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On Geometric–Arithmetic Index of Graphs

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Abstract

Let $G = (V, E)$ be a simple connected graph (molecular graph) with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let d_i be the degree of vertex v_i for $i = 1, 2, \ldots, n$. In [1], Vukičević et al. defined a new topological index, named "geometric–arithmetic index" of a graph G, denoted by $GA(G)$ and is defined by

$$GA(G) = \sum_{v_i v_j \in E(G)} \frac{2\sqrt{d_i\, d_j}}{d_i + d_j} .$$

In this paper we obtain the lower and upper bounds on $GA(G)$ of a connected graph and characterize graphs for which these bounds are best possible. Moreover, we give Nordhaus–Gaddum–type results for $GA(G)$ of the graph and its complement, and characterize extremal graphs.

1 Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. Let d_i be the degree of vertex v_i for $i = 1, 2, \ldots, n$. The maximum vertex degree is denoted by Δ, the minimum by δ and the minimum non-pendent vertex degree δ_1. The second Zagreb index $M_2(G)$ is equal to the sum of the products of the degrees of pairs of adjacent vertices of the underlying molecular graph G, that is, $M_2(G) = \sum\limits_{v_i v_j \in E(G)} d_i\, d_j$.

Graph theory has provided chemist with a variety of useful tools, such as topological indices [2]. Molecules and molecular compounds are often modeled by molecular graph.

Topological indices of molecular graphs are one of the oldest and most widely used descriptors in QSPR/QSAR research. Recently, people are studying various topological descriptors, like Zagreb indices [3], Randić connectivity index [4], modified Zagreb indices [5], etc. Beside above-mentioned there are other topological descriptors based on end vertex degrees of edges of graph that have found some applications in QSPR/QSAR research [6–16]. The geometric–arithmetic index has a number of interesting properties in [1]. The lower and upper bounds of the geometric–arithmetic index of a connected graph and characterize graphs for which these bounds are best possible in [1].

In [1], Vukičević et al. defined a new topological index "geometric–arithmetic index" of a graph G, denoted by $GA(G)$ and is defined by

$$GA(G) = \sum_{v_i v_j \in E(G)} \frac{2\sqrt{d_i\, d_j}}{d_i + d_j} \,. \tag{1}$$

Let $G = (V(G), E(G))$. If $V(G)$ is the disjoint union of two nonempty sets $V_1(G)$ and $V_2(G)$ such that every vertex in $V_1(G)$ has degree r and every vertex in $V_2(G)$ has degree s, then G is (r, s)-semiregular graph. When $r = s$, is called a regular graph. If (r, s)-semiregular graph is a tree, then it is called $(r, 1)$-semiregular tree. Denote, as usual, by $K_{1,n-1}$, P_n and K_n the star, path and complete graph on n vertices, respectively.

In this paper, we obtain the lower and upper bounds on $GA(G)$ of a connected graph, and characterize graphs for which these bounds are best possible. Moreover, we give the Nordhaus–Gaddum-type result for $GA(G)$ of the graph and its complement, and characterize extremal graphs. The bounds of a descriptor are important information of a molecule (graph) in the sense that they establish the approximate range of the descriptor in terms of molecular structural parameters.

2 Lower and upper bounds on geometric–arithmetic index

In [1] the following lower and upper bounds for $GA(G)$ and $GA(T)$ were established:

Lemma 2.1. *[1] Let G be a simple connected graph with n vertices, then*

$$\frac{2(n-1)^{3/2}}{n} \le GA(G) \le \binom{n}{2} . \tag{2}$$

Lower bound is achieved if and only if $G \cong K_{1,n-1}$ and upper bound is achieved if and only if $G \cong K_n$.

Lemma 2.2. *[1] Let T be a tree with $n > 2$ vertices, then*

$$\frac{2(n-1)^{3/2}}{n} \le GA(T) \le \frac{4\sqrt{2}}{3} + n - 3\,. \tag{3}$$

Lower bound is achieved if and only if $T \cong K_{1,n-1}$ and upper bound is achieved if and only if $T \cong P_n$.

Now we give lower and upper bounds on $GA(G)$ of a graph G in terms of number of edges m, maximum vertex degree Δ and minimum vertex degree δ. First we obtain the lower bound on $GA(G)$ of a graph G.

