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Optimal Upper Bounds of the Geometric–Arithmetic Index

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Abstract

The concept of geometric-arithmetic index was introduced in the chemical graph theory recently, but it has shown to be useful. The aim of this paper is to obtain new upper bounds of the geometric-arithmetic index and characterize graphs extremal with respect to them.

1 Introduction

A single number, representing a chemical structure in graph-theoretical terms via the molecular graph, is called a topological descriptor and if it in addition correlates with a molecular property it is called topological index, which is used to understand physico-chemical properties of chemical compounds. Topological indices are interesting since they capture some of the properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes (see [41]).

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 descriptors are the Randić connectivity index (R) and the Zagreb indices.

The first and second Zagreb indices, denoted by M_1 and M_2, respectively, were introduced by Gutman and Trinajstić in 1972 (see [15]) as

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

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.

There is a vast amount of research on the Zagreb indices. For details of their chemical applications and mathematical theory see [11], [12], [13], and the references therein.

In [19], [18], [22], the *first and second variable Zagreb indices* are defined as

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

with $\alpha \in \mathbb{R}$.

The concept of variable molecular descriptors was proposed as a new way of characterizing heteroatoms in molecules (see [27], [28]), but also to assess the structural differences (e.g., the relative role of carbon atoms of acyclic and cyclic parts in alkylcycloalkanes [29]). 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., [22]).

In the paper of Gutman and Tošović [14], 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 the second variable Zagreb index M_2^α with exponent $\alpha = -1$ (and to a lesser extent with exponent $\alpha = -2$) performs significantly better than the Randić index ($R = M_2^{-0.5}$).

The second variable Zagreb index is used in the structure-boiling point modeling of benzenoid hydrocarbons [25]. Also, variable Zagreb indices exhibit a potential applicability for deriving multi-linear regression models [7]. Various properties and relations of these indices are discussed in several papers (see, e.g., [3], [18], [20], [36], [42], [43]).

Note that M_1^2 is the first Zagreb index M_1, M_1^{-1} is the inverse index ID, M_1^3 is the forgotten index F, etc.; also, $M_2^{-1/2}$ is the usual Randić index, M_2^1 is the second Zagreb index M_2, M_2^{-1} is the modified Zagreb index, etc.

The *general sum-connectivity index* was defined by Zhou and Trinajstić in [47] 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 H, $\chi_{-1/2}$ is the sum-connectivity index χ, etc.

The (first) *geometric-arithmetic index* GA is defined in [38] as

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

Although GA was introduced in 2009, there are many papers dealing with this index (see, e.g., [4], [5], [6], [16], [21], [24], [26], [31], [35], [38] and the references therein). There are other geometric-arithmetic indices, like $Z_{p,q}$ ($Z_{0,1} = GA$), but the results in [5, p.598] show that the GA index gathers the same information on observed molecule as other $Z_{p,q}$ indices.

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 $5.85 \cdot 10^{21}$ [37]. Therefore, modeling their physico-chemical properties is important in order to predict properties of currently unknown species. The predicting ability of the GA index compared with Randić index is reasonably better (see [5, Table 1]). The graphic in [5, Fig.7] (from [5, Table 2], [33]) shows that there exists a good linear correlation between GA and the heat of formation of benzenoid hydrocarbons (the correlation coefficient is equal to 0.972).

Furthermore, the improvement in prediction with GA index comparing to Randić index in the case of standard enthalpy of vaporization is more than 9%. That is why one can think that GA index should be considered in the QSPR/QSAR researches.

Throughout this work, $G = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) such that each connected connected component of G has at least an edge. We denote by Δ, δ, n, m the maximum degree, the minimum degree and the cardinality of the set of vertices and edges of G, respectively.

A main topic in the study of topological indices is to find bounds of the indices involving several parameters. [23] proves that many upper bounds of GA are not useful, and shows the importance of obtaining upper bounds of GA less than m. With this aim, we obtain in this paper several new upper bounds of GA, which are less than m, and we characterize graphs extremal with respect to them.

2 Upper bounds involving other indices

Theorem 2.1. *If G is a graph with m edges and maximum degree Δ, then*

$$GA(G) \le m - \frac{M_1(G) - 2M_2^{1/2}(G)}{2\Delta},$$

and the equality is attained if and only if G is regular.

