1$ pendant vertices.

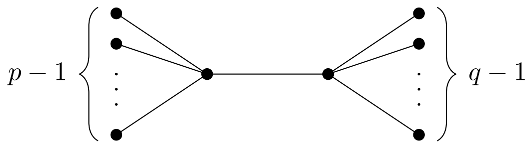

Figure 2.1: Tree $S_{p-1,q-1}$.

We show that $S_{p-1,q-1}$ is the extremal tree for Theorem 2.1.

Theorem 2.1. *Let G be any tree which has a (p,q)-bipartition, where $p \geq q \geq 2$. If f has property P, then*

$$I_f(G) \leq (p-1)f(p,1) + (q-1)f(q,1) + f(p,q)$$

with equality if and only if G is $S_{p-1,q-1}$.

Proof. Let G' be any tree having a (p,q)-bipartition with the largest I_f. If the diameter of G' would be at least 4, then we can denote the first five vertices of its longest path by u_1, u, w_1, v, v_1, and by Corollary 1.1 (or Lemma 1.2 and its proof) and Remark 1.1, there would exist a tree with the same bipartition having larger I_f.

So, the diameter of G' is at most 3. For $p \geq q \geq 2$, there exists no tree with diameter smaller than 3, therefore G' has diameter 3. The unique tree with a (p,q)-bipartition and diameter 3 is $S_{p-1,q-1}$, so T' is $S_{p-1,q-1}$ and

$$I_f(S_{p-1,q-1}) = (p-1)f(p,1) + (q-1)f(q,1) + f(p,q).$$ □

There is no unicyclic graph having a $(p,1)$-bipartition. For $p \geq q \geq 2$, let $C_{4,p-2,q-2}$ be the graph which consists of the cycle C_4, where one vertex of that C_4 is adjacent to $p-2$ pendant vertices, and one of its neighbours on that C_4 is adjacent to $q-2$ pendant vertices; see Figure 2.2.

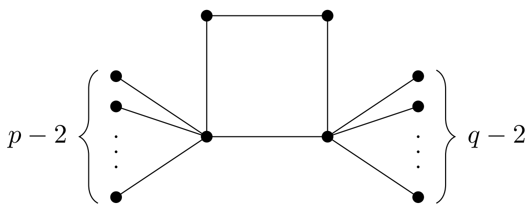

Figure 2.2: Unicyclic graph $C_{4,p-2,q-2}$.

Let us prove that $C_{4,p-2,q-2}$ is the extremal unicyclic graph with a (p,q)-bipartition.

Theorem 2.2. *Let G be any unicyclic graph which has a (p,q)-bipartition, where $p \geq q \geq 2$. If f has property P, then*

$$I_f(G) \leq (p-2)f(p,1) + (q-2)f(q,1) + f(p,q) + f(p,2) + f(q,2) + f(2,2)$$

with equality if and only if G is $C_{4,p-2,q-2}$.

Proof. Let G' be a unicyclic graph with a (p,q)-bipartition having the largest I_f. Let $v_1v_2 \ldots v_kv_1$, where $k \geq 4$ is even, be the cycle of G'.

Claim 1. The cycle of G' has length 4.

Assume to the contrary that the length of the cycle is even $k \geq 6$. Let us define G_1 such that $V(G_1) = V(G')$ and

$$E(G_1) = \cup_{v \in N_{G'}(v_{k-1}) \setminus \{v_k\}} \{v_1 v\} \cup E(G') \setminus \cup_{v \in N_{G'}(v_{k-1}) \setminus \{v_k\}} \{v_{k-1} v\}.$$

Since v_1 and v_{k-1} are in the same partite set, G_1 has a (p,q)-bipartition. The graph G_1 contains the cycle $v_1v_2\dots v_{k-2}v_1$ of length $k-2$. Let $d_{G'}(v_1)=t$ and $d_{G'}(v_{k-1})=r$. We have $t,r\ge 2$, $d_{G_1}(v_1)=t+r-1$ and $d_{G_1}(v_{k-1})=1$. Then

