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Some results on lower bounds for topological indices

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Abstract

The aim of this paper is to obtain new inequalities involving some topological indices of a graph and characterize graphs extremal with respect to them. Our main results provide lower bounds on several indices involving just the minimum and the maximum degree of the graph G. This family of indices includes, among others, the Wiener index and several of its generalizations, the harmonic index and the general sum-connectivity index, and the geometric-arithmetic index. We also include some chemical applications of our results and some open problems.

Keywords Wiener index · Generalized Wiener index · Harmonic index · General sum-connectivity index · Geometric-arithmetic index.

Mathematics Subject Classification 05C07 · 92E10

1 Introduction

A topological descriptor is a single number that represents a chemical structure in graph-theoretical terms via the molecular graph, they play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations. A topological descriptor is called a topological index if it correlates with a molecular property.

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Topological indices are used to understand physicochemical properties of chemical compounds, since they capture some properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener [41]. Since then, its mathematical properties and chemical applications have been intensively studied. The *Wiener index* of G is defined as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v),$$

where $\{u, v\}$ runs over every pair of vertices in G.

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best know such descriptor is the Randić connectivity index [30].

Two of the main successors of the Randić index are the first and second Zagreb indices, denoted by M_1 and M_2, respectively, and introduced by Gutman et al. in (see [21]). They are defined as

$$M_1(G) = \sum_{u \in V(G)} d_u^2 = \sum_{uv \in E(G)} (d_u + d_v), \quad M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

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.

The *general sum-connectivity index* was defined by Zhou and Trinajstić in [45] as

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha.$$

Note that χ_1 is the first Zagreb index M_1, $2\chi_{-1}$ is the harmonic index, $\chi_{-1/2}$ is the sum-connectivity index, etc.

The concept of variable molecular descriptors was proposed as a new way of characterizing heteroatoms in molecules (see [31,32]), but also to assess the structural differences (e.g., the relative role of carbon atoms of acyclic and cyclic parts in alkyl-cycloalkanes [34]). 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.

In the paper of Gutman and Tošović [20], the correlation abilities of 20 vertex-degree-based topological indices occurring in the chemical literature were tested for the case of standard heats of formation and normal boiling points of octane isomers. It is remarkable to realize that variable indices provide indices that perform significantly better than the Randić index.

Countless applications of topological indices were reported, most of them concerned with exploring medicinal and pharmacological issues. A turning point in the mathematical examination of topological indices happened in the second half of the

1990s, when a significant and ever growing research field on this matter started, resulting in numerous publications. In this context, especially the papers of Erdös [1] and [2] should be mentioned.

Throughout this work, $G = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) non-trivial ($E(G) \neq \emptyset$) graph. A main topic in the study of topological indices is to find bounds of the indices involving several parameters. The aim of this paper is to obtain new inequalities for a large family of topological indices and to characterize the set of extremal graphs with respect to them. Our main results provide lower bounds on this family of topological indices involving just the minimum and the maximum degree of the graph. This family of indices includes, among others, the Wiener index and several of its generalizations (in Sect. 2), the harmonic index and the general sum-connectivity index (see Sects. 4 and 5, respectively), and the geometric-arithmetic index (in Sect. 6). Theorem 6 and Corollary 3 show some applications of our results in mathematical chemistry.

2 Wiener index and its generalizations

Along this section we just consider connected graphs G, in order to have defined $d(u, v)$ for every $u, v \in V(G)$.

Motivated by the Wiener index, Randić introduced in [33] an extension of the Wiener index for trees, and this has come to be known as the *hyper-Wiener index*. In [25], this extension was generalized to graphs as

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

$WW(G)$ has been useful in correlations (see, e.g., [16] and the references therein). For information about the hyper-Wiener index in mathematics see, e.g., [3,16,23].

Also, it is interesting to generalize the Wiener index in the following way

$$W^\lambda(G) = \sum_{\{u,v\} \subseteq V(G)} d(u, v)^\lambda,$$

with $\lambda \in \mathbb{R}$. Obviously, if $\lambda = 1$, then W^λ coincides with the ordinary Wiener index W. Note that W^{-2} is the Harary index; W^{-1} is the reciprocal Wiener index; the quantity W^2 is closely related to the hyper-Wiener index, since $WW = (W^1 + W^2)/2$. Another topological index, proposed in [38] is expressed in terms of W^1, W^2 and W^3 as $(2W^1 + 3W^2 + W^3)/6$. See [24] for more connections of the same kind.

Three different variants of the q-Wiener index ($q > 0$, $q \neq 1$) were defined in [42] as

$$W_1(G, q) = \sum_{\{u,v\} \subseteq V(G)} [d(u, v)]_q,$$

$$W_2(G, q) = \sum_{\{u,v\} \subseteq V(G)} [d(u, v)]_q \, q^{L-d(u,v)},$$

$$W_3(G, q) = \sum_{\{u,v\} \subseteq V(G)} [d(u, v)]_q \, q^{d(u,v)},$$

where L is the diameter of G, and

$$[k]_q = \frac{1 - q^k}{1 - q} = 1 + q + q^2 + \cdots + q^{k-1}.$$

Since $\lim_{q \to 1} [k]_q = k$, we have

$$\lim_{q \to 1} W_1(G, q) = \lim_{q \to 1} W_2(G, q) = \lim_{q \to 1} W_3(G, q) = W(G).$$

The *Schultz index* and the *modified Schultz index* of G are defined as

$$W_+(G) = \sum_{\{u,v\} \subseteq V(G)} (d_u + d_v) \, d(u, v),$$

$$W_*(G) = \sum_{\{u,v\} \subseteq V(G)} d_u \, d_v \, d(u, v),$$

respectively.

For each fixed real number α, let us define the *generalized Schultz-type indices* by

$$W_{\ddagger}^{(\alpha)}(G) = \sum_{\{u,v\} \subseteq V(G)} \left(d_u^{\alpha} + d_v^{\alpha} \right) d(u, v),$$

$$W_+^{(\alpha)}(G) = \sum_{\{u,v\} \subseteq V(G)} (d_u + d_v)^{\alpha} \, d(u, v),$$

$$W_*^{(\alpha)}(G) = \sum_{\{u,v\} \subseteq V(G)} d_u^{\alpha} d_v^{\alpha} d(u, v),$$

see, e.g., [22]. For $\alpha = 1$ the indices $W_{\ddagger}^{(\alpha)}(G)$, $W_+^{(\alpha)}(G)$, and $W_*^{(\alpha)}(G)$, reduce to $W_+(G)$, and $W_*(G)$, respectively.

Given any positive symmetric function $g : [\delta, \Delta] \times [\delta, \Delta] \cap \mathbb{Z}^2 \to (0, \infty)$ and any non-negative function $h : [\delta, \Delta] \cap \mathbb{Z} \to [1, \infty)$, the (g, h)-*Wiener index* of G is defined as

$$W_{g,h}(G) = \sum_{\{u,v\} \subseteq V(G)} g(d_u, d_v) \, h \, (d(u, v)) .$$

This general approach allows to study in a unified way the previous indices.

Let us start with regular graphs. As usual, denote by K_n the complete graph with n vertices. Also, we write $G_1 \cong G_2$ if the graphs G_1 and G_2 are isomorphic.

Theorem 1 *Given $1 \leq \Delta$, if h is a non-decreasing function, then we have for any graph G with minimum and maximum degree Δ,*

$$W_{g,h}(G) \geq \frac{\Delta(\Delta + 1)}{2} g(\Delta, \Delta) h(1) = W_{g,h}(K_{\Delta+1}).$$

Furthermore, if h is strictly increasing, then $W_{g,h}(G) = W_{g,h}(K_{\Delta+1})$ if and only if $G \cong K_{\Delta+1}$.

Proof Since every vertex in G has degree Δ, there are at least $\Delta+1$ vertices and $\frac{(\Delta+1)\Delta}{2}$ pairs of vertices. Furthermore, we have $g(d_u, d_v) = g(\Delta, \Delta)$ for every $\{u, v\} \subseteq V(G)$. Hence, we have

$$W_{g,h}(G) \geq \frac{\Delta(\Delta + 1)}{2} g(\Delta, \Delta) h(1) = W_{g,h}(K_{\Delta+1}).$$

Assume that h is strictly increasing. If $\Delta = 1$, then $G \cong K_2$ and the last statement holds. Assume now that $\Delta > 1$. If G is not isomorphic to $K_{\Delta+1}$, then there are at least $\Delta + 2$ vertices and $\frac{(\Delta+2)(\Delta+1)}{2}$ pairs of vertices, and at least $\frac{\Delta+2}{2}$ of these pairs are non-adjacent. Therefore,

$$W_{g,h}(G) \geq \left(\frac{(\Delta + 2)(\Delta + 1)}{2} - \frac{\Delta + 2}{2} \right) g(\Delta, \Delta) h(1) + \frac{\Delta + 2}{2} g(\Delta, \Delta) h(2)$$

$$> \frac{\Delta(\Delta + 1)}{2} g(\Delta, \Delta) h(1) = W_{g,h}(K_{\Delta+1}).$$

This finishes the proof.   □

For any $1 \leq \delta < \Delta$, let $\mathcal{H}_{\delta,\Delta}$ denote the family of graphs with $\Delta+1$ vertices where one of them has degree δ, δ of them have degree Δ, and $\Delta - \delta$ have degree $\Delta - 1$.