Theorem 2.3. *Let G be a simple connected graph of m edges with maximum vertex degree Δ and minimum vertex degree δ. Then*

$$GA(G) \ge \frac{2m\sqrt{\Delta\delta}}{\Delta+\delta}\,, \tag{4}$$

with equality holding in (4) if and only if G is isomorphic to a regular graph or G is isomorphic to a bipartite semiregular graph.

Proof: Since $\dfrac{\Delta}{\delta} \ge \dfrac{d_i}{d_j} \ge \dfrac{\delta}{\Delta}$ for all $v_i, v_j \in V(G)$, we have

$$\begin{aligned} \left(\sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}}\right)^2 &= \left(\sqrt{\frac{d_i}{d_j}} - \sqrt{\frac{d_j}{d_i}}\right)^2 + 4 \\ \le \quad \left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}}\right)^2 + 4 &= \left(\sqrt{\frac{\Delta}{\delta}} + \sqrt{\frac{\delta}{\Delta}}\right)^2 . \end{aligned} \tag{5}$$

Using (5) in (1), we get the required result (4).

Moreover, the equality holds in (4) if and only if

$$\frac{d_i}{d_j} = \frac{\Delta}{\delta} \quad \text{for any } v_iv_j \in E(G) \text{ and } d_i \ge d_j$$

that is,

$$d_i = \Delta\,,\; d_j = \delta \text{ for any edge } v_iv_j \in E(G) \text{ and } d_i \ge d_j$$

that is, G is a regular graph or G is a bipartite semiregular graph, as G is connected.

Conversely, one can see easily that the equality holds in (4) for regular graph or bipartite semiregular graph. $\square$

Remark 2.4. *Our lower bound (4) is better than the lower bound in (2). Since G is connected, we have to show that*

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

that is,

$$[\delta(n-1)-\Delta]\left[\frac{1}{\delta}-\frac{1}{(n-1)\Delta}\right] \geq 0$$

which, evidently, is always obeyed.

Lemma 2.5. *(Ozeki inequality) [17] Let $(a_1,a_2,\ldots,a_n)$ and $(b_1,b_2,\ldots,b_n)$ be two positive n-tuples such that there exist positive numbers M_1,m_1,M_2,m_2 satisfying:*

$$0<m_1\leq a_i\leq M_1\,,\quad 0<m_2\leq b_i\leq M_2\,,\quad 1\leq i\leq n\;.$$

Then

$$\sum_{i=1}^{n}a_i^2\sum_{i=1}^{n}b_i^2-\left(\sum_{i=1}^{n}a_ib_i\right)^2 \leq \frac{1}{4}n^2(M_1M_2-m_1m_2)^2\,. \tag{6}$$

A vertex of a graph is said to be pendent if its neighborhood contains exactly one vertex. An edge of a graph is said to be pendent if one of its vertices is a pendent vertex. Now we give a lower bound on $GA(G)$ of a graph G.

Theorem 2.6. *Let G be a simple connected graph of order n $(n>2)$, m edges with maximum vertex degree Δ, minimum non-pendent vertex degree δ_1 and degree sequence $d_1,d_2,\ldots,d_n$. Then*

$$GA(G)\geq\frac{2p\sqrt{\Delta}}{\Delta+1}+$$

$$\sqrt{\mu^2-\frac{\mu}{4\delta_1^2}\left(\sum_{i=1}^{n}d_i^3-2M_2(G)-p(\delta_1-1)^2\right)-\frac{\mu^2}{4}\left(1-\frac{2\sqrt{\Delta\delta_1}}{\Delta+\delta_1}\right)^2} \tag{7}$$

where p is the number of pendent vertices in G, $\mu=m-p$ is the number of non-pendent edges, and $M_2(G)$ is the second Zagreb index of G. Moreover, the equality holds in (7) if and only if G is isomorphic to a regular graph or G is isomorphic to a $(\Delta,1)$-semiregular graph.