$$\begin{aligned} I_f(G')-I_f(G_1) &= \sum_{u\in N_{G'}(v_1)\setminus\{v_k\}} [f(d_{G'}(v_1),d_{G'}(u))-f(d_{G_1}(v_1),d_{G_1}(u))] \\ &\quad+\sum_{v\in N_{G'}(v_{k-1})\setminus\{v_k\}} [f(d_{G'}(v_{k-1}),d_{G'}(v))-f(d_{G_1}(v_1),d_{G_1}(v))] \\ &\quad+f(d_{G'}(v_1),d_{G'}(v_k))-f(d_{G_1}(v_1),d_{G_1}(v_k))+f(d_{G'}(v_{k-1}),d_{G'}(v_k))-f(d_{G_1}(v_{k-1}),d_{G_1}(v_k)) \\ &= \sum_{u\in N_{G'}(v_1)\setminus\{v_k\}} [f(t,d_{G'}(u))-f(t+r-1,d_{G_1}(u))]+\sum_{v\in N_{G'}(v_{k-1})\setminus\{v_k\}} [f(r,d_{G'}(v))-f(t+r-1,d_{G_1}(v))] \\ &\quad+f(t,d_{G'}(v_k))-f(t+r-1,d_{G_1}(v_k))+f(r,d_{G'}(v_k))-f(1,d_{G_1}(v_k)) \end{aligned}$$

The function f has property P, so by Definition 1.1 (i),

$$f(t,d_{G'}(u))<f(t+r-1,d_{G_1}(u)) \text{ and } f(r,d_{G'}(v))<f(t+r-1,d_{G_1}(v)),$$

By Definition 1.1 (ii),

$$f(r,d_{G'}(v_k))-f(1,d_{G_1}(v_k))\le f(t+r-1,d_{G_1}(v_k))-f(t,d_{G'}(v_k))$$

So $I_f(G')-I_f(G_1)<0$, hence $I_f(G')<I_f(G_1)$. Thus G' does not have the largest I_f, a contradiction.

Claim 2. Each pendant vertex of G' is adjacent to a vertex of the cycle.

If G' would contain a pendant vertex not adjacent to a vertex of the cycle, we can denote by u the unique vertex which is adjacent to a (pendant) vertex furthest from the cycle, and denote by v any non-pendant vertex whose distance is 2 from u. Then by Corollary 1.1 and Remark 1.1, there would be a unicyclic graph with the same bipartition having larger I_f.

Claim 3. One of any two non-adjacent vertices of the cycle has degree 2 in G'.

If two non-adjacent vertices of the cycle C_4 would have degree at least 3 in G', say $d_{G'}(v_1)\ge 3$ and $d_{G'}(v_3)\ge 3$, we can use $v_1=u$ and $v_3=v$. Then by Lemma 1.2 and Remark 1.1, there would be a unicyclic graph with the same bipartition having larger I_f.

The only unicyclic graph having a (p,q)-bipartition satisfying Claims 1, 2 and 3 is $C_{4,p-2,q-2}$. So G' is $C_{4,p-2,q-2}$ and

$$I_f(C_{4,p-2,q-2})=(p-2)f(p,1)+(q-2)f(q,1)+f(p,q)+f(p,2)+f(q,2)+f(2,2). \qquad \square$$

There is no bicyclic graph with a $(p,1)$-bipartition or $(2,2)$-bipartition. For $j\ge 2$ and $j'\ge 3$, the graph $C'_{4,j-2,j'-3}$ is obtained from the complete bipartite graph $K_{3,2}$ by joining one vertex of degree 2 in that $K_{3,2}$ to $j-2$ new vertices, and one vertex of degree 3 in that $K_{3,2}$ to $j'-3$ new vertices; see Figure 2.3.

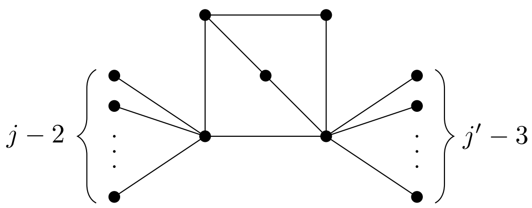

Figure 2.3: Bicyclic graph $C'_{4,j-2,j'-3}$.

Let us present upper bounds on I_f for bicyclic graphs.

Theorem 2.3. *Let G be any bicyclic graph which has a (p,q)-bipartition. Let f be a function having property P.*

For $p\ge 3$ and $q=2$, we have

$$I_f(G)\le (p-3)f(p,1)+3f(p,2)+3f(3,2)$$

with equality if and only if G is $C'_{4,0,p-3}$.

