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Optimization Problems for Variable Randić Type Lodeg Index and Other Indices

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Abstract

A large number of graph invariants of the form $\sum_{uv} F(d_u, d_v)$ are studied in mathematical chemistry, where uv denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u. Among them the variable Randić type lodeg index RLI_a, with $F(d_u, d_v) = \log^a d_u \log^a d_v$, for $a > 0$, was found to have applicative properties. The aim of this paper is to obtain new inequalities for the variable Randić type lodeg index, and to characterize graphs extremal with respect to them. In particular, some of the open problems posed by Vukičević are solved in this paper; we characterize graphs with maximum and minimum values of the RLI_a index, for every $a > 0$, in the following sets of graphs with n vertices: graphs, connected graphs, graphs with fixed minimum degree, connected graphs with fixed minimum degree, graphs with fixed maximum degree, and connected graphs with fixed maximum degree. Also, our results can be applied to a large class of topological indices of the form $\sum_{uv \in E(G)} F(d_u, d_v)$, as variable sum lodeg index and variable inverse sum lodeg index, solving some of the open problems posed by Vukičević.

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1 Introduction

Topological indices are parameters associated with chemical compounds that associate the chemical structure with several physical, chemical or biological properties. These indices play an important role in mathematical chemistry, especially regarding quantitative structure-activity relationship (QSAR) and the quantitative structure–property relationship (QSPR).

A family of degree–based topological indices, named *Adriatic indices*, was put forward in [21, 22]. Twenty of them were selected as significant predictors. One of them, the *Randić type lodeg index*, RLI, was singled out in [21] as a significant predictor of heat capacity at T constant. This index is defined as

$$RLI(G) = \sum_{uv \in E(G)} \log d_u \log d_v,$$

where uv denotes the edge of the graph G connecting the vertices u and v, and d_u is the degree of the vertex u.

We study here the properties of the *variable Randić type lodeg index* defined, for each $a \in \mathbb{R}^+$, as

$$RLI_a(G) = \sum_{uv \in E(G)} \log^a d_u \log^a d_v.$$

Note that RLI_1 is the Randić type lodeg index RLI.

The idea behind the variable molecular descriptors is that the variables are determined during the regression so that the standard error of estimate for a particular studied property is as small as possible (see, e.g., [16]).

The aim of this paper is to obtain new inequalities for the variable Randić type lodeg index, and to characterize graphs extremal with respect to them. Also, we want to remark that many previous results on topological indices are proved for connected graphs, but our inequalities hold for both connected and non-connected graphs.

In particular, we characterize the graphs with maximum and minimum values of the RLI_a index, for every $a > 0$, in the following sets of graphs with n vertices: graphs, connected graphs, graphs with a fixed minimum degree, connected graphs with a fixed minimum degree, graphs with a fixed maximum degree, and connected graphs with a fixed maximum degree. These results solve the problems (1), (7) and (8) stated by Vukičević in [24], for every value of the parameter a. We can use these results for detecting chemical compounds that could satisfy desirable properties. Hence, extremal graphs should correspond to molecules with a extremal value of a desired property since there exists a property well correlated with this descriptor for some values of a, in particular, $a = 1$.

Hollas [6] generalized several known indices to $BID(G)$, defined as

$$BID(G) = \sum_{uv \in E(G)} F(d_u, d_v).$$

In some literature, $BID(G)$ was called the *bond incident degree index* [1], [18] or the *connectivity function* [18], [25] of G. See [13, 14] for recent results on BID indices. Also, our results can be applied to this class of topological indices. In particular, we solve these optimization problems for the variable inverse sum lodeg index

$$ISL_a(G) = \sum_{uv \in E(G)} \frac{1}{\log^a d_u + \log^a d_v}\,,$$

with $a < 0$, and for the variable sum lodeg index

$$SLI_a(G) = \sum_{uv \in E(G)} \big(\log^a d_u + \log^a d_v \big),$$

with $a > 0$. These optimization problems for the variable inverse sum lodeg index and the variable sum lodeg index also appear in [24] as open problems.

The variable inverse sum lodeg index is used in the prediction of heat capacity at constant P and of total surface area for octane isomers [21], [23]. The variable sum lodeg index is used in the prediction of octanol-water partition coefficient for octane isomers [21].

Furthermore, our results can be applied to:

- variable inverse sum deg index (with $a < 0$)

$$ISD_a(G) = \sum_{uv \in E(G)} \frac{1}{d_u^a + d_v^a}\,,$$

- variable sum exdeg index (with $a > 1$)

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

- variable first Zagreb index (with $a > 1$)

$$M_1^a(G) = \sum_{uv \in E(G)} \big(d_u^{a-1} + d_v^{a-1}\big)$$

(first Zagreb and Forgotten indices are particular cases),

- variable second Zagreb index (with $a > 0$)

$$M_2^a(G) = \sum_{uv \in E(G)} (d_u d_v)^a\,,$$

- variable sum connectivity index (with $a > 0$)

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

- first and second Gourava indices [7]

$$GO_1(G) = \sum_{uv \in E(G)} (d_u + d_v + d_u d_v)\,, \qquad GO_2(G) = \sum_{uv \in E(G)} (d_u + d_v) d_u d_v\,,$$

- first and second hyper-Gourava indices [8]

$$HGO_1(G) = \sum_{uv \in E(G)} \big(d_u + d_v + d_u d_v\big)^2\,,$$

$$HGO_2(G) = \sum_{uv \in E(G)} \big((d_u + d_v) d_u d_v\big)^2\,,$$

- , the Gutman-Milovanović index [11]

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

which is a natural generalization of Zagreb indices.

Throughout this paper, $G = (V(G), E(G))$ denotes an undirected finite simple (without multiple edges and loops) graph without isolated vertices. We denote by n, Δ and δ the cardinality of the set of vertices of G, its maximum degree and its minimum degree, respectively. Thus, we have $1 \leq \delta \leq \Delta < n$.

2 Some extremal problems on general indices

Let I be any topological index defined as

$$I(G) = \sum_{uv \in E(G)} F(d_u, d_v), \tag{1}$$

where $F(x, y)$ is any non-negative symmetric function $F : \mathbb{Z}^+ \times \mathbb{Z}^+ \to [0, \infty)$.

We say that the index I defined by (1) belongs to $\mathcal{F}_1$ if F is a positive function that is strictly increasing in each variable. Also, we say that $I \in \mathcal{F}_2$ if $F(1, y) = 0$ for each $y \in \mathbb{Z}^+$, $F(x, y)$ is a strictly increasing function for each $x, y \geq 2$ in each variable, and also $F(x, y) > 0$ when $x, y \geq 2$.

Considering the index I in these classes allows to study many indices in a unified way.

It is clearly more difficult to work with indices in $\mathcal{F}_2$ than with indices in $\mathcal{F}_1$.