In [27] we obtained the following:

Proposition 1 *Given $1 \leq \delta < \Delta$, there is a unique graph (up to isomorphism), $H_{\delta,\Delta}$, in $\mathcal{H}_{\delta,\Delta}$.*

Notice that in $H_{\delta,\Delta}$ there are $\frac{(\Delta+1)\Delta}{2}$ pairs of vertices, $\frac{(\Delta-1)\Delta+2\delta}{2}$ of them are at distance 1 and $\Delta - \delta$ are at distance 2 (those with degree $\Delta - 1$ from the vertex with degree δ).

Therefore,

$$W_{g,h}(H_{\delta,\Delta}) = \left[\delta g(\delta, \Delta) + \binom{\delta}{2} g(\Delta, \Delta) + \binom{\Delta - \delta}{2} g(\Delta - 1, \Delta - 1) \right.$$

$$\left. + \delta(\Delta - \delta) g(\Delta - 1, \Delta) \right] h(1) + (\Delta - \delta) g(\delta, \Delta - 1) h(2).$$

First, we prove a non-sharp (but simple) lower bound of $W_{g,h}(G)$ (for any non-regular graph G) involving just the minimum and maximum degrees of G.

Theorem 2 *Given $1 \leq \delta < \Delta$, if g is a non-increasing function in the first variable and h is a non-decreasing function, then we have for any graph G with minimum degree δ and maximum degree Δ,*

$$W_{g,h}(G) \geq \frac{\Delta(\Delta-1) + 2\delta}{2} g(\Delta, \Delta)h(1) + (\Delta - \delta)g(\delta, \Delta)h(2).$$

Proof Since G has a vertex with degree Δ, there are at least $\Delta + 1$ vertices and $\frac{(\Delta+1)\Delta}{2}$ pairs of vertices (since g is a non-increasing function in the first variable, we have $g(d_u, d_v) \geq g(\Delta, \Delta)$ for every $\{u, v\} \subseteq V(G)$). Since a vertex u_0 has degree δ, there are at least $\Delta - \delta$ pairs of non-adjacent vertices, and we have $g(d_{u_0}, d_v) \geq g(\delta, \Delta)$ for these pairs of vertices $\{u_0, v\} \subseteq V(G)$. Therefore,

$$W_{g,h}(G) \geq \frac{\Delta(\Delta-1) + 2\delta}{2} g(\Delta, \Delta)h(1) + (\Delta - \delta)g(\delta, \Delta)h(2).$$

$\square$

Next, we obtain sharp lower bounds of $W_{g,h}$.

Definition 1 Let $\mathcal{I}$ be any topological index. A graph G with minimum degree δ and maximum degree Δ is *minimal* for $\mathcal{I}$ if $\mathcal{I}(G) \leq \mathcal{I}(\Gamma)$ for every graph Γ with minimum degree δ and maximum degree Δ. A graph G with minimum degree δ, maximum degree Δ and n vertices is *n-minimal* for $\mathcal{I}$ if $\mathcal{I}(G) \leq \mathcal{I}(\Gamma)$ for every graph Γ with minimum degree δ, maximum degree Δ and n vertices.

Theorem 3 *Given $1 \leq \delta < \Delta$, if g is a non-increasing function in the first variable and h is a non-decreasing function, then $H_{\delta,\Delta}$ is $(\Delta+1)$-minimal for $W_{g,h}$. Moreover, if g is strictly decreasing in the first variable or h is strictly increasing, then G is $(\Delta+1)$-minimal for $W_{g,h}$ if and only if $G \cong H_{\delta,\Delta}$.*

Proof Suppose G has $\Delta + 1$ vertices, $x_0, x_1, \ldots, x_\Delta$. Without loss of generality we can assume that x_0 has degree δ and that $x_{\delta+1}, \ldots, x_\Delta$ are not adjacent to x_0. Therefore, $d(x_0, x_i) \geq 2$ and x_i has degree at most $\Delta - 1$ for every $i > \delta$. Thus, since g is non-increasing in the first variable and h is non-decreasing,

$$W_{g,h}(G) \geq \left[\delta g(\delta, \Delta) + \binom{\delta}{2} g(\Delta, \Delta) + \binom{\Delta - \delta}{2} g(\Delta - 1, \Delta - 1) \right.$$
$$\left. + \delta(\Delta - \delta)g(\Delta-1, \Delta) \right] h(1) + (\Delta - \delta)g(\delta, \Delta-1)h(2) = W_{g,h}(H_{\delta,\Delta}).$$

If $G \not\cong H_{\delta,\Delta}$, then there is some other pair of vertices which are not adjacent and there exist either two vertices with degree less than $\Delta - 1$ or $\Delta - \delta + 2$ vertices with degree less than Δ. Therefore, if g is strictly decreasing in the first variable or h is strictly increasing, it is immediate to check that $W_{g,h}(G) > W_{g,h}(H_{\delta,\Delta})$. $\square$

Theorem 4 *Suppose $1 \leq \delta < \Delta$, g is a non-increasing function in the first variable and h is a non-decreasing function. If G is any graph with minimum degree δ and maximum degree Δ and the following conditions hold*

(i) $\left[\binom{\Delta+1}{2} - \binom{\delta}{2}\right] g(\Delta, \Delta) \geq \left[\binom{\Delta}{2} - \binom{\delta}{2}\right] g(\Delta - 1, \Delta - 1),$

(ii) $(\Delta - \delta + 1)g(\delta, \Delta) \geq (\Delta - \delta)g(\delta, \Delta - 1),$

then

$$W_{g,h}(G) \geq \left[\delta g(\delta, \Delta) + \binom{\delta}{2} g(\Delta, \Delta) + \binom{\Delta - \delta}{2} g(\Delta - 1, \Delta - 1)\right.$$
$$\left. + \delta(\Delta - \delta)g(\Delta - 1, \Delta)\right] h(1) + (\Delta - \delta)g(\delta, \Delta - 1)h(2) = W_{g,h}(H_{\delta, \Delta}).$$

Furthermore, if either g is strictly decreasing in the first variable or h is strictly increasing, then $W_{g,h}(G) = W_{g,h}(H_{\delta, \Delta})$ if and only if $G \cong H_{\delta, \Delta}$.

Proof If G has $\Delta + 1$ vertices, then the results follow from Theorem 3. Suppose G has at least $\Delta + 2$ vertices, $x_0, \ldots, x_{\Delta+1}$. Then, there are $\binom{\Delta+2}{2}$ pairs of vertices in G. We can assume that x_0 has degree δ, and that x_0 is not adjacent to $x_{\delta+1}, \ldots, x_{\Delta+1}$. Also, since the maximum degree is Δ, the vertices $x_1, \ldots, x_\delta$ are not adjacent to every vertex. Therefore, there are at least $\frac{\delta}{2}$ pairs of non-adjacent vertices in $\{x_1, \ldots, x_{\Delta+1}\}$. Thus,

$$W_{g,h}(G) \geq \left[\delta g(\delta, \Delta) + \left(\binom{\Delta+1}{2} - \frac{\delta}{2}\right) g(\Delta, \Delta)\right] h(1)$$
$$+ \left[(\Delta - \delta + 1)g(\delta, \Delta) + \frac{\delta}{2} g(\Delta, \Delta)\right] h(2).$$

Now, notice that since h is non-decreasing,

$$\left[\delta g(\delta, \Delta) + \left(\binom{\Delta+1}{2} - \frac{\delta}{2}\right) g(\Delta, \Delta)\right] h(1)$$
$$+ \left[(\Delta - \delta + 1)g(\delta, \Delta) + \frac{\delta}{2} g(\Delta, \Delta)\right] h(2) \qquad (1)$$
$$\geq \left[\delta g(\delta, \Delta) + \binom{\Delta+1}{2} g(\Delta, \Delta)\right] h(1) + (\Delta - \delta + 1)g(\delta, \Delta)h(2),$$

and since g is non-increasing,

$$\left[\delta g(\delta, \Delta) + \binom{\delta}{2} g(\Delta, \Delta) + \binom{\Delta - \delta}{2} g(\Delta - 1, \Delta - 1)\right.$$
$$\left. + \delta(\Delta - \delta)g(\Delta - 1, \Delta)\right] h(1) + (\Delta - \delta)g(\delta, \Delta - 1)h(2)$$
$$\leq \left[\delta g(\delta, \Delta) + \binom{\delta}{2} g(\Delta, \Delta) + \left(\binom{\Delta - \delta}{2} + \delta(\Delta - \delta)\right) g(\Delta - 1, \Delta - 1)\right] h(1)$$
$$+ (\Delta - \delta)g(\delta, \Delta - 1)h(2), \qquad (2)$$

where

$$\binom{\Delta - \delta}{2} + \delta(\Delta - \delta) = \binom{\Delta}{2} - \binom{\delta}{2}.$$