For $p\ge q\ge 3$,

$$I_f(G)\le \begin{cases} (p-2)f(p,1)+(q-3)f(q,1)+f(p,q)+f(p,3)+2f(q,2)+2f(3,2) & \text{if } c\ge 0, \\ (q-2)f(q,1)+(p-3)f(p,1)+f(p,q)+f(q,3)+2f(p,2)+2f(3,2) & \text{if } c<0, \end{cases}$$

where $c=f(p,1)-f(q,1)+f(p,3)-f(q,3)+2f(q,2)-2f(p,2)$.

Equalities for $I_f(G)$ hold if and only if G is $C'_{4,p-2,q-3}$ for $c>0$, G is any of the graphs $C'_{4,p-2,q-3}$, $C'_{4,q-2,p-3}$ for $c=0$, and G is $C'_{4,q-2,p-3}$ for $c<0$.

Proof. Let G' be a bicyclic graph with a (p,q)-bipartition having the largest I_f. Let C_k and C_l be the two shortest cycles in G'. (Note that if C_k and C_l have a common edge, then G' contains one other cycle, otherwise if C_k and C_l have no common edge, then G' contains no other cycle.) Since G' is bipartite, $k, l \geq 4$ are even. Let A be a path connecting C_k and C_l. Let $C_k = v_1 v_2 \dots v_k v_1$ and $C_l = u_1 u_2 \dots u_l u_1$. The cycles C_k and C_l have $x \geq 0$ common vertices. If $x \geq 1$, then the length of A is 0 and we can assume that $v_i = u_i$ for $1 = 1, 2, \dots, x$. We have $x \leq \frac{k}{2}$ and $x \leq \frac{l}{2}$, otherwise if $x > \frac{k}{2}$ or $x > \frac{l}{2}$, it would imply that the third cycle would not be the longest cycle. Let S be the set of all the vertices of C_k, C_l and A.

Claim 1. The cycles C_k and C_l have length 4.

Assume to the contrary that the length of C_k or C_l, say C_k, is at least 6. So $k \geq 6$ is even. We can use the proof of Claim 1 presented in the proof of Theorem 2.2 to show that there exists a graph G_1 containing the cycle $v_1 v_2 \dots v_{k-2} v_1$ of length $k-2$, such that $I_f(G') < I_f(G_1)$. Since the cycle C_l remains the same in G_1, the graph G_1 is bicyclic and it has a (p,q)-bipartition. Since G' does not have the largest I_f, a contradiction.

Claim 2. Each pendant vertex of G' is adjacent to a vertex in S.

If G' would contain a pendant vertex not adjacent to a vertex in S, then by Corollary 1.1 and Remark 1.1, G' would not have the largest I_f.

Claim 3. The cycles C_k and C_l have at least one edge in common.

Assume that the cycles C_k and C_l have no edge in common. Without loss of generality, suppose that the path A connecting C_k and C_l contains the vertices v_1 and u_1. By Claim 1, we have $k, l = 4$.

Note that v_3 and u_3 are not adjacent to pendant vertices (otherwise, if say v_3 is adjacent to a pendant vertex, then using $v_3 = u$ and $v_1 = v$, by Lemma 1.2 and Remark 1.1, there would be a bicyclic graph with the same bipartition having larger I_f).

Similarly, by Lemma 1.2, one of v_2, v_4 is not adjacent to pendant vertices and one of u_2, u_4 is not adjacent to pendant vertices. We can assume that v_4 and u_4 are not adjacent to pendant vertices, so $d_{G'}(v_3) = d_{G'}(u_3) = d_{G'}(v_4) = d_{G'}(u_4) = 2$. Let $d_{G'}(v_1) = z$, $d_{G'}(v_2) = r$ and $d_{G'}(u_2) = t$. We have $z \geq 3$ and $r, t \geq 2$.