Note that $I \in \mathcal{F}_2$ for:

- $F(x, y) = \log^a x \log^a y$ with $a > 0$ (variable Randić type lodeg index),

• $F(x, y) = (\log^a x + \log^a y)^{-1}$ with $a < 0$ (variable inverse sum lodeg index).

Also, it is clear that $I \in \mathcal{F}_1$ for:

• $F(x, y) = (x^a + y^a)^{-1}$ with $a < 0$ (variable inverse sum deg index),

• $F(x, y) = \log^a x + \log^a y$ with $a > 0$ (variable sum lodeg index, for graphs without isolated edges),

• $F(x, y) = a^x + a^y$ with $a > 1$ (variable sum exdeg index),

• $F(x, y) = x^{a-1} + y^{a-1}$ with $a > 1$ (variable first Zagreb index),

• $F(x, y) = (xy)^a$ with $a > 0$ (variable second Zagreb index),

• $F(x, y) = (x + y)^a$ with $a > 0$ (variable sum connectivity index),

• $F(x, y) = x + y + xy$ and $F(x, y) = x^2y + xy^2$ (first and second Gourava indices, respectively),

• $F(x, y) = (x + y + xy)^2$ and $F(x, y) = (x^2y + xy^2)^2$ (first and second hyper-Gourava indices, respectively),

• $F(x, y) = (xy)^\alpha(x + y)^\beta$ with $\alpha, \beta > 0$ (Gutman-Milovanović index).

If $1 \le \delta < \Delta$ are integers, we say that a graph G is (Δ, δ)-*quasi-regular* if there exists $v \in V(G)$ with $d_v = \delta$ and $d_u = \Delta$ for every $u \in V(G) \setminus \{v\}$; G is (Δ, δ)-*pseudo-regular* if there exists $v \in V(G)$ with $d_v = \Delta$ and $d_u = \delta$ for every $u \in V(G) \setminus \{v\}$.

In [4] appears the following result.

Lemma 1. *Consider integers* $2 \le k < n$.

(1) *If* kn *is even, then there is a Hamiltonian* k*-regular graph with* n *vertices.*

(2) *If* kn *is odd, then there is a connected* $(k, k-1)$*-quasi-regular graph with* n *vertices and a connected* $(k+1, k)$*-pseudo-regular graph with* n *vertices.*

Proposition 1. *If* G *is a graph,* $u, v \in V(G)$ *with* $uv \notin E(G)$*, and* $I \in \mathcal{F}_1 \cup \mathcal{F}_2$*, then* $I(G \cup \{uv\}) > I(G)$.

Proof. Let $\{x_1, \dots, x_{d_u}\}$ and $\{y_1, \dots, y_{d_v}\}$ be the neighbors of u and v in G, respectively. If $x, y \ge 1$, then

$$F(x + 1, y) \ge F(x, y), \tag{2}$$

and we have the strict inequality if $y > 1$.

We have by (2)

$$\begin{aligned} I(G \cup \{uv\}) - I(G) &= F(d_u + 1, d_v + 1) \\ &\quad + \sum_{i=1}^{d_u} \big(F(d_u + 1, d_{x_i}) - F(d_u, d_{x_i})\big) \\ &\quad + \sum_{j=1}^{d_v} \big(F(d_v + 1, d_{y_j}) - F(d_v, d_{y_j})\big) \\ &\geq F(d_u + 1, d_v + 1) > 0. \end{aligned}$$

■

Given an integer $n \geq 2$, let $\mathcal{G}(n)$ (respectively, $\mathcal{G}_c(n)$) be the set of graphs (respectively, connected graphs) with n vertices.

Given integers $1 \leq \delta \leq \Delta < n$, let $\mathcal{H}(n, \delta)$ (respectively, $\mathcal{H}_c(n, \delta)$) be the set of graphs (respectively, connected graphs) with n vertices and minimum degree δ, and let $\mathcal{I}(n, \Delta)$ (respectively, $\mathcal{I}_c(n, \Delta)$) be the set of graphs (respectively, connected graphs) with n vertices and maximum degree Δ.

Theorem 2. *Consider $I \in \mathcal{F}_1 \cup \mathcal{F}_2$ and an integer $n \geq 2$.*

(1) *The only graph that maximizes the I index in $\mathcal{G}_c(n)$ or $\mathcal{G}(n)$ is the complete graph K_n.*

(2) *If a graph minimizes the I index in $\mathcal{G}_c(n)$, then it is a tree.*

(3) *Assume that $I \in \mathcal{F}_1$. If n is even, then the only graph that minimizes the I index in $\mathcal{G}(n)$ is the union of $n/2$ paths P_2. If n is odd, then the only graph that minimizes the I index in $\mathcal{G}(n)$ is the union of $(n-3)/2$ paths P_2 with a path P_3.*

(4) *If $I \in \mathcal{F}_2$, then the only graph that minimizes the I index in $\mathcal{G}_c(n)$ is the star graph S_n.*

(5) *If $I \in \mathcal{F}_2$, then the only graphs that minimize the I index in $\mathcal{G}(n)$ are the unions of star graphs.*

Proof. Proposition 1 gives items (1) and (2).

Assume that $I \in \mathcal{F}_1$ and n is even. Handshaking lemma gives $2m \geq$

$n\delta \geq n$. For any graph $G \in \mathcal{G}(n)$, we have

$$I(G) = \sum_{uv \in E(G)} F(d_u, d_v) \geq \sum_{uv \in E(G)} F(1,1) = m\, F(1,1) \geq \frac{n}{2}\, F(1,1),$$

and the equality in the bound is attained if and only if $d_u = 1$ for every $u \in V(G)$, i.e., G is the union of $n/2$ path graphs P_2.

Assume now that $I \in \mathcal{F}_1$ and n is odd, and consider a graph $G \in \mathcal{G}(n)$. If $d_u = 1$ for every $u \in V(G)$, then handshaking lemma gives $2m = n$, a contradiction since n is odd. Thus, there exists a vertex w with $d_w \geq 2$. Handshaking lemma gives $2m \geq (n-1)\delta + 2 \geq n + 1$. Denote by $N(w)$ the set of neighbors of w. We have

$$\begin{aligned}
I(G) &= \sum_{u \in N(w)} F(d_u, d_w) + \sum_{uv \in E(G), u,v \neq w} F(d_u, d_v) \\
&\geq \sum_{u \in N(w)} F(1,2) + \sum_{uv \in E(G), u,v \neq w} F(1,1) \\
&\geq 2\, F(1,2) + (m-2) F(1,1) \\
&\geq 2\, F(1,2) + \Big(\frac{n+1}{2} - 2\Big) F(1,1) \\
&= 2\, F(1,2) + \frac{n-3}{2}\, F(1,1),
\end{aligned}$$

and the equality in the bound is attained if and only if $d_u = 1$ for every $u \in V(G) \setminus \{w\}$, and $d_w = 2$. Therefore, G is the union of $(n-3)/2$ path graphs P_2 and a path graph P_3.