Thus, it suffices to check that

$$
\left[\delta g(\delta, \Delta) + \binom{\Delta+1}{2} g(\Delta, \Delta) \right] h(1) + (\Delta - \delta + 1) g(\delta, \Delta) h(2)
$$

$$
\geq \left[\delta g(\delta, \Delta) + \binom{\delta}{2} g(\Delta, \Delta) + \left(\binom{\Delta}{2} - \binom{\delta}{2} \right) g(\Delta - 1, \Delta - 1) \right] h(1)
$$

$$
+ (\Delta - \delta) g(\delta, \Delta - 1) h(2)
$$

$$
\Leftrightarrow \left[\binom{\Delta+1}{2} - \binom{\delta}{2} \right] g(\Delta, \Delta) h(1) + (\Delta - \delta + 1) g(\delta, \Delta) h(2)
$$

$$
\geq \left[\binom{\Delta}{2} - \binom{\delta}{2} \right] g(\Delta - 1, \Delta - 1) h(1) + (\Delta - \delta) g(\delta, \Delta - 1) h(2)
$$

and this holds if conditions (i), (ii) are satisfied.

If h (respectively, g) is strictly increasing (respectively, decreasing in the first variable), then the inequality (1) (respectively, (2)) is strict, and then $W_{g,h}(G) > W_{g,h}(H_{\delta,\Delta})$. This finishes the proof. $\square$

Corollary 1 *Suppose* $1 \leq \delta < \Delta$, *g is a constant function* $g = c$ *and h is a non-decreasing function. If G is any graph with minimum degree δ and maximum degree Δ, then*

$$
W_{g,h}(G) \geq \frac{\Delta(\Delta - 1) + 2\delta}{2} c\, h(1) + (\Delta - \delta) c\, h(2) = W_{g,h}(H_{\delta,\Delta}).
$$

Furthermore, if h is strictly increasing, then $W_{g,h}(G) = W_{g,h}(H_{\delta,\Delta})$ *if and only if* $G \cong H_{\delta,\Delta}$.

Thus, by taking $g = 1$ and $h(t) = t$ in Corollary 1, we obtain the following inequality for one of the main topological indices: the Wiener index.

Theorem 5 *Given* $1 \leq \delta < \Delta$, *we have for any graph G with minimum degree δ and maximum degree Δ,*

$$
W(G) \geq \frac{\Delta(\Delta - 1) + 2\delta}{2} + 2(\Delta - \delta),
$$

with equality if and only if $G \cong H_{\delta,\Delta}$.

Although only about 1000 benzenoid hydrocarbons are known, the number of possible benzenoid hydrocarbons is huge. For instance, the number of possible benzenoid hydrocarbons with 35 benzene rings is 5851000265625801806530 [39]. Therefore, the modeling of their physico-chemical properties is very important in order to predict properties of currently unknown species. The main reason for use topological indices is to obtain prediction of some property of molecules (see, e.g., [13,17,20,34]). Therefore, given some fixed parameters, a natural problem is to find the graphs that minimize (or maximize) the value of a topological index on the set of chemical graphs (graphs

with maximum degree at most 4) satisfying the restrictions given by the parameters (see, e.g., [1,2,4,5,10–12,18]).

Theorems 1 and 5 have the following consequence for chemical graphs.

Theorem 6 *Let G be a chemical graph with minimum degree δ and maximum degree Δ.*

If $(\Delta, \delta) = (4, 4)$, then $W(G) \geq 10$, with equality if and only if $G \cong K_5$.

If $(\Delta, \delta) = (4, 3)$, then $W(G) \geq 11$, with equality if and only if G has five vertices, two of them with degree 3 and three with degree 4.

If $(\Delta, \delta) = (4, 2)$, then $W(G) \geq 12$, with equality if and only if G has five vertices, one of them with degree 2, two with degree 3 and two with degree 4.

If $(\Delta, \delta) = (4, 1)$, then $W(G) \geq 13$, with equality if and only if G has five vertices, one of them with degree 1, three with degree 3 and one with degree 4.

If $(\Delta, \delta) = (3, 3)$, then $W(G) \geq 6$, with equality if and only if $G \cong K_4$.

If $(\Delta, \delta) = (3, 2)$, then $W(G) \geq 7$, with equality if and only if G has four vertices, two of them with degree 2 and two with degree 3.

If $(\Delta, \delta) = (3, 1)$, then $W(G) \geq 8$, with equality if and only if G has four vertices, one of them with degree 1, two with degree 2 and one with degree 3.

If $(\Delta, \delta) = (2, 2)$, then $W(G) \geq 3$, with equality if and only if $G \cong K_3$.

If $(\Delta, \delta) = (2, 1)$, then $W(G) \geq 4$, with equality if and only if G is a path graph with 3 vertices.

If $(\Delta, \delta) = (1, 1)$, then $W(G) \geq 1$, with equality if and only if $G \cong K_2$.

The pictures of the minimizing chemical graphs in Theorem 6 appear in Fig. 1. Other choices of h in Corollary 1 with $g = 1$, give the following results.

Theorem 7 *Given $1 \leq \delta < \Delta$, we have for any graph G with minimum degree δ and maximum degree Δ,*

$$WW(G) \geq \frac{\Delta(\Delta - 1) + 2\delta}{2} + 3(\Delta - \delta),$$

with equality if and only if $G \cong H_{\delta,\Delta}$.

Theorem 8 *Given $1 \leq \delta < \Delta$ and $\lambda > 0$, we have for any graph G with minimum degree δ and maximum degree Δ,*

$$W^\lambda(G) \geq \frac{\Delta(\Delta - 1) + 2\delta}{2} + 2^\lambda(\Delta - \delta),$$

with equality if and only if $G \cong H_{\delta,\Delta}$.

Since $[k]_q$ (respectively, $[k]_q q^{L-k}$ and $[k]_q q^k$) is an increasing function on k for $q > 0$ (respectively, $0 < q < 1$ and $q > 1$), Corollary 1 has the following consequence.

Theorem 9 *Given $1 \leq \delta < \Delta$ and $q > 0$, we have for any graph G with minimum degree δ and maximum degree Δ,*
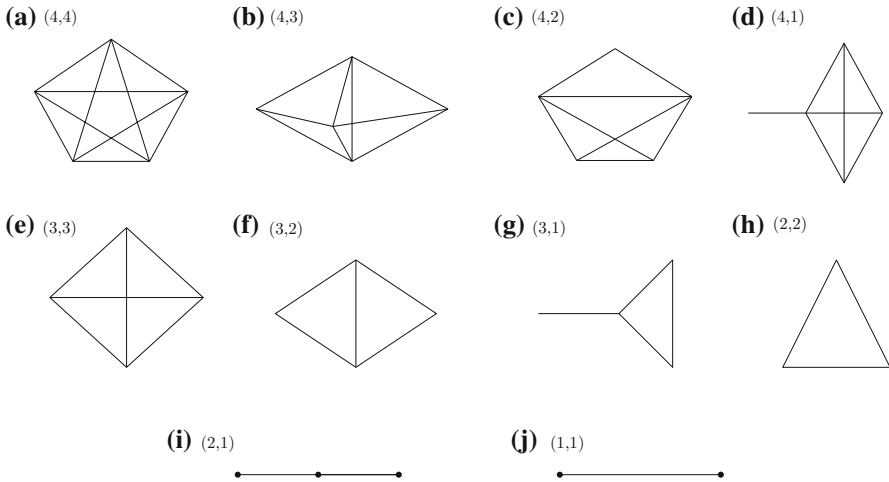
(a) (4,4)　　　**(b)** (4,3)　　　**(c)** (4,2)　　　**(d)** (4,1)

(e) (3,3)　　　**(f)** (3,2)　　　**(g)** (3,1)　　　**(h)** (2,2)

(i) (2,1)　　　　　　　　**(j)** (1,1)

Fig. 1 Minimizing chemical graphs

$$W_1(G, q) \geq \frac{\Delta(\Delta - 1) + 2\delta}{2} + (\Delta - \delta)(1 + q) \quad \text{if } q \neq 1,$$

$$W_2(G, q) \geq \frac{\Delta(\Delta - 1) + 2\delta}{2} q^{L-1} + (\Delta - \delta)(1 + q)q^{L-2} \quad \text{if } 0 < q < 1,$$

$$W_3(G, q) \geq \frac{\Delta(\Delta - 1) + 2\delta}{2} q + (\Delta - \delta)(1 + q)q^2 \quad \text{if } q > 1,$$

with equality in each inequality if and only if $G \cong H_{\delta, \Delta}$.