Proof. We have

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} + \frac{\left(\sqrt{d_u} - \sqrt{d_v}\right)^2}{d_u + d_v} = 1,$$
$$GA(G) + \sum_{uv \in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\right)^2}{d_u + d_v} = m.$$

Since

$$\sum_{uv \in E(G)} \frac{\left(\sqrt{d_u} - \sqrt{d_v}\right)^2}{d_u + d_v} \ge \frac{1}{2\Delta} \sum_{uv \in E(G)} \left(\sqrt{d_u} - \sqrt{d_v}\right)^2$$
$$= \frac{1}{2\Delta}\Big(\sum_{uv \in E(G)} (d_u + d_v) - 2 \sum_{uv \in E(G)} \sqrt{d_u d_v} \Big) = \frac{M_1(G) - 2M_2^{1/2}(G)}{2\Delta},$$

we conclude

$$GA(G) \le m - \frac{M_1(G) - 2M_2^{1/2}(G)}{2\Delta}.$$

If G is regular, then

$$m - \frac{M_1(G) - 2M_2^{1/2}(G)}{2\Delta} = m - \frac{2\Delta m - 2\Delta m}{2\Delta} = m = GA(G).$$

If the equality is attained, then $d_u + d_v = 2\Delta$ for every $uv \in E(G)$; thus, $d_u = \Delta$ for every $u \in V(G)$, and G is a regular graph. ∎

Remark 2.2. *Since Cauchy-Schwarz inequality gives*

$$M_1(G) - 2M_2^{1/2}(G) = \sum_{uv \in E(G)} \left(\sqrt{d_u} - \sqrt{d_v}\right)^2$$
$$= \sum_{uv \in E(G)} \left(\sqrt{d_u} - \sqrt{d_v}\right)^2 \frac{1}{m} \sum_{uv \in E(G)} 1^2$$
$$\ge \frac{1}{m}\Big(\sum_{uv \in E(G)} \left|\sqrt{d_u} - \sqrt{d_v}\right| \Big)^2,$$

we have $M_1(G) - 2M_2^{1/2}(G) \ge 0$.

As usual, let us define

$$\Delta_e = \max_{uv \in E(G)} (d_u + d_v), \qquad \delta_e = \max_{uv \in E(G)} (d_u + d_v).$$

Thus, the argument in the proof of Theorem 2.1 has the following consequence.

Theorem 2.3. *If G is a graph with m edges and maximum degree Δ, then*

$$GA(G) \le m - \frac{M_1(G) - 2M_2^{1/2}(G)}{\Delta_e},$$

and the equality is attained if and only if the line graph of G is regular.

The *misbalance rodeg index* is defined as

$$MR(G) = \sum_{uv \in E(G)} \left| \sqrt{d_u} - \sqrt{d_v} \right|.$$

This is a significant predictor of enthalpy of vaporization and of standard enthalpy of vaporization for octane isomers (see [39]).

Since Remark 2.2 gives

$$M_1(G) - 2M_2^{1/2}(G) \ge \frac{1}{m} MR(G)^2,$$

Theorems 2.1 and 2.3 have the following consequences, respectively.

Corollary 2.4. *If G is a graph with m edges and maximum degree Δ, then*

$$GA(G) \le m - \frac{1}{2\Delta m} MR(G)^2,$$

and the equality is attained if and only if G is regular.

Corollary 2.5. *If G is a graph with m edges and maximum degree Δ, then*

$$GA(G) \le m - \frac{1}{\Delta_e m} MR(G)^2,$$

and the equality is attained if and only if the line graph of G is regular.

In the same paper, where Zagreb indices were introduced, the *forgotten topological index* (or *F-index*) is defined as

$$F(G) = \sum_{u \in V(G)} d_u^3.$$

Both the forgotten topological index and the first Zagreb index were employed in the formulas for total π-electron energy in [15], as a measure of branching extent of the carbon-atom skeleton of the underlying molecule. However, this index never got attention except recently, when Furtula and Gutman in [10] established some basic properties of the F-index and showed that its predictive ability is almost similar to that of first Zagreb index and for the entropy and acetic factor, both of them yield correlation coefficients greater than 0.95. Besides, [10] pointed out the importance of the F-index: it can be used to obtain a high accuracy of the prediction of logarithm of the octanol-water partition coefficient (see also [1]).

The *Albertson index* is defined in [2] as

$$Alb(G) = \sum_{uv \in E(G)} |d_u - d_v| .$$

This index is much used as a measure of non-regularity of a graph. The Albertson index is also known as *misbalance deg index* (see [39] and [40]). This is a significant predictor of standard enthalpy of vaporization for octane isomers (see [39]).