Assume that $I \in \mathcal{F}_2$. It is clear that $I(G) \geq 0$ for every graph G, and $I(G) = 0$ if and only if $F(d_u, d_v) = 0$ for every $uv \in E(G)$, i.e., $\min\{d_u, d_v\} = 1$ for every $uv \in E(G)$, and this holds if and only if G is a union of star graphs. This proves items (4) and (5). ■

Corollary 1. *Let G be a graph with n vertices and $I \in \mathcal{F}_1 \cup \mathcal{F}_2$.*

(1) *Then*

$$I(G) \leq \frac{1}{2}\, n(n-1) F(n-1, n-1),$$

and the equality in the bound is attained if and only if G is the complete graph K_n.

(2) *If* $I \in \mathcal{F}_1$ *and* n *is even, then*

$$I(G) \geq \frac{1}{2}\, nF(1,1),$$

and the equality in the bound is attained if and only if G *is the union of* $n/2$ *path graphs* P_2.

(3) *If* $I \in \mathcal{F}_1$ *and* n *is odd, then*

$$I(G) \geq \frac{1}{2}\,(n-3)F(1,1) + 2F(1,2)\,,$$

and the equality in the bound is attained if and only if G *is the union of* $(n-3)/2$ *path graphs* P_2 *and a path graph* P_3.

(4) *If* $I \in \mathcal{F}_2$*, then*

$$I(G) \geq 0,$$

and the equality in the bound is attained if and only if G *is a union of star graphs.*

Proof. Theorem 2 gives

$$I(G) \leq I(K_n) = \sum_{uv \in E(K_n)} F(d_u, d_v) = \frac{1}{2}\, n(n-1)F(n-1, n-1),$$

and the equality in the bound is attained if and only if G is the complete graph K_n. This gives item (1).

Also, the argument in the proof of Theorem 2 gives directly the other items. ■

Given integers $1 \leq \delta \leq n$, denote by K_n^δ the n-vertex graph with maximum and minimum degrees $n-1$ and δ, respectively, obtained from the complete graph K_{n-1} and an additional vertex v in the following way: Fix δ vertices $u_1, \dots, u_\delta \in V(K_n^\delta)$ and let $V(K_n^\delta) = V(K_{n-1}) \cup \{v\}$ and $E(K_n^\delta) = E(K_{n-1}) \cup \{u_1 v, \dots, u_\delta v\}$.

Theorem 3. *Consider* $I \in \mathcal{F}_1 \cup \mathcal{F}_2$ *and integers* $1 \leq \delta < n$.

(1) *Then the only graph in* $\mathcal{H}_c(n, \delta)$ *that maximizes the* I *index is* K_n^δ.

(2) *If* $\delta \geq 2$ *and* δn *is even, then the only graphs in* $\mathcal{H}_c(n, \delta)$ *that minimize the* I *index are the connected* δ*-regular graphs.*

(3) *If $\delta \geq 2$ and δn is odd, then the only graphs in $\mathcal{H}_c(n, \delta)$ that minimize the I index are the connected $(\delta + 1, \delta)$-pseudo-regular graphs.*

Proof. Given a graph $G \in \mathcal{H}_c(n, \delta) \setminus \{K_n^\delta\}$, fix any vertex $u \in V(G)$ with $d_u = \delta$. Since

$$G \neq G \cup \{vw : v, w \in V(G) \setminus \{u\} \text{ and } vw \notin E(G)\} = K_n^\delta,$$

Proposition 1 gives $I(K_n^\delta) > I(G)$. This proves item (1).

Denote by m the cardinality of the set $E(G)$. Handshaking lemma gives $2m \geq n\delta$.

Since $d_u \geq \delta$ for every $u \in V(G)$, we have

$$I(G) = \sum_{uv \in E(G)} F(d_u, d_v) \geq \sum_{uv \in E(G)} F(\delta, \delta) = mF(\delta, \delta) \geq \frac{1}{2}\, n\delta F(\delta, \delta),$$

and, since $\delta \geq 2$, the equality in the bound is attained if and only if $d_u = \delta$ for every $u \in V(G)$, i.e., G is regular.

If δn is even, then Lemma 1 gives that there is a connected δ-regular graph with n vertices. Hence, the only graphs in $\mathcal{H}_c(n, \delta)$ that minimize the I index are the connected δ-regular graphs.

If δn is odd, then handshaking lemma gives that there is no regular graph. Hence, there exists a vertex w with $d_w \geq \delta + 1$. Handshaking lemma gives $2m \geq (n-1)\delta + \delta + 1 = n\delta + 1$. Denote by $N(w)$ the set of neighbors of w. We have

$$\begin{aligned}
I(G) &= \sum_{u \in N(w)} F(d_u, d_w) + \sum_{uv \in E(G), u, v \neq w} F(d_u, d_v) \\
&\geq \sum_{u \in N(w)} F(\delta, \delta + 1) + \sum_{uv \in E(G), u, v \neq w} F(\delta, \delta) \\
&\geq (\delta + 1)F(\delta, \delta + 1) + (m - \delta - 1)F(\delta, \delta) \\
&\geq (\delta + 1)F(\delta, \delta + 1) + \Big(\frac{n\delta + 1}{2} - \delta - 1\Big)F(\delta, \delta),
\end{aligned}$$

and, since $\delta \geq 2$, the equality in the bound is attained if and only if $d_u = \delta$ for every $u \in V(G) \setminus \{w\}$, and $d_w = \delta + 1$. Lemma 1 gives that there is a connected $(\delta + 1, \delta)$-pseudo-regular graph with n vertices. Therefore, the only graphs in $\mathcal{H}_c(n,\delta)$ that minimize the I index are the connected $(\delta+1,\delta)$-pseudo-regular graphs. ■

Remark. If we replace $\mathcal{H}_c(n,\delta)$ with $\mathcal{H}(n,\delta)$ everywhere in the statement of Theorem 3, then the argument in its proof gives that the same conclusion holds if we remove everywhere the word "connected".

Theorem 3 and Remark 2 have the following consequence.

Corollary 2. *Let G be a graph with n vertices and minimum degree δ, and $I \in \mathcal{F}_1 \cup \mathcal{F}_2$.*

(1) *Then*

$$\begin{aligned} I(G) \le \frac{1}{2}\,&(n-\delta-1)(n-\delta-2)F(n-2,n-2)+\delta F(\delta,n-1) \\ &+\frac{1}{2}\,\delta(\delta-1)F(n-1,n-1)+\delta(n-\delta-1)F(n-2,n-1), \end{aligned}$$

and the equality in the bound is attained if and only if G is K_n^{δ}.

(2) *If δn is even, then*

$$I(G) \ge \frac{1}{2}\,n\delta F(\delta,\delta),$$

and the equality in the bound is attained if and only if G is δ-regular.