Given $1 \leq \delta < \Delta$, let us define

$$\sigma_{\delta, \Delta} := \frac{\log \frac{\binom{\Delta+1}{2} - \binom{\delta}{2}}{\binom{\Delta}{2} - \binom{\delta}{2}}}{\log \frac{\Delta-1}{\Delta}}, \quad \eta_{\delta, \Delta} := \frac{\log \frac{\Delta-\delta+1}{\Delta-\delta}}{\log \frac{\Delta+\delta-1}{\Delta+\delta}}, \quad \mu_{\delta, \Delta} := \frac{\log \frac{\Delta-\delta+1}{\Delta-\delta}}{\log \frac{\Delta-1}{\Delta}}.$$

Notice that $\sigma_{\delta, \Delta}, \eta_{\delta, \Delta}, \mu_{\delta, \Delta} < 0$. Then, Theorem 4 yields the following results:

Theorem 10 *Given* $1 \leq \delta < \Delta$ *and* $\alpha < 0$, *for any graph G with minimum degree* δ *and maximum degree* Δ:

– *If* $\alpha \geq \sigma_{\delta, \Delta}$ *and* $(\Delta - \delta + 1)(\delta^\alpha + \Delta^\alpha) \geq (\Delta - \delta)[\delta^\alpha + (\Delta - 1)^\alpha]$, *then*

$$W_{\ddagger}^{(\alpha)}(G) \geq \delta(\delta^\alpha + \Delta^\alpha) + 2\binom{\delta}{2}\Delta^\alpha + 2\binom{\Delta - \delta}{2}(\Delta - 1)^\alpha$$
$$+ \delta(\Delta - \delta)((\Delta - 1)^\alpha + \Delta^\alpha) + 2(\Delta - \delta)(\delta^\alpha + (\Delta - 1)^\alpha),$$

– *If* $\alpha \geq \sigma_{\delta, \Delta}$ *and* $\alpha \geq \eta_{\Delta, \delta}$, *then*

$$W_{+}^{(\alpha)}(G) \geq \delta(\delta + \Delta)^\alpha + 2^\alpha \binom{\delta}{2}\Delta^\alpha + 2^\alpha \binom{\Delta - \delta}{2}(\Delta - 1)^\alpha$$
$$+ \delta(\Delta - \delta)(2\Delta - 1)^\alpha + 2(\Delta - \delta)(\delta + \Delta - 1)^\alpha,$$

– *If $\alpha \geq \frac{1}{2}\sigma_{\delta,\Delta}$ and $\alpha \geq \mu_{\Delta,\delta}$, then*

$$W_*^{(\alpha)}(G) \geq \delta^{\alpha+1}\Delta^\alpha + \binom{\delta}{2}\Delta^{2\alpha} + \binom{\Delta - \delta}{2}(\Delta - 1)^{2\alpha}$$
$$+ \delta(\Delta - \delta)(\Delta - 1)^\alpha \Delta^\alpha + 2(\Delta - \delta)\delta^\alpha(\Delta - 1)^\alpha,$$

with equality in each inequality if and only if $G \cong H_{\delta,\Delta}$.

The *multiplicative Wiener index* of G is defined in [19] as

$$\pi(G) = \prod_{\{u,v\} \subseteq V(G)} d(u, v).$$

The mathematical arguments leading to this index have been outlined in due detail in [19].

Given any function $f : [\delta, \Delta] \cap \mathbb{Z} \to [1, \infty)$, the *$f$-multiplicative Wiener index* of G is defined as

$$\pi_f(G) = \prod_{\{u,v\} \subseteq V(G)} f\left(d(u, v)\right).$$

Theorem 11 *Suppose $1 \leq \delta < \Delta$, and f is a non-decreasing function. If G is any graph with minimum degree δ and maximum degree Δ, then*

$$\pi_f(G) \geq f(1)^{(\Delta(\Delta-1)+2\delta)/2} f(2)^{\Delta-\delta} = \pi_f(H_{\delta,\Delta}).$$

Furthermore, if f is strictly increasing, then $\pi_f(G) = \pi_f(H_{\delta,\Delta})$ if and only if $G \cong H_{\delta,\Delta}$.

Proof Since

$$\log \pi_f(G) = \sum_{\{u,v\} \subseteq V(G)} \log f\left(d(u, v)\right) = W_{1,\log f}(G),$$

$\log f \geq 0$ and the logarithm is a strictly increasing function, Corollary 1 gives the result. $\square$

Therefore, by taking $f(t) = t$, we obtain the following.

Corollary 2 *Suppose $1 \leq \delta < \Delta$. If G is any graph with minimum degree δ and maximum degree Δ, then*

$$\pi(G) \geq 2^{\Delta-\delta} = \pi(H_{\delta,\Delta}).$$

Furthermore, $\pi(G) = \pi(H_{\delta,\Delta})$ if and only if $G \cong H_{\delta,\Delta}$.

Corollary 3 *The minimizing graphs in* Theorems 7, 8, 9, 10, 11 *and* 6 *are identical. They are represented in* Fig. 1.

3 General estimates

Given integers $1 \leq \delta \leq \Delta$, let us define $\mathcal{G}_{\delta,\Delta}$ as the set of graphs G with $|V(G)| = \Delta + 1$, minimum degree δ, maximum degree Δ, and such that:

(1) G is isomorphic to the complete graph with $\Delta + 1$ vertices $K_{\Delta+1}$, if $\delta = \Delta$,

(2) there are Δ vertices with degree δ, if $\delta < \Delta$ and $\Delta(\delta + 1)$ is even,

(3) there are $\Delta - 1$ vertices with degree δ and a vertex with degree $\delta+1$, if $\delta < \Delta-1$ and $\Delta(\delta + 1)$ is odd,

(4) there are $\Delta - 1$ vertices with degree δ and two vertices with degree Δ, if $\delta = \Delta - 1$ and Δ is odd (and thus $\Delta(\delta + 1)$ is odd).

Remark 1 Every graph $G \in \mathcal{G}_{\delta,\Delta}$ has maximum degree Δ and $|V(G)| = \Delta + 1$. Hence, every graph $G \in \mathcal{G}_{\delta,\Delta}$ is connected.

Proposition 2 *For any integers $1 \leq \delta \leq \Delta$, we have $\mathcal{G}_{\delta,\Delta} \neq \emptyset$. Let G be a graph with minimum degree δ and maximum degree Δ. Then*

$$|E(G)| \geq \frac{\Delta(\delta + 1)}{2} \quad \text{if } \Delta(\delta + 1) \text{ is even,}$$

and

$$|E(G)| \geq \frac{\Delta(\delta + 1) + 1}{2} \quad \text{if } \Delta(\delta + 1) \text{ is odd,}$$

with equality if and only if $G \in \mathcal{G}_{\delta,\Delta}$.

In [28] we obtained the following:

Theorem 12 *Let us consider $\alpha \in \mathbb{R}$ with $\alpha < 0$, any integers $1 \leq \delta \leq \Delta$, and a graph G with minimum degree δ and maximum degree Δ. The following inequalities hold: If $\Delta(\delta + 1)$ is even and*

$$(2\Delta)^\alpha \geq (\Delta - \delta)[(\Delta + \delta)^\alpha - (2\Delta)^\alpha] + 2^{\alpha-1}\Delta(\delta - 1)(\delta^\alpha - \Delta^\alpha), \qquad (3)$$

then $G \in \mathcal{G}_{\delta,\Delta}$ is minimal for χ_α and thus,

$$\chi_\alpha(G) \geq \Delta(\Delta + \delta)^\alpha + 2^{\alpha-1}\Delta(\delta - 1)\delta^\alpha.$$

Moreover, if the inequality (3) is strict, then G is minimal for χ_α if and only if $G \in \mathcal{G}_{\delta,\Delta}$. If $\Delta(\delta + 1)$ is odd and

$$\begin{aligned} (2\Delta)^\alpha &\geq (\Delta - \delta - 1)[(\Delta + \delta)^\alpha - (2\Delta)^\alpha] + (\Delta + \delta + 1)^\alpha - (2\Delta)^\alpha \\ &\quad + \delta[(2\delta + 1)^\alpha - (2\Delta)^\alpha] + 2^{\alpha-1}[(\Delta - 2)(\delta - 1) - 1](\delta^\alpha - \Delta^\alpha), \end{aligned} \qquad (4)$$

then $G \in \mathcal{G}_{\delta,\Delta}$ is minimal for χ_α and thus,

$$\chi_\alpha(G) \geq (\Delta - 1)(\Delta + \delta)^\alpha + (\Delta + \delta + 1)^\alpha$$
$$+ \delta(2\delta + 1)^\alpha + 2^{\alpha-1}[(\Delta - 2)(\delta - 1) - 1]\delta^\alpha.$$

Moreover, if the inequality (4) *is strict, then G is minimal for* χ_α *if and only if* $G \in \mathcal{G}_{\delta,\Delta}$.