Let the length of A be even. We define G_2 such that $V(G_2) = V(G')$ and $E(G_2) = \{u_2 v_3\} \cup E(G') \setminus \{u_2 u_3\}$. Since the length of A is even, v_3 and u_3 are in the same partite set, so G_2 has a (p,q)-bipartition. We have $d_{G_2}(v_3) = 3$ and $d_{G_2}(u_3) = 1$. Then

$$\begin{aligned} I_f(G') - I_f(G_2) &= f(d_{G'}(u_2), d_{G'}(u_3)) - f(d_{G_2}(u_2), d_{G_2}(v_3)) + f(d_{G'}(u_3), d_{G'}(u_4)) - f(d_{G_2}(u_3), d_{G_2}(u_4)) \\ &\quad + f(d_{G'}(v_2), d_{G'}(v_3)) - f(d_{G_2}(v_2), d_{G_2}(v_3)) + f(d_{G'}(v_3), d_{G'}(v_4)) - f(d_{G_2}(v_3), d_{G_2}(v_4)) \\ &= f(t,2) - f(t,3) + f(2,2) - f(1,2) + f(r,2) - f(r,3) + f(2,2) - f(3,2). \end{aligned}$$

Since f has property P, by Definition 1.1 (i), we get $f(t,2) < f(t,3)$ and $f(r,2) < f(r,3)$. By Definition 1.1 (ii), we have $f(2,2) - f(1,2) \leq f(3,2) - f(2,2)$. Thus $I_f(G') - I_f(G_2) < 0$, so $I_f(G') < I_f(G_2)$.

Let the length of A be odd. We define G_3 such that $V(G_3) = V(G')$ and $E(G_3) = \{u_2 v_4\} \cup E(G') \setminus \{u_2 u_3\}$. Since the length of A is odd, v_4 and u_3 are in the same partite set, so G_3 has a (p,q)-bipartition. We have $d_{G_3}(v_4) = 3$ and $d_{G_3}(u_3) = 1$. Then

$$\begin{aligned} I_f(G') - I_f(G_3) &= f(d_{G'}(u_2), d_{G'}(u_3)) - f(d_{G_3}(u_2), d_{G_3}(v_4)) + f(d_{G'}(u_3), d_{G'}(u_4)) - f(d_{G_3}(u_3), d_{G_3}(u_4)) \\ &\quad + f(d_{G'}(v_1), d_{G'}(v_4)) - f(d_{G_3}(v_1), d_{G_3}(v_4)) + f(d_{G'}(v_3), d_{G'}(v_4)) - f(d_{G_3}(v_3), d_{G_3}(v_4)) \\ &= f(t,2) - f(t,3) + f(2,2) - f(1,2) + f(z,2) - f(z,3) + f(2,2) - f(3,2), \end{aligned}$$

which is the same situation as in the case when the length of A is even. We obtain $I_f(G') < I_f(G_3)$, so G' does not have the largest I_f, a contradiction.

Claim 4. The cycles C_k and C_l have two edges in common.

By Claim 1, the cycles C_k and C_l have length 4, so they cannot share more than 2 edges. By Claim 3, C_k and C_l share at least one edge. We prove by contradiction that C_k and C_l share two edges.

Assume that C_k and C_l share exactly one edge $v_1 v_2$. Let $d_{G'}(v_1) = z$. We have $z \geq 3$. Note that v_3, v_4, u_3 and u_4 are not adjacent to pendant vertices (otherwise, if say v_3 is adjacent to a pendant vertex, then using $v_3 = u$ and $v_1 = v$, by Lemma 1.2, there would be a bicyclic graph with the same bipartition having larger I_f). So $d_{G'}(v_3) = d_{G'}(v_4) = d_{G'}(u_3) = d_{G'}(u_4) = 2$.

We define G_4 such that $V(G_4) = V(G')$ and $E(G_4) = \{u_3v_4\} \cup E(G') \setminus \{u_3u_4\}$. Since v_4 and u_4 are in the same partite set, G_4 has a (p,q)-bipartition. We get $d_{G_4}(v_4) = 3$ and $d_{G_4}(u_4) = 1$. Then

$$\begin{aligned} I_f(G') - I_f(G_4) &= f(d_{G'}(u_3), d_{G'}(u_4)) - f(d_{G_4}(u_3), d_{G_4}(v_4)) + f(d_{G'}(v_1), d_{G'}(u_4)) - f(d_{G_4}(v_1), d_{G_4}(u_4)) \\ &\quad + f(d_{G'}(v_1), d_{G'}(v_4)) - f(d_{G_4}(v_1), d_{G_4}(v_4)) + f(d_{G'}(v_3), d_{G'}(v_4)) - f(d_{G_4}(v_3), d_{G_4}(v_4)) \\ &= f(2,2) - f(2,3) + f(z,2) - f(z,1) + f(z,2) - f(z,3) + f(2,2) - f(2,3). \end{aligned}$$

We obtain $f(2,2) < f(2,3)$ by Definition 1.1 (i) and $f(z,2) - f(z,1) \le f(z,3) - f(z,2)$ by Definition 1.1 (ii). Therefore, $I_f(G') < I_f(G_4)$, hence G' does not have the largest I_f, a contradiction.