Theorem 2.6. *If G is a graph with maximum degree Δ and minimum degree δ, then*

$$GA(G) \le \frac{F(G)}{2\delta^2} - \frac{Alb(G)^2}{\delta\, M_1(G)} ,$$

and the equality is attained if and only if G is regular.

Proof. Since

$$\frac{d_u^2 + d_v^2}{2\delta} \ge \frac{d_u^2 + d_v^2}{d_u + d_v} = \frac{2d_u d_v}{d_u + d_v} + \frac{(d_u - d_v)^2}{d_u + d_v} \ge \frac{2\delta\sqrt{d_u d_v}}{d_u + d_v} + \frac{(d_u - d_v)^2}{d_u + d_v} ,$$

for every $uv \in E(G)$, and

$$F(G) = \sum_{u \in V(G)} d_u^3 = \sum_{uv \in E(G)} \big(d_u^2 + d_v^2\big),$$

we have

$$\frac{F(G)}{2\delta} \ge \delta\, GA(G) + \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u + d_v} .$$

Cauchy-Schwarz inequality gives

$$\begin{aligned} Alb(G)^2 &= \Big(\sum_{uv \in E(G)} \frac{|d_u - d_v|}{(d_u + d_v)^{1/2}} \, (d_u + d_v)^{1/2} \Big)^2 \\ &\le \Big(\sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u + d_v} \Big) \Big(\sum_{uv \in E(G)} (d_u + d_v) \Big) = M_1(G) \sum_{uv \in E(G)} \frac{(d_u - d_v)^2}{d_u + d_v} , \end{aligned}$$

and we conclude

$$\frac{F(G)}{2\delta} \geq \delta\, GA(G) + \frac{Alb(G)^2}{M_1(G)}\,.$$

If the graph is regular, then

$$\frac{F(G)}{2\delta^2} - \frac{Alb(G)^2}{\delta\, M_1(G)} = \frac{F(G)}{2\delta^2} = \frac{2\delta^2 m}{2\delta^2} = m = GA(G).$$

The previous argument gives that if the bound is attained, then $d_u + d_v = 2\delta$ for every $uv \in E(G)$. Thus, $d_u = \delta$ for every $u \in V(G)$ and G is regular. ■

The argument in the proof of Theorem has the following consequence.

Theorem 2.7. *If G is a graph with maximum degree Δ and minimum degree δ, then*

$$GA(G) \leq \frac{F(G)}{\delta_e\, \delta} - \frac{Alb(G)^2}{\delta\, M_1(G)}\,,$$

and the equality is attained if and only if the line graph of G is regular.

The following Kober's inequalities appear in [17] (see also [46, Lemma 1]).

Lemma 2.8. *If $a_j > 0$ for $1 \leq j \leq k$, then*

$$\sum_{j=1}^{k} a_j + k(k-1)\Big(\prod_{j=1}^{k} a_j\Big)^{1/k} \leq \Big(\sum_{j=1}^{k} \sqrt{a_j}\Big)^2 \leq (k-1)\sum_{j=1}^{k} a_j + k\Big(\prod_{j=1}^{k} a_j\Big)^{1/k}.$$

Another remarkable topological descriptor is the *harmonic index*, defined in [9] 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., [44], [45] and [32]).

Multiplicative versions of the first and the second Zagreb indices, Π_1 and Π_2, were first considered in [34], defined as

$$\Pi_1(G) = \prod_{u\in V(G)} d_u^2, \qquad \Pi_2(G) = \prod_{uv\in E(G)} d_u d_v.$$

Also, the multiplicative sum–Zagreb index Π_1^* was introduced in [8] as

$$\Pi_1^*(G) = \prod_{uv\in E(G)} (d_u + d_v).$$

Theorem 2.9. *If G is a graph with m edges, then*

$$GA(G) \leq M_2^{1/2}(G)\, H(G) - 2m(m-1)\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}}\,,$$

and the equality is attained for every regular graph.