Corollary 4 *For any* $\alpha \in \mathbb{R}$ *with* $\alpha < 0$, *a graph G with minimum and maximum degree* $\delta = \Delta \geq 1$ *is mimimal for* χ_α *if and only if* $G \cong K_{\Delta+1}$.

4 Harmonic index

Another remarkable topological descriptor is the *harmonic* index, defined in [14] as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

This index has attracted a great interest in the lasts years (see, e.g., [9,15,43,44] and the references therein).

If G is a graph with m edges and maximum degree Δ, then it is trivial to check that

$$H(G) \geq \frac{m}{\Delta}. \tag{5}$$

Proposition 3 *Let G be a graph with minimum degree* δ *and maximum degree* Δ. *Then*

$$H(G) \geq \frac{\delta + 1}{2},$$

with equality if and only if $G \cong K_{\Delta+1}$.

Proof The inequality follows from (5) and Proposition 2. If G is isomorphic to the complete graph $K_{\Delta+1}$, then it is clear that the equality holds. If the equality holds, then the number of edges is minimal, and so, $G \in \mathcal{G}_{\delta,\Delta}$ by Proposition 2. Also, every edge joins two vertices with degree Δ. Therefore, $\delta = \Delta$ and G is isomorphic to the complete graph $K_{\Delta+1}$.   □

Proposition 4 *For every integers* $1 \leq \delta \leq \Delta$ *and* $G \in \mathcal{G}_{\delta,\Delta}$, *we have*

$$H(G) = \frac{2\Delta}{\delta + \Delta} + \frac{\Delta(\delta - 1)}{2\delta} \quad \text{if } \Delta(\delta + 1) \text{ is even,}$$

and

$$H(G) = \frac{2(\Delta - 1)}{\delta + \Delta} + \frac{2}{\delta + 1 + \Delta} + \frac{2\delta}{2\delta + 1} + \frac{(\Delta - 2)(\delta - 1) - 1}{2\delta}$$
$$> \frac{2\Delta}{\delta + \Delta + 1} + \frac{\Delta(\delta - 1)}{2\delta} \quad \text{if } \Delta(\delta + 1) \text{ is odd.}$$

Proof The equalities follow from the definitions of H and $\mathcal{G}_{\delta,\Delta}$. The inequality is trivial. □

Remark 2 Notice that the expression $\frac{2(\Delta-1)}{\delta+\Delta} + \frac{2}{\delta+1+\Delta} + \frac{2\delta}{2\delta+1} + \frac{(\Delta-2)(\delta-1)-1}{2\delta}$ can be greater (see, e.g., $\delta = 3$ and $\Delta = 7$) or smaller (see, e.g., $\delta = 10$ and $\Delta = 11$) than $\frac{2\Delta}{\delta+\Delta} + \frac{\Delta(\delta-1)}{2\delta}$.

Note that the harmonic index of the complete bipartite graph is $H(K_{\delta,\Delta}) = \frac{2\delta\Delta}{\delta+\Delta}$. Also notice that if $\delta = 1$, then $K_{\delta,\Delta}$ and $G \in \mathcal{G}_{\delta,\Delta}$ are both the star graph.

Proposition 5 *Consider any integers* $1 < \delta \leq \Delta$ *with* $\Delta(\delta+1)$ *even and define* $\alpha = \delta/\Delta$. *Then for any* $G \in \mathcal{G}_{\delta,\Delta}$,

- $H(K_{\delta,\Delta}) > H(G)$ *if and only if* $\alpha > \frac{1}{3}$,
- $H(K_{\delta,\Delta}) = H(G)$ *if and only if* $\alpha = \frac{1}{3}$,
- $H(K_{\delta,\Delta}) < H(G)$ *if and only if* $\alpha < \frac{1}{3}$.

Proof We have

$$H(K_{\delta,\Delta}) = \frac{2\Delta\delta}{\Delta+\delta} = \frac{2\alpha}{1+\alpha}\Delta, \quad H(G) = \frac{2\Delta}{\delta+\Delta} + \frac{\Delta(\delta-1)}{2\delta} = \frac{2}{1+\alpha} + \frac{\alpha\Delta-1}{2\alpha}.$$

Therefore, if suffices to check if

$$\frac{2\alpha}{1+\alpha}\Delta \geq \frac{2}{1+\alpha} + \frac{\alpha\Delta-1}{2\alpha}$$
$$\Leftrightarrow \frac{2}{1+\alpha}(\alpha\Delta-1) \geq \frac{1}{2\alpha}(\alpha\Delta-1)$$
$$\Leftrightarrow \frac{2}{1+\alpha}(\delta-1) \geq \frac{1}{2\alpha}(\delta-1).$$

This follows immediately since $\delta > 1$ and $\frac{2}{1+\alpha} \geq \frac{1}{2\alpha}$ if and only if $\alpha \in [\frac{1}{3}, 1]$. Moreover, the equality only holds for $\alpha = \frac{1}{3}$. □

Notice that Theorem 12 is not very useful to find the minimal graph for the harmonic index since for almost every case, the inequalities (3) and (4) do not hold. (Notice that a graph is minimal for the harmonic index if and only if it is minimal for χ_{-1}.) Let us analyze the (easier) case when $\Delta(\delta+1)$ is even.

Proposition 6 *Suppose* $\alpha = -1$, $1 \leq \delta \leq \Delta$ *and* $\Delta(\delta+1)$ *is even. Given a graph* G *with minimum degree* δ *and maximum degree* Δ, *then* (3) *holds if and only if*

$$2\delta(\Delta+\delta) \geq 2(\Delta-\delta)^2\delta + \Delta(\delta-1)(\Delta+\delta)(\Delta-\delta). \tag{6}$$

Proof It is immediate to check that

$$\frac{1}{2\Delta} \geq (\Delta - \delta) \left[\frac{1}{\Delta + \delta} - \frac{1}{2\Delta} \right] + \frac{\Delta(\delta - 1)}{4} \left[\frac{1}{\delta} - \frac{1}{\Delta} \right]$$

$$\Leftrightarrow 1 \geq \frac{(\Delta - \delta)^2}{\Delta + \delta} + \frac{\Delta(\delta - 1)(\Delta - \delta)}{2\delta}$$

$$\Leftrightarrow 1 \geq \frac{2\delta(\Delta - \delta)^2 + \Delta(\delta - 1)(\Delta - \delta)(\Delta + \delta)}{2\delta(\Delta + \delta)}$$

$$\Leftrightarrow 2\delta(\Delta + \delta) \geq 2\delta(\Delta - \delta)^2 + \Delta(\delta - 1)(\Delta - \delta)(\Delta + \delta).$$

$\square$

Thus, it can be seen that (3) holds in a few cases:

Corollary 5 *Given $\alpha = -1$, $1 = \delta \leq \Delta$, and a graph G with minimum degree δ and maximum degree Δ, then (3) holds if and only if $1 \leq \Delta \leq 3$.*

Corollary 6 *Given $\alpha = -1$, $2 = \delta \leq \Delta$ with Δ even, and a graph G with minimum degree δ and maximum degree Δ, then (3) holds if and only if $\Delta = 2$.*

Proof By Proposition 6, (3) holds if and only if (6) holds. Thus, since $\delta = 2$, it suffices to see that

$$4(\Delta + 2) \geq 4(\Delta - 2)^2 + \Delta(\Delta - 2)(\Delta + 2)$$

$$\Leftrightarrow 0 \geq \Delta^3 + 4\Delta^2 - 24\Delta + 8.$$

The solutions of this cubic equation are $x_1 \approx -7.4$, $x_2 \approx 0.4$ and $x_3 \approx 3.04$. Thus, the only solutions of the inequality where $\Delta \geq \delta$ are $\Delta = 2$ or $\Delta = 3$ and in this last case, $\Delta(\delta + 1)$ is not even. $\square$

Corollary 7 *Given $\alpha = -1$, $3 \leq \delta \leq \Delta$ with $\Delta(\delta + 1)$ even, and a graph G with minimum degree δ and maximum degree Δ, then (3) holds if and only if $\delta = \Delta$.*

Proof By Corollary 4, (3) holds if $\delta = \Delta$. Assume now that $\delta < \Delta$. By Proposition 6, (3) holds if and only if (6) holds. It is immediate to check that:

$$2\delta(\Delta + \delta) \geq 2(\Delta - \delta)^2\delta + \Delta(\delta - 1)(\Delta - \delta)(\Delta + \delta)$$

$$\Leftrightarrow \Delta + \delta \geq (\Delta - \delta)^2 + \frac{\Delta(\delta - 1)}{2\delta}(\Delta - \delta)(\Delta + \delta).$$

However, since $3 \leq \delta < \Delta$, it is trivial that

$$\frac{\Delta(\delta - 1)}{2\delta} > 1$$

and therefore

$$\Delta + \delta < \frac{\Delta(\delta - 1)}{2\delta}(\Delta + \delta) < (\Delta - \delta)^2 + \frac{\Delta(\delta - 1)}{2\delta}(\Delta - \delta)(\Delta + \delta).$$

□

5 General sum-connectivity index

Theorem 12 is not very useful either to find minimal graphs for the sum-connectivity index since the inequalities (3) and (4) almost never hold. Let us analyze the (easier) case when $\Delta(\delta + 1)$ is even.