So, by Claim 4, C_k and C_l share two edges v_1v_2 and v_2v_3. By Claim 1, we have $k, l = 4$, so v_4 and u_4 are adjacent to v_1 and v_3. Note that at most one of the vertices v_2, v_4, u_4 is adjacent to pendant vertices (otherwise if say each of v_2 and v_4 would be adjacent to a pendant vertex we can use $v_2 = u$ and $v_4 = v$, and by Lemma 1.2, there would be a bicyclic graph with the same bipartition having larger I_f). Similarly, by Lemma 1.2, at most one of the vertices v_1 and v_3 is adjacent to pendant vertices.

Let $q = 2$. Then G' is $C'_{4,0,p-3}$ and we obtain

$$I_f(C'_{4,0,p-3}) = (p-3)f(p,1) + 3f(p,2) + 3f(3,2).$$

Let $p \ge q \ge 3$. It follows that G' is $C'_{4,p-2,q-3}$ or $C'_{4,q-2,p-3}$. We compare their I_f. We obtain

$$I_f(C'_{4,p-2,q-3}) = (p-2)f(p,1) + (q-3)f(q,1) + f(p,q) + f(p,3) + 2f(q,2) + 2f(3,2)$$

and

$$I_f(C'_{4,q-2,p-3}) = (q-2)f(q,1) + (p-3)f(p,1) + f(p,q) + f(q,3) + 2f(p,2) + 2f(3,2).$$

Then

$$I_f(C'_{4,p-2,q-3}) - I_f(C'_{4,q-2,p-3}) = f(p,1) - f(q,1) + f(p,3) - f(q,3) + 2f(q,2) - 2f(p,2) = c.$$

So, G' is $C'_{4,p-2,q-3}$ if $c > 0$, G' is $C'_{4,q-2,p-3}$ if $c < 0$, and G' is any of the graphs $C'_{4,p-2,q-3}$, $C'_{4,q-2,p-3}$ if $c = 0$. □

Note that if $p = q$, then $c = 0$ in Theorem 2.3 and

$$I_f(G) \le (2p-5)f(p,1) + f(p,p) + f(p,3) + 2f(p,2) + 2f(3,2).$$

3. Conclusion

In Theorems 2.1 and 2.2, we obtained sharp upper bounds on I_f for trees and unicyclic graphs, respectively. By Theorems 2.1, 2.2 and Lemma 1.1, we get Corollary 3.1 for several general indices.

Corollary 3.1. *Among trees and unicyclic graphs with a (p,q)-bipartition, where $p \ge q \ge 2$, $S_{p-1,q-1}$ is the unique tree and $C_{4,p-2,q-2}$ is the unique unicyclic graph having the largest value of*

- *FGO_a for $a \ge 1$,*
- *$SO_{a,b}$, $M_{a,b}$ and $GZ_{a,b}$ for $a, b \ge 1$,*
- *$BES_{l,a}$ for $a \ge 1$ and $l > -1$ (with its special cases GRM_l for $l > -1$ and R_a for $a \ge 1$).*

In Theorem 2.3, we presented upper bounds on I_f for bicyclic graphs. It is more complicated to find extremal graphs for general indices for bicyclic graphs. Let us consider Theorem 2.3 for $f(x,y) = (x+a)(y+a)$. We obtain

$$c = (p+a)(1+a) - (q+a)(1+a) + (p+a)(3+a) - (q+a)(3+a) + 2(q+a)(2+a) - 2(p+a)(2+a) = 0.$$

Thus, by Theorem 2.3 and Lemma 1.1, among bicyclic graphs with a (p,q)-bipartition, where $p \ge q \ge 3$, the graphs $C'_{4,p-2,q-3}$ and $C'_{4,q-2,p-3}$ have the largest value of GRM_a for $a > -1$.