Proof. The first inequality in Lemma 2.8 and Cauchy-Schwarz inequality give

$$\sum_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{d_u+d_v} + m(m-1)\Big(\prod_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{d_u+d_v}\Big)^{1/m} \le \Big(\sum_{uv\in E(G)} \frac{(d_u d_v)^{1/4}}{(d_u+d_v)^{1/2}}\Big)^2$$
$$\le \sum_{uv\in E(G)} (d_u d_v)^{1/2} \sum_{uv\in E(G)} \frac{1}{d_u+d_v} = M_2^{1/2}(G)\,\frac{1}{2}\,H(G),$$
$$GA(G) + 2m(m-1)\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}} \le M_2^{1/2}(G)\,H(G).$$

If G is a regular graph, then

$$M_2^{1/2}(G)\,H(G) - 2m(m-1)\frac{\Pi_2(G)^{1/(2m)}}{\Pi_1^*(G)^{1/m}}$$
$$= \Delta m\frac{m}{\Delta} - 2m(m-1)\frac{(\Delta^{2m})^{1/(2m)}}{((2\Delta)^m)^{1/m}} = m = GA(G).$$

■

3 Other upper bounds

We obtain in this section additional upper bounds of GA which do not involve other topological indices.

Theorem 3.1. *Let G be a graph with m edges, minimum degree δ, maximum degree $\delta+1$, and α the cardinality of the set of edges $uv\in E(G)$ with $d_u+d_v = 2\delta+1$. Then α is an even integer and*

$$GA(G) = m - \alpha + \alpha\frac{2\sqrt{\delta(\delta+1)}}{2\delta+1}\,.$$

Proof. Since the minimum degree of G is δ and its maximum degree is $\delta+1$, we have $d_u+d_v\in\{2\delta, 2\delta+1, 2\delta+2\}$ for every $uv\in E(G)$. If $d_u+d_v = 2\delta$ or $d_u+d_v = 2\delta+2$, then $d_u = d_v = \delta$ or $d_u = d_v = \delta+1$, respectively, and

$$\frac{2\sqrt{d_u d_v}}{d_u+d_v} = 1.$$

Since there are exactly α edges $uv\in E(G)$ with $d_u+d_v = 2\delta+1$ and $m-\alpha$ edges with $d_u+d_v\in\{2\delta, 2\delta+2\}$, we have

$$GA(G) = m - \alpha + \alpha\frac{2\sqrt{\delta(\delta+1)}}{2\delta+1}\,.$$

Seeking for a contradiction assume that α is an odd integer.

Let G_1 be the subgraph of G induced by the n_1 vertices with degree δ in $V(G)$, and denote by m_1 the cardinality of the set of edges of G_1. Handshaking Lemma gives $n_1\delta - \alpha = 2m_1$. Since α is an odd integer, δ is also an odd integer.

Let G_2 be the subgraph of G induced by the n_2 vertices with degree $\delta+1$ in $V(G)$, and denote by m_2 the cardinality of the set of edges of G_2. Handshaking Lemma gives $n_2(\delta+1)-\alpha = 2m_2$. Since α is an odd integer, $\delta+1$ is also an even integer, a contradiction.

Thus, we conclude that α is an even integer. ∎

Theorem 3.2. *Let G be a connected graph with m edges, minimum degree δ and maximum degree $\delta+1$. Then*

$$GA(G) \le m - 2 + \frac{4\sqrt{\delta(\delta+1)}}{2\delta+1},$$

and the equality is attained for each δ.

Proof. Denote by α the cardinality of the set of edges $uv \in E(G)$ with $d_u + d_v = 2\delta+1$. Theorem 3.1 gives that α is an even integer. Since G is a connected graph, we have $\alpha \neq 0$ and so, $\alpha \ge 2$. Since

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

and $\alpha \ge 2$, Theorem 3.1 gives

$$GA(G) = m - \alpha + \alpha\frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} \le m - 2 + \frac{4\sqrt{\delta(\delta+1)}}{2\delta+1}.$$

Given a fixed δ, let us consider the complete graphs $K_{\delta+1}$ and $K_{\delta+2}$ with $\delta+1$ and $\delta+2$ vertices, respectively. Fix $u_1, u_2 \in V(K_{\delta+1})$ and $v_1, v_2 \in V(K_{\delta+2})$, and denote by $K'_{\delta+1}$ and $K'_{\delta+2}$ the graphs obtained from $K_{\delta+1}$ and $K_{\delta+2}$ by deleting the edges u_1u_2 and v_1v_2, respectively. Let Γ_δ be the graph with $V(\Gamma_\delta) = V(K'_{\delta+1}) \cup V(K'_{\delta+2})$ and $E(\Gamma_\delta) = E(K'_{\delta+1}) \cup E(K'_{\delta+2}) \cup \{u_1v_1\} \cup \{u_2v_2\}$. Thus, Γ_δ has $\delta^2+2\delta+1$ edges, minimum degree δ, maximum degree $\delta+1$, and Theorem 3.1 gives

$$GA(\Gamma_\delta) = \delta^2 + 2\delta - 1 + \frac{4\sqrt{\delta(\delta+1)}}{2\delta+1}.$$

Hence, the equality is attained for each δ. ∎

We have the following consequence for chemical graphs.