(3) *If δn is odd, then*

$$I(G) \ge \frac{1}{2}\,\big(\delta(n-2)-1\big)F(\delta,\delta)+(\delta+1)F(\delta,\delta+1),$$

and the equality in the bound is attained if and only if G is $(\delta+1,\delta)$-pseudo-regular graphs.

For any odd natural number Δ and $i=1,2$, define $\mathcal{F}_i^{\Delta}$ as the set of indices $I \in \mathcal{F}_i$ such that the function

$$F^*(k) := k\,F(\Delta,k)-\frac{1}{2}\,k\,F(\Delta,\Delta)$$

is strictly increasing for $1 \le k \le \Delta-1$.

Theorem 4. *Consider $I \in \mathcal{F}_1 \cup \mathcal{F}_2$ and integers $2 \le \Delta < n$.*

(1) *If* Δn *is even, then the only graphs that maximize the* I *index in* $\mathcal{I}_c(n,\Delta)$ *are the connected* Δ*-regular graphs.*

(2) *If* Δn *is odd and* $I \in \mathcal{F}_1^\Delta \cup \mathcal{F}_2^\Delta$*, then the only graphs that maximize the* I *index in* $\mathcal{I}_c(n,\Delta)$ *are the connected* $(\Delta,\Delta-1)$*-quasi-regular graphs.*

(3) *If a graph minimizes the* I *index in* $\mathcal{I}_c(n,\Delta)$*, then it is a tree.*

Proof. Denote by m the cardinality of the set $E(G)$. Handshaking lemma gives $2m \le n\Delta$. Since $d_u \le \Delta$ for every $u \in V(G)$, We have

$$I(G) = \sum_{uv\in E(G)} F(d_u,d_v) \le \sum_{uv\in E(G)} F(\Delta,\Delta) = mF(\Delta,\Delta) \le \frac{1}{2}\,n\Delta F(\Delta,\Delta),$$

and the equality in the bound is attained if and only if $d_u = \Delta$ for every $u \in V(G)$.

If Δn is even, then Lemma 1 gives that there is a connected Δ-regular graph with n vertices. Hence, the only graphs in $\mathcal{I}_c(n,\Delta)$ that maximize the I index are the connected Δ-regular graphs.

If Δn is odd, then handshaking lemma gives that there is no regular graph in $\mathcal{I}_c(n,\Delta)$. Let $G \in \mathcal{I}_c(n,\Delta)$. Hence, there exists a vertex w with minimum degree $\delta = d_w \le \Delta - 1$. Then $2m \le \Delta(n-1)+\delta$. We have

$$\begin{aligned}
I(G) &= \sum_{u\in N(w)} F(d_u,d_w) + \sum_{uv\in E(G),u,v\neq w} F(d_u,d_v)\\
&\le \sum_{u\in N(w)} F(\Delta,\delta) + \sum_{uv\in E(G),u,v\neq w} F(\Delta,\Delta)\\
&= \delta\, F(\Delta,\delta) + (m-\delta)F(\Delta,\Delta)\\
&\le \delta\, F(\Delta,\delta) + \frac{1}{2}\big(\Delta(n-1)-\delta\big)F(\Delta,\Delta)\\
&= F^*(\delta) + \frac{1}{2}\,\Delta(n-1)F(\Delta,\Delta),
\end{aligned}$$

and the equality in the bound is attained if and only if $d_u = \Delta$ for every $u \in V(G)\setminus\{w\}$, and $d_w = \delta$.

If $I \in \mathcal{F}_1^\Delta \cup \mathcal{F}_2^\Delta$, then $F^*(k)$ is strictly increasing for $1 \le k \le \Delta - 1$

and

$$I(G) \le F^*(\delta) + \frac{1}{2}\,\Delta(n-1)F(\Delta,\Delta) \le F^*(\Delta-1) + \frac{1}{2}\,\Delta(n-1)F(\Delta,\Delta)$$
$$= (\Delta-1)F(\Delta,\Delta-1) + \frac{\Delta(n-2)+1}{2}\,F(\Delta,\Delta),$$

and the equality in the bound is attained if and only if $d_u = \Delta$ for every $u \in V(G)\setminus\{w\}$, and $d_w = \Delta - 1$. Lemma 1 gives that there is a connected $(\Delta, \Delta-1)$-quasi-regular graph with n vertices. Therefore, the only graphs in $\mathcal{I}_c(n,\delta)$ that maximize the I index are the connected $(\Delta,\Delta-1)$-quasi-regular graphs.

Given any graph $G \in \mathcal{I}_c(n,\Delta)$ which is not a tree, fix any vertex $u \in V(G)$ with $d_u = \Delta$. Since G is not a tree, there exists a cycle C in G. Since C has at least three edges, there exists $vw \in E(G)\cap C$ such that $u \notin \{v,w\}$. Thus, $G \setminus \{vw\} \in \mathcal{I}_c(n,\Delta)$ and Proposition 1 gives $I(G) > I(G\setminus\{vw\})$. By iterating this argument, we obtain that if a graph minimizes the I index in $\mathcal{I}_c(n,\Delta)$, then it is a tree. ■

Let us denote by $S^*_{\Delta+1}$ the star graph $S_{\Delta+1}$ with an additional edge attached to a vertex of degree 1 in $S_{\Delta+1}$.

Theorem 5. *Consider $I \in \mathcal{F}_1 \cup \mathcal{F}_2$ and integers $2 \le \Delta < n$.*

(1) *If Δn is even, then the only graphs that maximize the I index in $\mathcal{I}(n,\Delta)$ are the Δ-regular graphs.*

(2) *If Δn is odd and $I \in \mathcal{F}_1^\Delta \cup \mathcal{F}_2^\Delta$, then the only graphs that maximize the I index in $\mathcal{I}(n,\Delta)$ are the $(\Delta,\Delta-1)$-quasi-regular graphs.*

(3) *If $I \in \mathcal{F}_1$ and $n-\Delta$ is odd, then the only graph that minimizes the I index in $\mathcal{I}(n,\Delta)$ is the union of the star graph $S_{\Delta+1}$ and $(n-\Delta-1)/2$ path graphs P_2.*

(4) *If $I \in \mathcal{F}_1$ and $n = \Delta+2$, then the only graph that minimizes the I index in $\mathcal{I}(n,\Delta)$ is $S^*_{\Delta+1}$.*

(5) *If $I \in \mathcal{F}_1$, $n \ge \Delta+4$ and $n-\Delta$ is even, then the only graphs that minimize the I index in $\mathcal{I}(n,\Delta)$ are either:*

(*a*) *the union of the star graph $S_{\Delta+1}$, $(n-\Delta-4)/2$ path graphs P_2 and a path graph P_3 when $F(1,\Delta)+F(1,2) < F(2,\Delta)+F(1,1)$,* *(b) the union of* $S^*_{\Delta+1}$ *and* $(n-\Delta-2)/2$ *path graphs* P_2 *when* $F(1,\Delta)+F(1,2)>F(2,\Delta)+F(1,1)$,

(c) or both of them when $F(1,\Delta)+F(1,2)=F(2,\Delta)+F(1,1)$.