Similarly, one can study the value of c for other functions given in Lemma 1.1. We leave this task for future research. Also, it would be interesting to know graphs with the largest values of I_f among graphs with given bipartition containing more cycles (such as tricyclic and tetracyclic graphs). Therefore, we state the following open problem.

Problem 3.1. *Let f be a function with property P. Among connected graphs with a (p,q)-bipartition and $p+q+i$ edges, where $i \ge 2$, find graphs having the largest value of I_f.*

Note that a connected graph is tricyclic if it has $p+q+2$ edges and it is tetracyclic if it has $p+q+3$ edges.

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References

[1] A. Ali, D. Dimitrov, On the extremal graphs with respect to bond incident degree indices, *Discrete Appl. Math.* **238** (2018) 32–40.

[2] A. Ali, W. Iqbal, Z. Raza, E. E. Ali, J.-B. Liu, F. Ahmad, Q. A. Chaudhry, Some vertex/edge-degree-based topological indices of r-apex trees, *J. Math.* **2021** (2021) 4349074.

[3] M. Azari, A. Iranmanesh, Generalized Zagreb index of graphs, *Stud. Univ. Babes-Bolyai Chem.* **3** (2011) 59–70.

[4] B. Bollobás, P. Erdős, Graphs of extremal weights, *Ars Combin.* **50** (1998) 225–233.

[5] L. Feng, W. Liu, G. Yu, S. Li, The hyper-Wiener index of graphs with given bipartition, *Util. Math.* **95** (2014) 23–32.

[6] Y. K. Feyissa, T. Vetrík, Bounds on the general eccentric distance sum of graphs, *Discrete Math. Lett.* **10** (2022) 99–106.

[7] I. Gutman, E. Milovanović, I. Milovanović, Beyond the Zagreb indices, *AKCE Int. J. Graphs Comb.* **17(1)** (2020) 74–85.

[8] A. E. Hamza, A. Ali, On a conjecture regarding the exponential reduced Sombor index of chemical trees, *Discrete Math. Lett.* **9** (2022) 107–110.

[9] J. C. Hernández, J. M. Rodríguez, O. Rosario, J. M. Sigarreta, Extremal problems on the general Sombor index of a graph, *AIMS Math.* **7(5)** (2022) 8330–8343.

[10] B. Horoldagva, L. Buyantogtokh, K. C. Das, S.-G. Lee, On general reduced second Zagreb index of graphs, *Hacet. J. Math. Stat.* **48(4)** (2019) 1046–1056.

[11] H. Jiang, W. Li, Largest Wiener index of unicyclic graphs with given bipartition, *MATCH Commun. Math. Comput. Chem.* **82(1)** (2019) 77–92.

[12] V. P. Kulli, On hyper Gourava indices and coindices, *Int. J. Math. Arch.* **8(12)** (2017) 116–120.

[13] V. P. Kulli, The Gourava indices and coindices of graphs, *Ann. Pure Appl. Math.* **14(1)** (2017) 33–38.

[14] Z. Li, B. Wu, The Steiner Wiener index of trees with given bipartition, *MATCH Commun. Math. Comput. Chem.* **86(2)** (2021) 363–373.

[15] S. Noureen, A. Ali, Maximum atom-bond sum-connectivity index of n-order trees with fixed number of leaves, *Discrete Math. Lett.* **12** (2023) 26–28.

[16] X. Qi, Z. Du, On Zagreb eccentricity indices of trees, *MATCH Commun. Math. Comput. Chem.* **78(1)** (2017) 241–256.

[17] T. Vetrík, Degree-based function index for graphs with given connectivity, *Iranian J. Math. Chem.* **14(3)** (2023) 183–194.

[18] T. Vetrík, Degree-based function index for graphs with given diameter, *Discrete Appl. Math.* **333** (2023) 59–70.

[19] L. Ye, R. S. Chen, Ordering of trees with a given bipartition by their energies and Hosoya indices, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 193–208.

[20] B. Zhou, N. Trinajstić, On general sum-connectivity index, *J. Math. Chem.* **47** (2010) 210–218.

[21] W. Zhou, S. Pang, M. Liu, A. Ali, On bond incident degree indices of connected graphs with fixed order and number of pendent vertices, *MATCH Commun. Math. Comput. Chem.* **88(3)** (2022) 625–642.