Let us define

$$N_{\delta, \Delta} := \frac{\Delta(\delta + 1)}{2} - \delta, \quad \lambda_{\delta, \Delta} := \sqrt{\frac{2\Delta}{\Delta + \delta}}, \quad \text{and} \quad \varepsilon_{\delta, \Delta} := \sqrt{\frac{\Delta}{\delta}}.$$

Notice that $N_{\delta, \Delta}$ is increasing in both variables for $1 \le \delta \le \Delta$ and that $\varepsilon_{\delta, \Delta} > \lambda_{\delta, \Delta} > 1$ for every $\Delta > \delta$.

Since $\chi_{-1/2}$ is the sum-connectivity index χ, Theorem 12 implies the following:

Proposition 7 *Suppose $\alpha = -\frac{1}{2}$, $1 \le \delta < \Delta$ and $\Delta(\delta + 1)$ is even. Given a graph G with minimum degree δ and maximum degree Δ, then (3) does not hold if*

$$N_{\delta, \Delta} > \frac{1}{\lambda_{\delta, \Delta} - 1}. \tag{7}$$

Proof First, let us see that

$$\frac{1}{\sqrt{2\Delta}} < (\Delta - \delta) \left[\frac{1}{\sqrt{\Delta + \delta}} - \frac{1}{\sqrt{2\Delta}} \right] + \frac{\Delta(\delta - 1)}{2\sqrt{2}} \left[\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}} \right]$$

$$\Leftrightarrow 1 < (\Delta - \delta) \left(\frac{\sqrt{2\Delta}}{\sqrt{\Delta + \delta}} - 1 \right) + \frac{\Delta(\delta - 1)}{2} \left(\frac{\sqrt{\Delta}}{\sqrt{\delta}} - 1 \right)$$

$$\Leftrightarrow \Delta - \delta + \frac{\Delta(\delta - 1)}{2} + 1 < (\Delta - \delta) \frac{\sqrt{2\Delta}}{\sqrt{\Delta + \delta}} + \frac{\Delta(\delta - 1)}{2} \frac{\sqrt{\Delta}}{\sqrt{\delta}}.$$

Notice that, since $\delta < \Delta$,

$$1 < \sqrt{\frac{2\Delta}{\Delta + \delta}} < \sqrt{\frac{\Delta}{\delta}}.$$

Therefore, (3) does not hold if

$$\Delta - \delta + \frac{\Delta(\delta - 1)}{2} + 1 < (\Delta - \delta) \frac{\sqrt{2\Delta}}{\sqrt{\Delta + \delta}} + \frac{\Delta(\delta - 1)}{2} \frac{\sqrt{2\Delta}}{\sqrt{\Delta + \delta}}$$

and, since $\Delta - \delta + \frac{\Delta(\delta-1)}{2} = N_{\delta,\Delta}$, then (3) does not hold if

$$N_{\delta,\Delta} + 1 < N_{\delta,\Delta}\lambda_{\delta,\Delta}.$$

$\square$

Proposition 8 *If* $9 \le \delta < \Delta$, *then* $N_{\delta,\Delta} > \frac{1}{\lambda_{\delta,\Delta}-1}$.

Proof Since $\Delta > \delta$ then $N_{\delta,\Delta} \ge \frac{(\delta+1)^2}{2} - \delta$ and $\lambda_{\delta,\Delta} \ge \sqrt{\frac{2(\delta+1)}{2\delta+1}}$ which means that

$$\frac{1}{\lambda_{\delta,\Delta} - 1} \le \frac{1}{\sqrt{\frac{2(\delta+1)}{2\delta+1}} - 1}.$$

Thus, it suffices to check that

$$\frac{1}{\sqrt{\frac{2(\delta+1)}{2\delta+1}} - 1} < \frac{(\delta+1)^2}{2} - \delta$$

$$\Leftrightarrow \sqrt{\frac{2(\delta+1)}{2\delta+1}} > \frac{\delta^2+3}{\delta^2+1}$$

$$\Leftrightarrow 2(\delta+1)(\delta^2+1)^2 > (2\delta+1)(\delta^2+3)^2$$

$$\Leftrightarrow \delta^4 - 8\delta^3 - 2\delta^2 - 16\delta - 7 > 0.$$

The real solutions of the equation $\delta^4 - 8\delta^3 - 2\delta^2 - 16\delta - 7 = 0$ are $x_1 \approx -0.4$ and $x_2 \approx 8.5$. Therefore, $N_{\delta,\Delta} > \frac{1}{\lambda_{\delta,\Delta}-1}$ for every $\delta \ge 9$. $\square$

Corollary 8 *Suppose* $\alpha = -\frac{1}{2}$, $9 \le \delta \le \Delta$ *and* $\Delta(\delta + 1)$ *is even. If G is a graph with minimum degree* δ *and maximum degree* Δ, *then* (3) *holds if and only if* $\delta = \Delta$.

Proposition 9 *Suppose* $\alpha = -\frac{1}{2}$, $1 \le \delta < \Delta$ *and* $\Delta(\delta + 1)$ *is even. If G is a graph with minimum degree* δ *and maximum degree* Δ, *then* (3) *holds if*

$$N_{\delta,\Delta} \le \frac{1}{\varepsilon_{\delta,\Delta} - 1}. \tag{8}$$

Proof First, let us see that

$$\frac{1}{\sqrt{2\Delta}} \ge (\Delta - \delta)\left[\frac{1}{\sqrt{\Delta+\delta}} - \frac{1}{\sqrt{2\Delta}}\right] + \frac{\Delta(\delta-1)}{2\sqrt{2}}\left[\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right]$$

$$\Leftrightarrow 1 \ge (\Delta - \delta)\left(\frac{\sqrt{2\Delta}}{\sqrt{\Delta+\delta}} - 1\right) + \frac{\Delta(\delta-1)}{2}\left(\frac{\sqrt{\Delta}}{\sqrt{\delta}} - 1\right)$$

$$\Leftrightarrow \Delta - \delta + \frac{\Delta(\delta-1)}{2} + 1 \ge (\Delta - \delta)\frac{\sqrt{2\Delta}}{\sqrt{\Delta+\delta}} + \frac{\Delta(\delta-1)}{2}\frac{\sqrt{\Delta}}{\sqrt{\delta}}.$$

Notice that, since $\delta < \Delta$,

$$1 < \sqrt{\frac{2\Delta}{\Delta + \delta}} < \sqrt{\frac{\Delta}{\delta}}.$$

Therefore, (3) holds if

$$\Delta - \delta + \frac{\Delta(\delta - 1)}{2} + 1 \geq (\Delta - \delta)\frac{\sqrt{\Delta}}{\sqrt{\delta}} + \frac{\Delta(\delta - 1)}{2}\frac{\sqrt{\Delta}}{\sqrt{\delta}}$$

and, since $\Delta - \delta + \frac{\Delta(\delta - 1)}{2} = N_{\delta,\Delta}$, then (3) holds if

$$N_{\delta,\Delta} + 1 \geq N_{\delta,\Delta}\varepsilon_{\delta,\Delta}.$$

$\square$

However, this proposition does not provide many positive results:

Proposition 10 *If $4 \leq \delta < \Delta$, then $N_{\delta,\Delta} > \frac{1}{\varepsilon_{\delta,\Delta}-1}$.*

Proof Since $\Delta > \delta$ then $N_{\delta,\Delta} \geq \frac{(\delta+1)^2}{2} - \delta$ and $\varepsilon_{\delta,\Delta} \geq \sqrt{\frac{\delta+1}{\delta}}$ which means that

$$\frac{1}{\varepsilon_{\delta,\Delta} - 1} \leq \frac{1}{\sqrt{\frac{\delta+1}{\delta}} - 1}.$$