Corollary 3.3. *Let G be a connected chemical graph with m edges, minimum degree δ and maximum degree $\delta+1$. Then*

$$GA(G) \le m - 2 + \frac{8\sqrt{3}}{7},$$

and the inequality is sharp.

Proof. Since G is a chemical graph, we have $1 \le \delta \le 3$. Since

$$\max\left\{\frac{4\sqrt{2}}{3}, \frac{4\sqrt{6}}{5}, \frac{4\sqrt{12}}{7}\right\} = \frac{8\sqrt{3}}{7},$$

Theorem 3.2 gives the desired inequality.

The graph Γ_3 in the proof of Theorem 3.2 gives that the equality is attained. ■

The following technical results appear in [30, Lemma 2.2 and Corollary 2.3].

Lemma 3.4. *Let f be the function $f(t) = \frac{2t}{1+t^2}$ on the interval $[0,\infty)$. Then f strictly increases in $[0,1]$, strictly decreases in $[1,\infty)$, $f(t) = 1$ if and only if $t = 1$ and $f(t) = f(t_0)$ if and only if either $t = t_0$ or $t = t_0^{-1}$.*

Corollary 3.5. *Let g be the function $g(x,y) = \frac{2\sqrt{xy}}{x+y}$ with $0 < a \le x, y \le b$. Then*

$$\frac{2\sqrt{ab}}{a+b} \le g(x,y) \le 1.$$

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 $x = y$. Besides, $g(x,y) = g(x',y')$ if and only if x/y is equal to either x'/y' or y'/x'.

Theorem 3.6. *Let G be a graph with m edges, minimum degree δ and maximum degree $\Delta > \delta+1$. Denote by $\alpha_0, \alpha_1, \alpha_2$, the cardinality of the subsets of edges $A_0 = \{uv \in E(G) : d_u = \delta, d_v = \Delta\}$, $A_1 = \{uv \in E(G) : d_u = \delta, \delta < d_v < \Delta\}$, $A_2 = \{uv \in E(G) : d_u = \Delta, \delta < d_v < \Delta\}$, respectively. Then*

$$GA(G) \le m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}.$$

Proof. Lemma 3.4 gives that the function

$$\frac{2\sqrt{\delta d_v}}{\delta + d_v} = f\left(\left(\frac{d_v}{\delta}\right)^{1/2}\right)$$

is decreasing in $d_v \in [\delta, \Delta]$ and so,

$$\frac{2\sqrt{\delta d_v}}{\delta + d_v} \le \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1},$$

for every $uv \in A_1$.

In a similar way, Lemma 3.4 gives that the function

$$\frac{2\sqrt{\Delta d_v}}{\Delta + d_v} = f\Big(\Big(\frac{d_v}{\Delta}\Big)^{1/2}\Big)$$

is increasing in $d_v \in [\delta, \Delta]$ and so,

$$\frac{2\sqrt{\Delta d_v}}{\Delta + d_v} \le \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta - 1},$$

for every $uv \in A_2$.

Since

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} \le 1$$

for every $uv \in E(G)$, we have

$$\begin{aligned} GA(G) &= \sum_{uv\in E(G)\setminus A_0\cup A_1\cup A_2} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{uv\in A_0} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{uv\in A_1} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{uv\in A_2} \frac{2\sqrt{d_u d_v}}{d_u+d_v} \\ &= \sum_{uv\in E(G)\setminus A_0\cup A_1\cup A_2} \frac{2\sqrt{d_u d_v}}{d_u+d_v} + \sum_{uv\in A_0} \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \sum_{uv\in A_1} \frac{2\sqrt{\delta d_v}}{\delta+d_v} + \sum_{uv\in A_2} \frac{2\sqrt{\Delta d_v}}{\Delta+d_v} \\ &\le m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}. \end{aligned}$$

■

Theorem 3.7. *Let G be a connected graph with m edges, minimum degree δ and maximum degree $\Delta > \delta + 1$. Then*

$$GA(G) \le m - \min\Big\{2 - \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} - \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1},\, 1 - \frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\Big\}.$$

Proof. As in Theorem 3.6, let us denote by $\alpha_0, \alpha_1, \alpha_2$, the cardinality of the subsets of edges $A_0 = \{uv \in E(G) : d_u = \delta, d_v = \Delta\}$, $A_1 = \{uv \in E(G) : d_u = \delta, \delta < d_v < \Delta\}$, $A_2 = \{uv \in E(G) : d_u = \Delta, \delta < d_v < \Delta\}$.