(6) *If* $I \in \mathcal{F}_2$, *then the only graphs that minimize the* I *index in* $\mathcal{I}(n,\Delta)$ *are the unions of star graphs.*

Proof. The argument in Theorem 4 gives directly items (1) and (2).

Theorem 2 gives directly item (6).

Let $G \in \mathcal{I}(n,\Delta)$ and $w \in V(G)$ a vertex with $d_w = \Delta$.

Assume first that $I \in \mathcal{F}_1$ and $n-\Delta$ is odd. Handshaking lemma gives $2m \geq n-1+\Delta$. Note that $n-1+\Delta = n-\Delta+2\Delta-1$ is even. We have

$$\begin{aligned}
I(G) &= \sum_{u\in N(w)} F(d_u,d_w) + \sum_{uv\in E(G),u,v\neq w} F(d_u,d_v) \\
&\geq \sum_{u\in N(w)} F(1,\Delta) + \sum_{uv\in E(G),u,v\neq w} F(1,1) \\
&= \Delta F(1,\Delta) + (m-\Delta)F(1,1) \\
&\geq \Delta F(1,\Delta) + \Big(\frac{n-1+\Delta}{2} - \Delta\Big)F(1,1) \\
&= \Delta F(1,\Delta) + \frac{n-\Delta-1}{2}\, F(1,1),
\end{aligned}$$

and the equality in the bound is attained if and only if $d_u = 1$ for every $u \in V(G)\setminus\{w\}$, i.e., G is the union of the star graph $S_{\Delta+1}$ and $(n-\Delta-1)/2$ path graphs P_2.

Assume now that $I \in \mathcal{F}_1$ and $n = \Delta+2$. Let $z \in V(G)\setminus N(w)$ be the vertex with $V(G) = \{w,z\}\cup N(w)$. Choose $p \in N(z)$; since $z \notin N(w)$, we have $p \in N(w)$ and so, $d_p \geq 2$. Handshaking lemma gives $2m \geq (n-2)+\Delta+2 = n+\Delta$. We have

$$\begin{aligned}
I(G) &= \sum_{u\in N(w)} F(d_u,d_w) + \sum_{uv\in E(G),u,v\neq w} F(d_u,d_v) \\
&\geq (\Delta-1)F(1,\Delta) + F(2,\Delta) + F(1,2),
\end{aligned}$$

and the equality in the bound is attained if and only if $d_u = 1$ for every $u \in V(G)\setminus\{w,p\}$ and $d_p = 2$, i.e., G is the star graph $S_{\Delta+1}$ with an additional edge attached to a vertex of degree 1 in $S_{\Delta+1}$.

Assume that $I \in \mathcal{F}_1$, $n \geq \Delta + 4$ and $n - \Delta$ is even. If $d_u = 1$ for every $u \in V(G) \setminus \{w\}$, then handshaking lemma gives $2m = n - 1 + \Delta$, a contradiction since $n - 1 + \Delta = n - \Delta + 2\Delta - 1$ is odd. Thus, there exists a vertex $p \in V(G) \setminus \{w\}$ with $d_p \geq 2$. Handshaking lemma gives $2m \geq (n-2) + 2 + \Delta = n + \Delta$.

If $p \notin N(w)$, then

$$\begin{aligned}
I(G) &= \sum_{u \in N(w)} F(d_u, d_w) + \sum_{u \in N(p)} F(d_u, d_p) + \sum_{uv \in E(G), u,v \notin \{w,p\}} F(d_u, d_v) \\
&\geq \sum_{u \in N(w)} F(1, \Delta) + \sum_{u \in N(p)} F(1, 2) + \sum_{uv \in E(G), u,v \notin \{w,p\}} F(1, 1) \\
&\geq \Delta F(1, \Delta) + 2F(1, 2) + (m - \Delta - 2)F(1, 1) \\
&\geq \Delta F(1, \Delta) + 2F(1, 2) + \Big(\frac{n + \Delta}{2} - \Delta - 2\Big)F(1, 1) \\
&= \Delta F(1, \Delta) + 2F(1, 2) + \frac{n - \Delta - 4}{2} F(1, 1),
\end{aligned}$$

and the equality in the bound is attained if and only if $d_u = 1$ for every $u \in V(G) \setminus \{w, p\}$, and $d_p = 2$, i.e., G is the union of the star graph $S_{\Delta+1}$, $(n - \Delta - 4)/2$ path graphs P_2 and a path graph P_3.

If $p \in N(w)$, then

$$\begin{aligned}
I(G) = &\sum_{u \in N(w) \setminus \{p\}} F(d_u, d_w) + \sum_{u \in N(p) \setminus \{w\}} F(d_u, d_p) + \frac{1}{d_p^a + d_w^a} \\
&+ \sum_{uv \in E(G), u,v \notin \{w,p\}} F(d_u, d_v) \\
\geq &\sum_{u \in N(w) \setminus \{p\}} F(1, \Delta) + \sum_{u \in N(p) \setminus \{w\}} F(1, d_p) + F(d_p, \Delta) \\
&+ \sum_{uv \in E(G), u,v \notin \{w,p\}} F(1, 1) \\
\geq &\ (\Delta - 1)F(1, \Delta) + F(1, 2) + F(2, \Delta) + (m - \Delta - 1)F(1, 1) \\
\geq &\ (\Delta - 1)F(1, \Delta) + F(1, 2) + F(2, \Delta) + \Big(\frac{n + \Delta}{2} - \Delta - 1\Big)F(1, 1) \\
= &\ (\Delta - 1)F(1, \Delta) + F(1, 2) + F(2, \Delta) + \frac{n - \Delta - 2}{2} F(1, 1).
\end{aligned}$$

and the equality in the bound is attained if and only if $d_u = 1$ for every $u \in V(G)\backslash\{w, p\}$, and $d_p = 2$, i.e., G is the union of $S^*_{\Delta+1}$ and $(n-\Delta-2)/2$ path graphs P_2.

This finishes the proof of item (5). ■

Also, we can state the following inequalities.

Corollary 3. *Let G be a graph with n vertices and maximum degree Δ, and $I \in \mathcal{F}_1 \cup \mathcal{F}_2$.*

(1) *If Δn is even, then*

$$I(G) \leq \frac{1}{2}\, n\, \Delta\, F(\Delta, \Delta),$$

and the equality in the bound is attained if and only if G is a regular graph.

(2) *If Δn is odd and $I \in \mathcal{F}_1^{\Delta} \cup \mathcal{F}_2^{\Delta}$, then*

$$I(G) \leq (\Delta - 1)F(\Delta, \Delta - 1) + \frac{\Delta(n-2)+1}{2}\, F(\Delta, \Delta),$$

and the equality in the bound is attained if and only if G is a $(\Delta, \Delta-1)$-quasi-regular graph.