Proof: For $\delta_1\leq d_i,d_j\leq\Delta$, we have

$$\frac{2\sqrt{\Delta\delta_1}}{\Delta+\delta_1}\leq\frac{2\sqrt{d_id_j}}{d_i+d_j}\leq 1\,,\quad\text{by (5).} \tag{8}$$

Since

$$\frac{2\sqrt{d_i d_j}}{d_i+d_j} = \sqrt{1-\left(\frac{d_i-d_j}{d_i+d_j}\right)^2}$$

and μ is the number of non-pendent edges in G, using (6) we have

$$\begin{aligned}\left(\sum_{v_iv_j\in E(G),d_i,d_j\neq 1}\frac{2\sqrt{d_id_j}}{d_i+d_j}\right)^2 &\geq \mu \sum_{v_iv_j\in E(G),d_i,d_j\neq 1}\left(1-\left(\frac{d_i-d_j}{d_i+d_j}\right)^2\right)\\ &- \frac{\mu^2}{4}\left(1-\frac{2\sqrt{\Delta\delta_1}}{\Delta+\delta_1}\right)^2 \quad \text{by (8)}\ . \qquad (9)\end{aligned}$$

Now,

$$\begin{aligned}\sum_{v_iv_j\in E(G),d_i,d_j\neq 1}\left(1-\left(\frac{d_i-d_j}{d_i+d_j}\right)^2\right) &\geq \mu-\frac{1}{4\delta_1^2}\sum_{v_iv_j\in E(G),d_i,d_j\neq 1}(d_i-d_j)^2\\ &\geq \mu-\frac{1}{4\delta_1^2}\left(\sum_{i=1}^n d_i^3-2M_2(G)-p(\delta_1-1)^2\right). \quad (10)\end{aligned}$$

Using (10) in (9), we get

$$\sum_{v_iv_j\in E(G),d_i,d_j\neq 1}\frac{2\sqrt{d_i\,d_j}}{d_i+d_j} \geq$$

$$\sqrt{\mu^2-\frac{\mu}{4\delta_1^2}\left(\sum_{i=1}^n d_i^3-2M_2(G)-p(\delta_1-1)^2\right)-\frac{\mu^2}{4}\left(1-\frac{2\sqrt{\Delta\delta_1}}{\Delta+\delta_1}\right)^2}\ . \qquad (11)$$

Thus

$$GA(G) = \sum_{v_iv_j\in E(G),d_i=1}\frac{2\sqrt{d_j}}{d_j+1}+\sum_{v_iv_j\in E(G),d_i,d_j\neq 1}\frac{2\sqrt{d_i\,d_j}}{d_i+d_j}\ . \qquad (12)$$

For $2\leq d_j\leq\Delta$ we have

$$\frac{\sqrt{d_j}}{d_j+1}\geq\frac{\sqrt{\Delta}}{\Delta+1}\ .$$

By (11) and using above result in (12), we get the required result (7).

Now suppose that equality in (7) holds. Then all inequalities in the above argument must be equalities. In particular, from (10), we get

$$d_i=d_j=\delta_1 \quad \text{for any } v_iv_j\in E(G)\,,\ d_i,d_j\neq 1\,,\ m-p>0\,.$$

Also, we have

$$d_j=\Delta \quad \text{for } v_iv_j\in E(G)\,,\ d_i=1\,.$$

If $m = p$, then we have $n-1 \leq m = p \leq n-1$, as G is connected. Hence G is isomorphic to a $(n-1,1)$-semiregular graph. Otherwise, $m > p$. When $p = 0$, G is isomorphic to a regular graph. When $p \neq 0$, G is isomorphic to a $(\Delta, 1)$-semiregular graph, as G is connected.

Conversely, one can see easily that the equality holds in (7) for $(\Delta, 1)$-semiregular graph or regular graph. □

Corollary 2.7. *Let G be a simple connected graph of order n $(n > 2)$, m edges with maximum vertex degree Δ, minimum vertex degree δ and degree sequence $d_1, d_2, \ldots, d_n$. Then*

$$GA(G) \geq \sqrt{m^2 - \frac{m}{4\delta^2}\left(\sum_{i=1}^{n} d_i^3 - 2M_2(G)\right) - \frac{m^2}{4}\left(1 - \frac{2\sqrt{\Delta\delta}}{\Delta+\delta}\right)^2}\,, \tag{13}$$

where $M_2(G)$ is the second Zagreb index of G. Moreover, the equality holds in (13) if and only if G is isomorphic to a regular graph.