Since G is a connected graph, we have two possibilities: $A_0 \ne \emptyset$, or $A_1 \ne \emptyset$ and $A_2 \ne \emptyset$.

In the first case, $\alpha_0 \ge 1$ and, since

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} \le 1,$$

Theorem 3.6 gives

$$\begin{aligned} GA(G) &\le m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}. \\ &\le m - 1 + \frac{2\sqrt{\Delta\delta}}{\Delta+\delta}. \end{aligned}$$

In the second case, $\alpha_1, \alpha_2 \geq 1$ and Theorem 3.6 gives

$$\begin{aligned} GA(G) &\leq m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} . \\ &\leq m - 2 + \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} . \end{aligned}$$

■

We need the following technical result.

Lemma 3.8. *If* $u(t) = \frac{2\sqrt{t}}{1+t}$, *then*

(1) $u(t) \leq 1 - \frac{1}{8}(t-1)^2$ *for every* $t \in [0,1]$,

(2) $u(t) \geq 1 - \frac{1}{5}(t-1)^2$ *for every* $t \in [0.6,1]$.

Proof. We have for every $s \in [0,1]$ and $t = 1-s \in [0,1]$,

$$\begin{aligned} -s^3(s^3 - 4s^2 - 12s + 64) &\leq 0, \\ 256 - 256s - (s^2 - 4s + 4)(s^4 - 16s^2 + 64) &\leq 0, \\ 4(1-s) - (2-s)^2\Big(1 - \frac{1}{8}\,s^2\Big)^2 &\leq 0, \\ 4t - (1+t)^2\Big(1 - \frac{1}{8}\,(t-1)^2\Big)^2 &\leq 0, \\ u(t) = \frac{2\sqrt{t}}{1+t} &\leq 1 - \frac{1}{8}(t-1)^2. \end{aligned}$$

Let $s_0 = 0.40568698...$ be the unique real solution of $-s^3 + 7s^2 - 15s + 5 = 0$ in the interval $[0,1]$. We have for every $s \in [0,0.4] \subset [0,s_0]$ and $t = 1-s \in [0.6,1] \subset [1-s_0,1]$,

$$\begin{aligned} s^2(s+3)(-s^3 + 7s^2 - 15s + 5) &\geq 0, \\ 100 - 100s - (s^2 - 4s + 4)(s^4 - 10s^2 + 25) &\geq 0, \\ 4(1-s) - (2-s)^2\Big(1 - \frac{1}{5}\,s^2\Big)^2 &\geq 0, \\ 4t - (1+t)^2\Big(1 - \frac{1}{5}\,(t-1)^2\Big)^2 &\geq 0, \\ u(t) = \frac{2\sqrt{t}}{1+t} &\geq 1 - \frac{1}{5}(t-1)^2. \end{aligned}$$

■

Theorem 3.9. *Let G be a connected graph with m edges, minimum degree δ and maximum degree $\Delta > \delta + 1$.*

(1) *If δ is an even integer, then*

$$GA(G) \leq m - \min\Big\{2 - \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} - \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1}\, ,\, 3 - \frac{4\sqrt{\delta(\delta+1)}}{2\delta+1} - \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}\Big\}.$$

(2) *If Δ is an even integer, then*

$$GA(G) \le m - \min\left\{2 - \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} - \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1},\, 3 - \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} - \frac{4\sqrt{\Delta(\Delta-1)}}{2\Delta-1}\right\}.$$

(3) *If δ and Δ are even integers, then*

$$GA(G) \le m - 4 + \frac{4\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{4\sqrt{\Delta(\Delta-1)}}{2\Delta-1}.$$

Proof. Assume first that δ is an even integer. As in Theorem 3.6, let us denote by $\alpha_0, \alpha_1, \alpha_2$, the cardinality of the subsets of edges $A_0 = \{uv \in E(G) :\ d_u = \delta, d_v = \Delta\}$, $A_1 = \{uv \in E(G) :\ d_u = \delta, \delta < d_v < \Delta\}$, $A_2 = \{uv \in E(G) :\ d_u = \Delta, \delta < d_v < \Delta\}$.