(3) *If $I \in \mathcal{F}_1$ and $n - \Delta$ is odd, then*

$$I(G) \geq \Delta\, F(1, \Delta) + \frac{n-\Delta-1}{2}\, F(1, 1),$$

and the equality in the bound is attained if and only if G is the union of the star graph $S_{\Delta+1}$ and $(n-\Delta-1)/2$ path graphs P_2.

(4) *If $I \in \mathcal{F}_1$ and $n = \Delta + 2$, then*

$$I(G) \geq (\Delta - 1)F(1, \Delta) + F(2, \Delta) + F(1, 2),$$

and the equality in the bound is attained if and only if G is the star graph $S_{\Delta+1}$ with an additional edge attached to a vertex of degree 1 in $S_{\Delta+1}$.

(5) *If $I \in \mathcal{F}_1$, $n \geq \Delta + 4$ and $n - \Delta$ is even, then*

$$I(G) \geq \min\Big\{\Delta F(1,\Delta) + 2F(1,2) + \frac{n-\Delta-4}{2}\,F(1,1),\\ (\Delta-1)F(1,\Delta) + F(1,2) + F(2,\Delta) + \frac{n-\Delta-2}{2}\,F(1,1)\Big\}.$$

(6) *If $I \in \mathcal{F}_2$, then*

$$I(G) \geq 0,$$

and the equality in the bound is attained if and only if G is the union of the star graphs.

Proof. The argument in the proof of Theorem 4 gives items (1) and (2), since the I index of a regular graph is

$$\frac{1}{2}\,n\Delta F(\Delta,\Delta),$$

and the I index of a $(\Delta, \Delta-1)$-quasi-regular graph is

$$(\Delta-1)F(\Delta,\Delta-1) + \frac{\Delta(n-2)+1}{2}\,F(\Delta,\Delta).$$

The argument in the proof of Theorem 5 gives directly items (3), (4), (5) and (6). ■

Let M be any topological index defined as

$$M(G) = \prod_{uv\in E(G)} f(d_u, d_v), \tag{3}$$

where $f(x,y)$ is any symmetric function $f : \mathbb{Z}^+ \times \mathbb{Z}^+ \to [1,\infty)$.

We say that the index M defined by (3) belongs to $\mathcal{M}_1$ if $f : \mathbb{Z}^+ \times \mathbb{Z}^+ \to (1,\infty)$ is a strictly increasing function in each variable. Also, we say that $M \in \mathcal{M}_2$ if $f(1,y) = 1$ for each $y \in \mathbb{Z}^+$, $f(x,y)$ is a strictly increasing function in each variable for $x, y \geq 2$, and also $f(x,y) > 1$ when $x, y \geq 2$.

Note that M belongs to $\mathcal{M}_1$ (respectively, $\mathcal{M}_2, \mathcal{M}_1^{\Delta}, \mathcal{M}_2^{\Delta}$) if and only if

$$I(G) = \sum_{uv \in E(G)} \log f(d_u, d_v) = \log M(G) \tag{4}$$

belongs to $\mathcal{F}_1$ (respectively, $\mathcal{F}_2, \mathcal{F}_1^{\Delta}, \mathcal{F}_2^{\Delta}$).

Since the logarithmic function is increasing, from the results obtained for the index I we obtain as a particular case results for the index M taking $F(x,y) = \log f(x,y)$. For example from Theorems 2, 3 and 4 we obtain respectively the following corollaries.

Corollary 4. *Consider $M \in \mathcal{M}_1 \cup \mathcal{M}_2$ and an integer $n \geq 2$.*

(1) *The only graph that maximizes the M index in $\mathcal{G}_c(n)$ or $\mathcal{G}(n)$ is the complete graph K_n.*

(2) *If a graph minimizes the M index in $\mathcal{G}_c(n)$, then it is a tree.*

(3) *Assume that $M \in \mathcal{M}_1$. If n is even, then the only graph that minimizes the M index in $\mathcal{G}(n)$ is the union of $n/2$ paths P_2. If n is odd, then the only graph that minimizes the M index in $\mathcal{G}(n)$ is the union of $(n-3)/2$ paths P_2 with a path P_3.*

(4) *If $M \in \mathcal{M}_2$, then the only graph that minimizes the M index in $\mathcal{G}_c(n)$ is the star graph S_n.*

(5) *If $M \in \mathcal{M}_2$, then the only graphs that minimize the M index in $\mathcal{G}(n)$ are the unions of star graphs.*

Corollary 5. *Consider $M \in \mathcal{M}_1 \cup \mathcal{M}_2$ and integers $1 \leq \delta < n$.*

(1) *Then the only graph in $\mathcal{H}_c(n,\delta)$ that maximizes the M index is K_n^{δ}.*

(2) *If $\delta \geq 2$ and δn is even, then the only graphs in $\mathcal{H}_c(n,\delta)$ that minimize the M index are the connected δ-regular graphs.*

(3) *If $\delta \geq 2$ and δn is odd, then the only graphs in $\mathcal{H}_c(n,\delta)$ that minimize the M index are the connected $(\delta+1,\delta)$-pseudo-regular graphs.*

Corollary 6. *Consider $M \in \mathcal{M}_1 \cup \mathcal{M}_2$ and integers $2 \leq \Delta < n$.*

(1) *If Δn is even, then the only graphs that maximize the M index in $\mathcal{I}_c(n,\Delta)$ are the connected Δ-regular graphs.*

(2) *If Δn is odd and $I \in \mathcal{M}_1^{\Delta} \cup \mathcal{M}_2^{\Delta}$, then the only graphs that maximize the M index in $\mathcal{I}_c(n,\Delta)$ are the connected $(\Delta,\Delta-1)$-quasi-regular graphs.*

(3) *If a graph minimizes the M index in $\mathcal{I}_c(n,\Delta)$, then it is a tree.*

3 Some extremal problems for the variable Randić type lodeg index

Since $I \in \mathcal{F}_2$ for $F(x,y) = \log^a x \log^a y$ with $a > 0$, the results in the previous section have the following consequences for the variable Randić type lodeg index.

Since $I \in \mathcal{F}_2$ for $F(x,y) = (\log^a x + \log^a y)^{-1}$ with $a < 0$, we have similar results for the variable inverse sum lodeg index.

Note that these optimization results appear in [24] as open problems for these two indices.

The variable Randić type lodeg index is used in the prediction of heat capacity at constant T and of total surface area for octane isomers [21]. The variable inverse sum lodeg index is used in the prediction of heat capacity at constant P and of total surface area for octane isomers [21], [23].

We state the theorems just for the variable Randić type lodeg index, the case of the variable inverse sum lodeg index is similar.