Thus, it suffices to check that

$$\frac{1}{\sqrt{\frac{\delta+1}{\delta}} - 1} < \frac{(\delta + 1)^2}{2} - \delta$$

$$\Leftrightarrow \sqrt{\frac{\delta + 1}{\delta}} > \frac{\delta^2 + 3}{\delta^2 + 1}$$

$$\Leftrightarrow (\delta + 1)(\delta^2 + 1)^2 > \delta(\delta^2 + 3)^2$$

$$\Leftrightarrow \delta^4 + 2\delta^2 + 1 > 4\delta^3 + 8\delta$$

which is trivially satisfied for every $\delta \geq 4$. $\square$

Corollary 9 *If $1 = \delta < \Delta$, then $N_{\delta,\Delta} \leq \frac{1}{\varepsilon_{\delta,\Delta}-1}$ if and only if $\Delta = 2$.*

Proof Note that, in this case, $\Delta(\delta + 1) = 2\Delta$ is even. $N_{\delta,\Delta} \leq \frac{1}{\varepsilon_{\delta,\Delta}-1}$ if and only if $\frac{N_{\delta,\Delta}+1}{N_{\delta,\Delta}} \geq \varepsilon_{\delta,\Delta}$. Thus, it suffices to check that

$$\frac{\Delta}{\Delta - 1} \geq \sqrt{\Delta} \quad \Leftrightarrow \quad \Delta^2 \geq \Delta(\Delta - 1)^2 \quad \Leftrightarrow \quad \Delta^2 - 3\Delta + 1 \leq 0,$$

and therefore, $\Delta \in \{1, 2\}$. Since $\Delta > 1$, this is equivalent to $\Delta = 2$. $\square$

Corollary 10 *If* $2 = \delta < \Delta$ *with* $\Delta(\delta + 1)$ *even, then* $N_{\delta,\Delta} > \frac{1}{\varepsilon_{\delta,\Delta}-1}$.

Proof Note that

$$\frac{3\Delta - 2}{3\Delta - 4} \geq \sqrt{\frac{\Delta}{2}} \quad \Leftrightarrow \quad 9\Delta^3 - 42\Delta^2 + 40\Delta - 8 \leq 0.$$

The solutions of the equation $9\Delta^3 - 42\Delta^2 + 40\Delta - 8 = 0$ are $x_1 \approx 0.3$, $x_2 \approx 0.9$, $x_3 \approx 3.4$ and therefore, there are no even integer solutions such that $2 < \Delta$. $\square$

Corollary 11 *If* $3 = \delta < \Delta$, *then* $N_{\delta,\Delta} \leq \frac{1}{\varepsilon_{\delta,\Delta}-1}$ *if and only if* $\Delta = 4$.

Proof Note that, in this case, $\Delta(\delta + 1)$ is even. We have

$$\frac{2\Delta - 2}{2\Delta - 3} \geq \sqrt{\frac{\Delta}{3}} \quad \Leftrightarrow \quad 4\Delta^3 - 24\Delta^2 + 33\Delta - 12 \leq 0.$$

The solutions of the equation $4\Delta^3 - 24\Delta^2 + 33\Delta - 12 = 0$ are $x_1 \approx 0.6$, $x_2 \approx 1.2$, $x_3 \approx 4.2$ and therefore, the only integer solution with $\Delta > 3$ is $\Delta = 4$. $\square$

6 Geometric-arithmetic index

The *first geometric-arithmetic index* GA_1, defined in [40] as

$$GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)}$$

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, is one of the successors of the Randić index. Although GA_1 was introduced in 2009, there are many papers dealing with this index (see, e.g., [6–8,29,36,37,40] and the references therein).

Let us recall Corollary 2.3 in [35].

Corollary 12 *Let g be the function* $g(x, y) = \frac{2\sqrt{xy}}{x+y}$ *with* $0 < a \leq x, y \leq b$. *Then* $\frac{2\sqrt{ab}}{a+b} \leq g(x, y) \leq 1$. *The equality in the lower bound is attained if and only if either* $x = a$ *and* $y = b$, *or* $x = b$ *and* $y = a$, *and the equality in the upper bound is attained if and only if* $x = y$.

Let us recall the following example from [26, Example 2.11].

Example 1 Let us suppose $\delta = 4$ and $\Delta = 56$. Consider a graph G with 57 vertices, two of them, a_1, a_2 with degree 56 and the rest, $b_1, \ldots, b_{55}$ with degree 4. Let us assume the edges are as follows. There is an edge $a_i b_j$ for every i, j, an edge $a_1 a_2$ and the vertices $b_1, \ldots, b_{55}$ induce a cycle of length 55. Note that these edges produce the claimed degree in each vertex.

Notice that G has 166 edges, one of them joins two vertices of degree 56, 110 of them join vertices with degree 56 with vertices with degree 4 and 55 of them join vertices with degree 4. Therefore, $GA_1(G) = \frac{2 \cdot 110 \sqrt{4 \cdot 56}}{4 + 56} + 56 = \frac{220 \sqrt{224}}{60} + 56 \approx 110.8776$.

However, $GA_1(H) = \frac{112 \sqrt{224}}{60} + 84 \approx 111.9377$ for every $H \in \mathcal{G}_{4,56}$, and $GA_1(K_{4,56}) = \frac{448 \sqrt{224}}{60} \approx 111.7508$.

Given integers $0 < i \le \delta < \Delta$, let us define $\mathcal{H}_{\delta, \Delta}^i$ as the set of graphs H with minimum degree δ, maximum degree Δ, $|V(H)| = \Delta + 1$, and such that:

(1) there are i vertices with degree Δ and $\Delta - i + 1$ vertices with degree δ, if $(\Delta - i + 1)(\delta - i)$ is even,

(2) there are i vertices with degree Δ, $\Delta - i$ vertices with degree δ and an additional vertex with degree $\delta + 1$ (possibly Δ if $\delta = \Delta - 1$), if $(\Delta - i + 1)(\delta - i)$ is odd.

Note that the graph from Example 1 belongs to $\mathcal{H}_{4,56}^2$.

Remark 3 Every graph $H \in \mathcal{H}_{\delta, \Delta}$ has maximum degree Δ and $|V(H)| = \Delta + 1$. Hence, every graph $H \in \mathcal{H}_{\delta, \Delta}$ is connected. Notice also that the subgraph of H induced by the set of vertices with degree Δ is complete.

Remark 4 By definition, $\mathcal{G}_{\delta, \Delta} = \mathcal{H}_{\delta, \Delta}^1$ for every $\delta < \Delta$ and $\mathcal{G}_{\Delta-1, \Delta} = \mathcal{H}_{\Delta-1, \Delta}^2$ if Δ is odd (and therefore, Δ^2 is odd and $(\Delta - 1)(\Delta - 3)$ is even).

Proposition 11 *For any integers* $1 \le i \le \delta < \Delta$, *we have* $\mathcal{H}_{\delta, \Delta}^i \ne \emptyset$.

Proof We are going to define a graph H with $\Delta + 1$ vertices, $v_1, \ldots, v_{\Delta+1}$. The vertices $v_{\Delta-i+2}, \ldots, v_{\Delta+1}$ define a complete graph, and let us define an edge joining v_j with v_k for every $j \le \Delta - i + 1 < k$. Thus, $d_{v_j} = \Delta$ for every $j > \Delta - i + 1$.

First, suppose $\delta - i$ is even. Thus, $(\Delta - i + 1)(\delta - i)$ is even. We have already i edges in each v_j with $j \le \Delta - i + 1$. We are going to add edges so that $d_{v_j} = \delta$ for every $j \le \Delta - i + 1$. Note that this holds if $\delta = i$, so we can assume that $\delta > i$. Let us define for every $1 \le j, k \le \Delta - i + 1$, $||j - k|| = \min\{|j - k|, \Delta - i + 1 - |j - k|\}$, i.e., $||j - k||$ is the distance between the vertices v_j and v_k in the cycle $v_1, v_2, \ldots, v_{\Delta-i+1}, v_1$. Consider an edge $v_j v_k$ for every pair of vertices with $||j - k|| \le \frac{\delta - i}{2}$. This is possible since $\delta - i$ is even and $\delta - i < \Delta - i$. Then, every vertex v_j with $j \le \Delta - i + 1$ satisfies that $d_{v_j} = \delta$ and $H \in \mathcal{H}_{\delta, \Delta}^i$.

Now, suppose $\delta - i$ is odd and $\Delta - i + 1$ is even. Thus, $(\Delta - i + 1)(\delta - i)$ is even. Consider an edge $v_j v_k$ for every pair of vertices with $||j - k|| \le \frac{\delta - i - 1}{2}$ and an edge $v_j v_k$ if $||j - k|| = \frac{\Delta - i + 1}{2}$. Notice that this is well defined since $\Delta - i + 1$ is even and it is a new edge (recall that $\frac{\Delta - i + 1}{2} > \frac{\delta - i - 1}{2}$). Thus, every vertex v_j with $j \le \Delta - i + 1$ satisfies that $d_{v_j} = \delta$ and $H \in \mathcal{H}_{\delta, \Delta}^i$.