Let G_1 be the subgraph of G induced by the n_1 vertices with degree δ in $V(G)$, and denote by m_1 the cardinality of the set of edges of G_1. Handshaking Lemma gives $n_1\delta - \alpha_0 - \alpha_1 = 2m_1$. Since δ is an even integer, $\alpha_0 + \alpha_1$ is also an even integer; since G is a connected graph, we have $\alpha_0 + \alpha_1 \ge 1$ and so, $\alpha_0 + \alpha_1 \ge 2$.

If $\alpha_0 \ge 2$, then Corollary 3.5 gives

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} \le 1,$$

and we have, by Theorem 3.6,

$$\begin{aligned} GA(G) &\le m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \\ &\le m - \alpha_0 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \le m - 2 + 2\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}. \end{aligned}$$

If $\alpha_0 = 1$, then $\alpha_1 \ge 1$ and Theorem 3.6 gives

$$\begin{aligned} GA(G) &\le m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \\ &\le m - 2 - \alpha_2 + \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \\ &\le m - 2 + \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1}. \end{aligned}$$

If $\alpha_0 = 0$, then $\alpha_1 \ge 2$ and $\alpha_2 \ge 1$, and Theorem 3.6 gives

$$\begin{aligned} GA(G) &\le m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \\ &\le m - 3 + 2\frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}. \end{aligned}$$

Since Corollary 3.5 gives

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

we have

$$GA(G) \le m + \max\Big\{ -2 + \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1}\,,\ -3 + \frac{4\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \Big\}.$$

Assume now that Δ is an even integer. Let G_2 be the subgraph of G induced by the n_2 vertices with degree Δ in $V(G)$, and denote by m_2 the cardinality of the set of edges of G_2. Handshaking Lemma gives $n_2\Delta - \alpha_0 - \alpha_2 = 2m_2$. Since Δ is an even integer, $\alpha_0 + \alpha_2$ is also an even integer; since G is a connected graph, we have $\alpha_0 + \alpha_2 \ge 1$ and so, $\alpha_0 + \alpha_2 \ge 2$.

If $\alpha_0 \ge 2$, then Theorem 3.6 gives

$$\begin{aligned} GA(G) &\le m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \\ &\le m - 2 + 2\,\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\,. \end{aligned}$$

If $\alpha_0 = 1$, then $\alpha_2 \ge 1$ and Theorem 3.6 gives

$$\begin{aligned} GA(G) &\le m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \\ &\le m - 2 + \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}\,. \end{aligned}$$

If $\alpha_0 = 0$, then $\alpha_2 \ge 2$ and $\alpha_1 \ge 1$, and Theorem 3.6 gives

$$\begin{aligned} GA(G) &\le m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \\ &\le m - 3 + \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + 2\,\frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}\,. \end{aligned}$$

Since

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

we have

$$GA(G) \le m + \max\Big\{ -2 + \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}\,,\ -3 + \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{4\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \Big\}.$$

Finally, assume that δ and Δ are even integers. The previous arguments give $\alpha_0+\alpha_1 \ge 2$ and $\alpha_0 + \alpha_2 \ge 2$.

If $\alpha_0 \ge 2$, then Theorem 3.6 gives

$$\begin{aligned} GA(G) &\le m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \\ &\le m - 2 + 2\,\frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\,. \end{aligned}$$

If $\alpha_0 = 1$, then $\alpha_1, \alpha_2 \geq 1$ and Theorem 3.6 gives

$$\begin{aligned} GA(G) &\leq m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \\ &\leq m - 3 + \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}. \end{aligned}$$

If $\alpha_0 = 0$, then $\alpha_1, \alpha_2 \geq 2$, and Theorem 3.6 gives

$$\begin{aligned} GA(G) &\leq m - \alpha_0 - \alpha_1 - \alpha_2 + \alpha_0 \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \alpha_1 \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \alpha_2 \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \\ &\leq m - 4 + 2\,\frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + 2\,\frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}. \end{aligned}$$

We claim now

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

Assuming that this inequality holds, we have

$$m - 2 + 2\,\frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \leq m - 3 + \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1},$$

$$m - 3 + \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} + \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \leq m - 4 + 2\,\frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + 2\,\frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1},$$

and we conclude

$$GA(G) \leq m - 4 + \frac{4\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{4\sqrt{\Delta(\Delta-1)}}{2\Delta-1}.$$