Theorem 6. *Consider $a > 0$ and an integer $n \geq 2$.*

(1) *The only graph that maximizes the RLI_a index in $\mathcal{G}_c(n)$ or $\mathcal{G}(n)$ is the complete graph K_n.*

(2) *The only graph that minimizes the RLI_a index in $\mathcal{G}_c(n)$ is the star graph S_n.*

(3) *The only graphs that minimize the RLI_a index in $\mathcal{G}(n)$ are the unions of star graphs.*

Theorem 7. *Let G be a graph with n vertices and $a > 0$.*

(1) *Then*

$$RLI_a(G) \leq \frac{1}{2}\, n(n-1) \log^{2a}(n-1),$$

and the equality in the bound is attained if and only if G is the complete graph K_n.

(2) *Then*

$$RLI_a(G) \geq 0,$$

and the equality in the bound is attained if and only if G is a union of star graphs.

Theorem 8. *Consider $a > 0$ and integers $1 \le \delta < n$.*

(1) Then the only graph in $\mathcal{H}_c(n,\delta)$ that maximizes the RLI_a index is K_n^δ.

(2) If $\delta \ge 2$ and δn is even, then the only graphs in $\mathcal{H}_c(n,\delta)$ that minimize the RLI_a index are the connected δ-regular graphs.

(3) If $\delta \ge 2$ and δn is odd, then the only graphs in $\mathcal{H}_c(n,\delta)$ that minimize the RLI_a index are the connected $(\delta+1,\delta)$-pseudo-regular graphs.

Remark. Recall that if we replace $\mathcal{H}_c(n,\delta)$ with $\mathcal{H}(n,\delta)$ everywhere in the statement of Theorem 3, then the same conclusion holds if we remove everywhere the word “connected”.

Theorem 3 and Remark 2 have the following consequence.

Theorem 9. *Let G be a graph with n vertices and minimum degree δ, and $a > 0$.*

(1) Then

$$\begin{aligned} RLI_a(G) \le{} & \frac{1}{2}\,(n-\delta-1)(n-\delta-2)\log^{2a}(n-2) + \delta\log^{a}\delta\log^{a}(n-1) \\ & + \frac{1}{2}\,\delta(\delta-1)\log^{2a}(n-1) + \delta(n-\delta-1)\log^{a}(n-2)\log^{a}(n-1), \end{aligned}$$

and the equality in the bound is attained if and only if G is K_n^δ.

(2) If δn is even, then

$$RLI_a(G) \ge \frac{1}{2}\, n\delta\log^{2a}\delta,$$

and the equality in the bound is attained if and only if G is δ-regular.

(3) If δn is odd, then

$$RLI_a(G) \ge \frac{1}{2}\,\big(\delta(n-2)-1\big)\log^{2a}\delta + (\delta+1)\log^{a}\delta\log^{a}(\delta+1),$$

and the equality in the bound is attained if and only if G is $(\delta+1,\delta)$-pseudo-regular graphs.

Theorem 10. *Consider $a > 0$ and integers $2 \le \Delta < n$.*

(1) If Δn is even, then the only graphs that maximize the RLI_a index in $\mathcal{I}_c(n,\Delta)$ are the connected Δ-regular graphs.

(2) *If* Δn *is odd and* $RLI_a \in \mathcal{F}_1^\Delta \cup \mathcal{F}_2^\Delta$*, then the only graphs that maximize the* RLI_a *index in* $\mathcal{I}_c(n, \Delta)$ *are the connected* $(\Delta, \Delta - 1)$*-quasi-regular graphs.*

(3) *If a graph minimizes the* RLI_a *index in* $\mathcal{I}_c(n, \Delta)$*, then it is a tree.*

Theorem 11. *Consider* $a > 0$ *and integers* $2 \leq \Delta < n$*.*

(1) *If* Δn *is even, then the only graphs that maximize the* RLI_a *index in* $\mathcal{I}(n, \Delta)$ *are the* Δ*-regular graphs.*

(2) *If* Δn *is odd and* $RLI_a \in \mathcal{F}_1^\Delta \cup \mathcal{F}_2^\Delta$*, then the only graphs that maximize the* RLI_a *index in* $\mathcal{I}(n, \Delta)$ *are the* $(\Delta, \Delta - 1)$*-quasi-regular graphs.*

(3) *The only graphs that minimize the* I *index in* $\mathcal{I}(n, \Delta)$ *are the unions of star graphs.*

Theorem 12. *Let* G *be a graph with* n *vertices and maximum degree* Δ*, and* $a > 0$*.*

(1) *If* Δn *is even, then*

$$RLI_a(G) \leq \frac{1}{2}\, n\Delta \log^{2a} \Delta,$$

and the equality in the bound is attained if and only if G *is a regular graph.*

(2) *If* Δn *is odd and* $RLI_a \in \mathcal{F}_1^\Delta \cup \mathcal{F}_2^\Delta$*, then*

$$RLI_a(G) \leq (\Delta - 1) \log^a \Delta \log^a(\Delta - 1) + \frac{1}{2} \big(\Delta(n-2) + 1\big) \log^{2a} \Delta,$$

and the equality in the bound is attained if and only if G *is a* $(\Delta, \Delta - 1)$*-quasi-regular graph.*

(3) *Then*

$$RLI_a(G) \geq 0,$$

and the equality in the bound is attained if and only if G *is the union of star graphs.*

4 Some extremal problems for the SLI_a index

Let us consider the variable sum lodeg index

$$SLI_a(G) = \sum_{uv \in E(G)} \big(\log^a d_u + \log^a d_v \big).$$

Note that although $F(1,1) = 0$, the function F verifies the other properties in the definition of the class $\mathcal{F}_1$ (F is strictly increasing in each variable and $F > 0$ on $\mathbb{Z}^+ \times \mathbb{Z}^+ \setminus \{(0,0)\}$), and it is possible to apply our optimization results for the functions in $\mathcal{F}_1$ also for this F.

We have similar results for the variable inverse sum deg index with $a < 0$, the variable sum exdeg index with $a > 1$, the variable first Zagreb index with $a > 1$, the variable second Zagreb index with $a > 0$, the variable sum connectivity index with $a > 0$, the first and second Gourava indices, the first and second hyper-Gourava indices. Most of these optimization results are new, but some of them are known: the results for the variable sum exdeg index appear in [24] and [4], and the results for the inverse sum deg index appear in [17].

These optimization problems for the variable sum lodeg index also appear in [24] as open problems.

The variable sum lodeg index is used in the prediction of octanol-water partition coefficient for octane isomers [21].