Proof: The proof follows directly from Theorem 2.6. □

Corollary 2.8. *Let T be a tree of order n $(n > 2)$ with maximum vertex degree Δ, minimum non-pendent vertex degree δ_1 and degree sequence $d_1, d_2, \ldots, d_n$. Then*

$$GA(T) \geq \frac{2p\sqrt{\Delta}}{\Delta+1} +$$

$$\sqrt{\mu^2 - \frac{\mu}{4\delta_1^2}\left(\sum_{i=1}^{n} d_i^3 - 2M_2(T) - p(\delta_1 - 1)^2\right) - \frac{\mu^2}{4}\left(1 - \frac{2\sqrt{\Delta\delta_1}}{\Delta+\delta_1}\right)^2} \tag{14}$$

where p and $\mu = n - p - 1$ are the number of pendent and non-pendent vertices in T, respectively, and $M_2(T)$ is the second Zagreb index of T. Moreover, the equality holds in (14) if and only if T is isomorphic to a $(\Delta, 1)$-semiregular tree.

Corollary 2.9. *Let T be a tree of order n $(n > 2)$ with maximum vertex degree Δ. Then*

$$GA(T) \geq \frac{2p\sqrt{\Delta}}{\Delta+1}\,. \tag{15}$$

Moreover, the equality holds in (15) if and only if $T \cong K_{1,n-1}$.

Proof: From (14), we get the required result (15). Moreover, the equality holds in (15) if and only if $n-p-1=0$, that is, $p=n-1$, that is, $T \cong K_{1,n-1}$. $\square$

Now we give an upper bound on $GA(G)$ of a graph G.

Theorem 2.10. *Let G be a simple connected graph of m edges with maximum vertex degree Δ, minimum non-pendent vertex degree δ_1 and degree sequence $d_1, d_2, \ldots, d_n$. Then*

$$GA(G) \leq \frac{2p\sqrt{\delta_1}}{\delta_1+1} + \sqrt{(m-p)\left(m-p-\frac{1}{4\Delta^2}\left(\sum_{i=1}^{n} d_i^3 - 2M_2(G) - p(\Delta-1)^2\right)\right)} \tag{16}$$

where p is the number of pendent vertices in G and $M_2(G)$ is the second Zagreb index of G. Moreover, the equality holds in (16) if and only if G is isomorphic to a regular graph or G is isomorphic to a $(\Delta,1)$-semiregular graph.

Proof: For each edge $v_iv_j \in E(G)$, $d_i = 1$ and $d_j \geq \delta_1 \geq 2$, we have

$$\frac{2\sqrt{d_j}}{d_j+1} \leq \frac{2\sqrt{\delta_1}}{\delta_1+1}\,. \tag{17}$$

Since $m-p$ is the number of non-pendent edges in G, by Cauchy-Schwarz inequality,

$$\left[\sum_{v_iv_j \in E(G), d_i, d_j \neq 1} \sqrt{1-\left(\frac{d_i-d_j}{d_i+d_j}\right)^2}\right]^2 \leq (m-p) \sum_{v_iv_j \in E(G), d_i, d_j \neq 1} \left[1-\left(\frac{d_i-d_j}{d_i+d_j}\right)^2\right]$$
$$\leq (m-p)\left[m-p-\frac{1}{4\Delta^2}\left(\sum_{i=1}^{n} d_i^3 - 2M_2(G) - p(\Delta-1)^2\right)\right]\,. \tag{18}$$

Since

$$\frac{2\sqrt{d_i d_j}}{d_i+d_j} = \sqrt{1-\left(\frac{d_i-d_j}{d_i+d_j}\right)^2}$$

using (17) and (18) in (12), we get the required result (16).

Now suppose that equality in (16) holds. Then all inequalities in the above argument must be equalities. In particular, from (18), we get

$$d_i = d_j = \Delta \quad \text{for } v_iv_j \in E(G)\,,\ d_i\,, d_j \neq 1 \text{ and } m > p\,.$$

From equality in (17), we get $d_j = \delta_1$ for $v_iv_j \in E(G)$, $d_i = 1$.

If $m = p$, then G is isomorphic to a $(n-1, 1)$-semiregular graph. Otherwise, $m > p$. When $p = 0$, G is isomorphic to a regular graph. When $p \neq 0$, G is isomorphic to a $(\Delta, 1)$-semiregular graph, as G is connected.