Therefore, in order to finish the proof, it suffices to show

$$\begin{gathered} 1 + \frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \leq \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}, \\ u\Big(\frac{\delta}{\delta+1}\Big) + u\Big(\frac{\Delta-1}{\Delta}\Big) \geq 1 + u\Big(\frac{\delta}{\Delta}\Big), \end{gathered}$$

where $u(t) = \frac{2\sqrt{t}}{1+t}$ is the function in Lemma 3.8. Since u is an increasing function in $[0,1]$ and $\Delta \geq \delta + 2$, we have

$$u\Big(\frac{\Delta-1}{\Delta}\Big) \geq u\Big(\frac{\delta+1}{\delta+2}\Big), \qquad u\Big(\frac{\delta}{\delta+2}\Big) \geq u\Big(\frac{\delta}{\Delta}\Big).$$

Hence, it suffices to show

$$u\Big(\frac{\delta}{\delta+1}\Big) + u\Big(\frac{\delta+1}{\delta+2}\Big) \geq 1 + u\Big(\frac{\delta}{\delta+2}\Big), \tag{1}$$

for every $\delta \geq 1$.

One can check that (1) holds for $\delta = 1, 2, 3$. Let us prove that it holds for $\delta \geq 4$. Since $\delta \geq 4$, we have

$$3(\delta+1)^2 \geq 2(\delta+2)^2,$$
$$\frac{3/10}{(\delta+2)^2} \geq \frac{1/5}{(\delta+1)^2},$$
$$2 - \frac{1/5}{(\delta+1)^2} - \frac{1/5}{(\delta+2)^2} \geq 2 - \frac{1/2}{(\delta+2)^2}.$$

Since $(\delta+1)/(\delta+2) \geq \delta/(\delta+1) \geq 4/5 > 0.6$, Lemma 3.8 gives

$$\begin{aligned} u\Big(\frac{\delta}{\delta+1}\Big) + u\Big(\frac{\delta+1}{\delta+2}\Big) &\geq 1 - \frac{1}{5}\Big(\frac{\delta}{\delta+1} - 1\Big)^2 + 1 - \frac{1}{5}\Big(\frac{\delta+1}{\delta+2} - 1\Big)^2 \\ &= 2 - \frac{1/5}{(\delta+1)^2} - \frac{1/5}{(\delta+2)^2} \geq 2 - \frac{1/2}{(\delta+2)^2} \\ &= 1 + 1 - \frac{1}{8}\Big(\frac{\delta}{\delta+2} - 1\Big)^2 \geq 1 + u\Big(\frac{\delta}{\delta+2}\Big). \end{aligned}$$

These inequalities give (1) for $\delta \geq 4$, and the proof is finished. ∎

We can deduce from Theorem 3.9 the following result with a nicer statement.

Corollary 3.10. *Let G be a connected graph with m edges, minimum degree δ and maximum degree $\Delta > \delta + 1$.*

(1) *If δ is an even integer, then*

$$GA(G) \leq m - 1 + \frac{2\sqrt{\delta(\delta+1)}}{2\delta+1}.$$

(2) *If Δ is an even integer, then*

$$GA(G) \leq m - 1 + \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}.$$

(3) *If δ and Δ are even integers, then*

$$GA(G) \leq m - 4 + \frac{4\sqrt{\delta(\delta+1)}}{2\delta+1} + \frac{4\sqrt{\Delta(\Delta-1)}}{2\Delta-1}.$$

Proof. Since

$$\frac{2\sqrt{\Delta\delta}}{\Delta+\delta} \leq 1,$$

we have

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

Since

$$\frac{2\sqrt{\delta(\delta+1)}}{2\delta+1} \leq 1, \qquad \frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1} \leq 1,$$

we have

$$3-\frac{4\sqrt{\delta(\delta+1)}}{2\delta+1}-\frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}\geq 1-\frac{2\sqrt{\delta(\delta+1)}}{2\delta+1}.$$

Thus, Theorem 3.9 gives (1).

Similarly,

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

and

$$3-\frac{2\sqrt{\delta(\delta+1)}}{2\delta+1}-\frac{4\sqrt{\Delta(\Delta-1)}}{2\Delta-1}\geq 1-\frac{2\sqrt{\Delta(\Delta-1)}}{2\Delta-1}.$$

Thus, Theorem 3.9 gives (2). ■

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