Theorem 13. *Consider $a > 0$ and an integer $n \geq 2$.*

(1) *The only graph that maximizes the SLI_a index in $\mathcal{G}_c(n)$ or $\mathcal{G}(n)$ is the complete graph K_n.*

(2) *If a graph minimizes the SLI_a index in $\mathcal{G}_c(n)$, then it is a tree.*

(3) *If n is even, then the only graph that minimizes the SLI_a index in $\mathcal{G}(n)$ is the union of $n/2$ paths P_2. If n is odd, then the only graph that minimizes the SLI_a index in $\mathcal{G}(n)$ is the union of $(n-3)/2$ paths P_2 with a path P_3.*

Theorem 14. *Let G be a graph with n vertices and $a > 0$.*

(1) *Then*

$$SLI_a(G) \le n(n-1)\log^a(n-1),$$

and the equality in the bound is attained if and only if G *is the complete graph* K_n*.*

(2) *If* n *is even, then*

$$SLI_a(G) \ge 0,$$

and the equality in the bound is attained if and only if G *is the union of* $n/2$ *path graphs* P_2*.*

(3) *If* n *is odd, then*

$$SLI_a(G) \ge 2\log^a 2,$$

and the equality in the bound is attained if and only if G *is the union of* $(n-3)/2$ *path graphs* P_2 *and a path graph* P_3*.*

Theorem 15. *Consider* $a > 0$ *and integers* $1 \le \delta < n$*.*

(1) *Then the only graph in* $\mathcal{H}_c(n,\delta)$ *that maximizes the* SLI_a *index is* K_n^δ*.*

(2) *If* $\delta \ge 2$ *and* δn *is even, then the only graphs in* $\mathcal{H}_c(n,\delta)$ *that minimize the* SLI_a *index are the connected* δ*-regular graphs.*

(3) *If* $\delta \ge 2$ *and* δn *is odd, then the only graphs in* $\mathcal{H}_c(n,\delta)$ *that minimize the* SLI_a *index are the connected* $(\delta+1,\delta)$*-pseudo-regular graphs.*

Remark. If we replace $\mathcal{H}_c(n,\delta)$ with $\mathcal{H}(n,\delta)$ everywhere in the statement of Theorem 15, then the same conclusion holds if we remove everywhere the word “connected”.

Theorem 15 and Remark 4 have the following consequence.

Theorem 16. *Let* G *be a graph with* n *vertices and minimum degree* δ*, and* $a > 0$*.*

(1) *Then*

$$\begin{aligned} SLI_a(G) \le{} & (n-\delta-1)(n-\delta-2)\log^a(n-2) + \delta\big(\log^a(n-1) + \log^a\delta\big) \\ & + \delta(\delta-1)\log^a(n-1) + \delta(n-\delta-1)\big(\log^a(n-1) + \log^a(n-2)\big), \end{aligned}$$

and the equality in the bound is attained if and only if G *is* K_n^δ*.*

(2) *If δn is even, then*

$$SLI_a(G) \geq n\delta \log^a \delta,$$

and the equality in the bound is attained if and only if G is δ-regular.

(3) *If δn is odd, then*

$$SLI_a(G) \geq \big(\delta(n-2)-1\big) \log^a \delta + (\delta+1)\big(\log^a(\delta+1) + \log^a \delta\big),$$

and the equality in the bound is attained if and only if G is $(\delta+1,\delta)$-pseudo-regular graphs.

Theorem 17. *Consider $a > 0$ and integers $2 \leq \Delta < n$.*

(1) *If Δn is even, then the only graphs that maximize the SLI_a index in $\mathcal{I}_c(n,\Delta)$ are the connected Δ-regular graphs.*

(2) *If Δn is odd and $SLI_a \in \mathcal{F}_1^{\Delta} \cup \mathcal{F}_2^{\Delta}$, then the only graphs that maximize the SLI_a index in $\mathcal{I}_c(n,\Delta)$ are the connected $(\Delta,\Delta-1)$-quasi-regular graphs.*

(3) *If a graph minimizes the SLI_a index in $\mathcal{I}_c(n,\Delta)$, then it is a tree.*

Remark. Note that if $F(x,y) = f(x) + f(y)$ for some function f, then $F(1,\Delta) + F(1,2) = 2f(1) + f(\Delta) + f(2) = F(2,\Delta) + F(1,1)$.

Remark 4 and Theorem 5 have the following consequence.

Theorem 18. *Consider $a > 0$ and integers $2 \leq \Delta < n$.*

(1) *If Δn is even, then the only graphs that maximize the SLI_a index in $\mathcal{I}(n,\Delta)$ are the Δ-regular graphs.*

(2) *If Δn is odd and $SLI_a \in \mathcal{F}_1^{\Delta} \cup \mathcal{F}_2^{\Delta}$, then the only graphs that maximize the SLI_a index in $\mathcal{I}(n,\Delta)$ are the $(\Delta,\Delta-1)$-quasi-regular graphs.*

(3) *If $n-\Delta$ is odd, then the only graph that minimizes the SLI_a index in $\mathcal{I}(n,\Delta)$ is the union of the star graph $S_{\Delta+1}$ and $(n-\Delta-1)/2$ path graphs P_2.*

(4) *If $n = \Delta+2$, then the only graph that minimizes the SLI_a index in $\mathcal{I}(n,\Delta)$ is $S^*_{\Delta+1}$.*

(5) *If $n \geq \Delta+4$ and $n-\Delta$ is even, then the only graphs that minimize the SLI_a index in $\mathcal{I}(n,\Delta)$ are the union of the star graph $S_{\Delta+1}$, $(n-$

$\Delta-4)/2$ path graphs P_2 and a path graph P_3, and the union of $S^*_{\Delta+1}$ and $(n-\Delta-2)/2$ path graphs P_2.

Also, we can state the following inequalities.

Theorem 19. *Let G be a graph with n vertices and maximum degree Δ, and $a>0$.*

(1) *If Δn is even, then*

$$SLI_a(G) \le n\Delta \log^a \Delta,$$

and the equality in the bound is attained if and only if G is a regular graph.

(2) *If Δn is odd and $SLI_a \in \mathcal{F}_1^\Delta \cup \mathcal{F}_2^\Delta$, then*

$$SLI_a(G) \le (\Delta-1)\big(\log^a(\Delta-1)+\log^a\Delta\big)+\big(\Delta(n-2)+1\big)\log^a\Delta,$$

and the equality in the bound is attained if and only if G is a $(\Delta,\Delta-1)$-quasi-regular graph.

(3) *If $n-\Delta$ is odd, then*

$$SLI_a(G) \ge \Delta \log^a \Delta,$$

and the equality in the bound is attained if and only if G is the union of the star graph $S_{\Delta+1}$ and $(n-\Delta-1)/2$ path graphs P_2.

(4) *If $n=\Delta+2$, then*

$$SLI_a(G) \ge \Delta \log^a \Delta + 2\log^a 2,$$

and the equality in the bound is attained if and only if G is the star graph $S_{\Delta+1}$ with an additional edge attached to a vertex of degree 1 in $S_{\Delta+1}$.

(5) *If $n \ge \Delta+4$ and $n-\Delta$ is even, then*

$$SLI_a(G) \ge \Delta \log^a \Delta + 2\log^a 2,$$

and the equality in the bound is attained if and only if G is either the union of the star graph $S_{\Delta+1}$, $(n-\Delta-4)/2$ path graphs P_2 and a path graph P_3, or the union of $S^*_{\Delta+1}$ and $(n-\Delta-2)/2$ path graphs P_2.

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