Finally, suppose $\delta - i$ and $\Delta - i + 1$ are odd. Therefore, $(\Delta - i + 1)(\delta - i)$ is odd. Consider an edge $v_j v_k$ for every pair of vertices with $||j - k|| \le \frac{\delta - i - 1}{2}$. Now every vertex v_j with $j \le \Delta - i + 1$ has degree $\delta - 1$. Let us define, for every $1 \le j < k \le \Delta - i$, an edge $v_j v_k$ if $k - j = \frac{\Delta - i}{2}$ (this edge is new since $\frac{\delta - i - 1}{2} < \frac{\Delta - i}{2}$). Now, $d_{v_j} = \delta$ for every $1 \le j \le \Delta - i$. It suffices to define an edge joining $v_{\Delta-i+1}$ to any non-adjacent vertex v_{j_0}, for example $j_0 = \frac{\delta - i - 1}{2} + 1$, and therefore, $H \in \mathcal{H}_{\delta, \Delta}^i$. Notice that, in this case, $d_{v_k} = \Delta$ for every $k > \Delta - i + 1$, $d_{v_{j_0}} = \delta + 1$ and $d_{v_j} = \delta$ for every $j \le \Delta - i + 1$ with $j \ne j_0$. $\square$

Proposition 12 *For every integers $1 \le i \le \delta < \Delta$ and $H \in \mathcal{H}^i_{\delta,\Delta}$, we have*

$$GA_1(H) = i(\Delta - i + 1)\frac{2\sqrt{\delta\Delta}}{\delta + \Delta} + \frac{i(i-1)}{2} + \frac{(\Delta - i + 1)(\delta - i)}{2}$$
$$\text{if } (\Delta - i + 1)(\delta - i) \text{ is even,}$$

$$GA_1(H) = i(\Delta - i)\frac{2\sqrt{\delta\Delta}}{\delta + \Delta} + i\frac{2\sqrt{(\delta+1)\Delta}}{\delta + \Delta + 1} + (\delta - i + 1)\frac{2\sqrt{\delta(\delta+1)}}{2\delta + 1}$$
$$+ \frac{i(i-1)}{2} + \frac{(\Delta - i - 1)(\delta - i) - 1}{2}$$
$$> i(\Delta - i + 1)\frac{2\sqrt{\delta\Delta}}{\delta + \Delta} + \frac{i(i-1)}{2} + \frac{(\Delta - i + 1)(\delta - i)}{2}$$
$$\text{if } (\Delta - i + 1)(\delta - i) \text{ is odd.}$$

Proof The equalities follow from the definitions of GA_1 and $\mathcal{H}^i_{\delta,\Delta}$.
To obtain the inequality, it suffices to check that

$$i\frac{2\sqrt{(\delta+1)\Delta}}{\delta + 1 + \Delta} > i\frac{2\sqrt{\delta\Delta}}{\delta + \Delta} \quad \text{and} \quad (\delta - i + 1)\frac{2\sqrt{\delta(\delta+1)}}{2\delta + 1} \ge \delta - i + \frac{1}{2}.$$

The first claim follows from Corollary 12. For the second claim it suffices to check
that

$$(\delta - i + 1)\frac{2\sqrt{\delta(\delta+1)}}{2\delta + 1} \ge \delta - i + \frac{1}{2} \quad \Leftrightarrow$$
$$(4\delta^2 + 4\delta)(\delta^2 - 2\delta i + 2\delta + i^2 - 2i + 1)$$
$$\ge \left(\delta^2 - 2\delta i + \delta - i + i^2 + \frac{1}{4}\right)(4\delta^2 + 4\delta + 1) \quad \Leftrightarrow$$
$$(4\delta^2 + 4\delta)\left(\delta - i + \frac{3}{4}\right) \ge \delta^2 - 2\delta i + \delta - i + i^2 + \frac{1}{4} = (\delta - i)^2 + \delta - i + \frac{1}{4}.$$

Since $\delta \ge i$, then it is immediate to see that

$$(4\delta^2 + 4\delta)\left(\delta - i + \frac{3}{4}\right) \ge 3\delta^2 + 3\delta > \delta^2 + \delta + 1 > (\delta - i)^2 + \delta - i + \frac{1}{4}.$$

□

Proposition 13 *For any integers $1 < i \le \delta < \Delta$, if $\Delta(\delta + 1)$ is even, $\alpha = \frac{\delta}{\Delta}$ and $\frac{\Delta}{\Delta-i} > \frac{2(1-\sqrt{\alpha})^2}{1-\alpha^2}$, then for any $G \in \mathcal{G}_{\delta,\Delta}$ and $H \in \mathcal{H}^i_{\delta,\Delta}$, we have $GA_1(H) > GA_1(G)$.*

Proof Let us see that

$$\frac{i(i-1)}{2} + \frac{(\Delta - i + 1)(\delta - i)}{2} + i(\Delta - i + 1)\frac{2\sqrt{\delta\Delta}}{\delta + \Delta} > \frac{\Delta(\delta-1)}{2} + \Delta\frac{2\sqrt{\delta\Delta}}{\delta + \Delta}.$$

Notice that

$$\frac{\Delta(\delta - 1)}{2} = \frac{(\Delta - i + 1)(\delta - i)}{2} + \frac{(i - 1)(\delta - i)}{2} + \frac{(i - 1)\Delta}{2}$$

$$= \frac{(\Delta - i + 1)(\delta - i)}{2} + \frac{i - 1}{2}(\delta + \Delta - i),$$

with $\delta + \Delta - i > 0$. Therefore, if $\varepsilon = \frac{2\sqrt{\delta\Delta}}{\delta + \Delta}$, it suffices to check that

$$[(i - 1)\Delta - i(i - 1)]\varepsilon > \frac{i - 1}{2}(\delta + \Delta - 2i)$$

$$\Leftrightarrow \varepsilon > \frac{(i - 1)(\delta + \Delta - 2i)}{2[(i - 1)\Delta - i(i - 1)]} = \frac{\delta + \Delta - 2i}{2(\Delta - i)}$$

$$\Leftrightarrow \frac{2\sqrt{\alpha}\Delta}{(1 + \alpha)\Delta} = \frac{2\sqrt{\alpha}}{1 + \alpha} > \frac{(1 + \alpha)\Delta - 2i}{2(\Delta - i)}$$

$$= \frac{2(\Delta - i) - (1 - \alpha)\Delta}{2(\Delta - i)} = 1 - \frac{(1 - \alpha)\Delta}{2(\Delta - i)}$$

$$\Leftrightarrow \frac{1 - \alpha}{2}\frac{\Delta}{\Delta - i} > 1 - \frac{2\sqrt{\alpha}}{1 + \alpha} = \frac{1 + \alpha - 2\sqrt{\alpha}}{1 + \alpha} = \frac{(1 - \sqrt{\alpha})^2}{1 + \alpha}$$

$$\Leftrightarrow \frac{\Delta}{\Delta - i} > \frac{2(1 - \sqrt{\alpha})^2}{1 - \alpha^2}.$$

$\square$

Corollary 13 *For any integers $1 < i \leq \delta < \Delta$, if $\Delta(\delta + 1)$ is even and $\delta \geq 0.09\Delta$, then for any $G \in \mathcal{G}_{\delta,\Delta}$ and $H \in \mathcal{H}^i_{\delta,\Delta}$, we have $GA_1(H) > GA_1(G)$.*

Proof Let us define $\alpha = \delta/\Delta \in (0, 1)$. Notice that we have $\frac{\Delta}{\Delta - i} > 1$ for every $i > 1$. Thus, let us check that

$$\frac{2(1 - \sqrt{\alpha})^2}{1 - \alpha^2} \leq 1 \Leftrightarrow 2(1 - \sqrt{\alpha})^2 \leq 1 - \alpha^2$$

$$\Leftrightarrow 2 - 4\sqrt{\alpha} + 2\alpha \leq 1 - \alpha^2 \quad \Leftrightarrow \quad \alpha^2 + 2\alpha + 1 \leq 4\sqrt{\alpha}$$

$$\Leftrightarrow (\alpha + 1)^2 \leq 4\sqrt{\alpha} \quad \Leftrightarrow \quad (\alpha + 1)^4 \leq 16\alpha$$

$$\Leftrightarrow \alpha^4 + 4\alpha^3 + 6\alpha^2 - 12\alpha + 1 \leq 0.$$

Since the real roots of the equation $x^4 + 4x^3 + 6x^2 - 12x + 1 = 0$ are $x_1 \approx 0.087$ and $x_1 = 1$, it is clear that the condition is satisfied for every $\alpha \in [0.09, 1)$. $\square$

Conjecture 13 *Given any integers $1 < \delta < \Delta$, a graph G is minimal for GA_1 if and only if $G \in \mathcal{H}^i_{\delta,\Delta}$ for some $1 \leq i \leq \delta$.*

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