Conversely, one can see easily that the equality holds in (16) for regular graph or $(\Delta, 1)$-semiregular graph. □

Corollary 2.11. *Let G be a simple connected graph of m edges with minimum non-pendent vertex degree δ_1. Then*

$$GA(G) \leq \frac{2p\sqrt{\delta_1}}{\delta_1 + 1} + m - p \tag{19}$$

where p is the number of pendent vertices in G. Moreover, the equality holds in (19) if and only if G is isomorphic to a regular graph or G is isomorphic to a $(\delta_1, 1)$-semiregular graph.

Proof: The proof follows directly from Theorem 2.10. □

Corollary 2.12. *Let T be a tree of order n with minimum non-pendent vertex degree δ_1. Then*

$$GA(T) \leq \frac{4\sqrt{\delta_1}}{\delta_1 + 1} + n - 3 \tag{20}$$

with equality holding in (20) if and only if $G \cong P_n$.

Proof: Let us consider a function

$$f(x) = \frac{2x\sqrt{\delta_1}}{\delta_1 + 1} + n - 1 - x \quad \text{for } 2 \leq x \leq n-1 .$$

We have

$$f^{'}(x) = \frac{2\sqrt{\delta_1}}{\delta_1 + 1} - 1 < 0 \quad \text{as } \delta_1 \geq 2 .$$

Thus $f(x)$ is a decreasing function for $2 \leq x \leq n-1$. By (19), we get the required result (20). Moreover, the equality holds in (20) if and only if $p = 2$, that is, $T \cong P_n$. □

Corollary 2.13. *Let G be a simple connected graph of m edges with maximum vertex degree Δ and degree sequence $d_1, d_2, \ldots, d_n$. Then*

$$GA(G) \leq \sqrt{m\left(m - \frac{1}{4\Delta^2}\left(\sum_{i=1}^{n} d_i^3 - 2M_2(G)\right)\right)} \tag{21}$$

where $M_2(G)$ is the second Zagreb index of G. Moreover, the equality holds in (21) if and only if G is isomorphic to a regular graph.

Proof: The proof follows directly from Theorem 2.10. $\square$

Remark 2.14. *Since*

$$\frac{\sqrt{\delta_1}}{\delta_1 + 1} \leq \frac{\sqrt{2}}{3}$$

our upper bound (20) is better than the upper bound in (3).

Remark 2.15. *Our upper bound (21) is better than the upper bound in (2). The reason is the following:*
From (16), we get

$$\sqrt{m\left(m - \frac{1}{4\Delta^2}\left(\sum_{v_i \in V(G)} d_i^3 - 2M_2(G)\right)\right)} \leq m \leq \binom{n}{2}.$$

Remark 2.16. *The lower and upper bounds given by (7) and (16), respectively, are equal when G is a regular graph or $(\Delta, 1)$-semiregular graph.*

3 Nordhaus–Gaddum-type results for geometric--arithmetic index

For a graph G, the chromatic number $\chi(G)$ is the minimum number of colors needed to color the vertices of G in such a way that no two adjacent vertices are assigned the same color. In 1956, Nordhaus and Gaddum [18] gave bounds involving the chromatic number $\chi(G)$ of a graph G and its complement $\overline{G}$:

$$2\sqrt{n} \leq \chi(G) + \chi(\overline{G}) \leq n + 1 .$$

Motivated by the above results, we now obtain analogous conclusions for the geometric–arithmetic index.

Theorem 3.1. *Let G be a connected graph on n vertices with a connected $\overline{G}$. Then*

$$GA(G) + GA(\overline{G}) \geq \frac{2k}{k^2+1}\binom{n}{2} \tag{22}$$

where $k = \max\left\{\sqrt{\frac{\Delta}{\delta}}, \sqrt{\frac{n-1-\delta}{n-1-\Delta}}\right\}$ *;* Δ, δ *are the maximum vertex degree and minimum vertex degree in* G *, respectively. Moreover, the equality holds in (22) if and only if* G *is isomorphic to a regular graph.*

Proof: We have $\overline{m} = \binom{n}{2} - m$, $\overline{\Delta} = n-1-\delta$ and $\overline{\delta} = n-1-\Delta$, where $\overline{m}$, $\overline{\Delta}$ and $\overline{\delta}$ are the number of edges, maximum vertex degree and minimum vertex degree in $\overline{G}$, respectively. Using (4), we get

$$GA(G) + GA(\overline{G}) \geq \frac{2m\sqrt{\Delta\delta}}{\Delta+\delta} + \frac{(n(n-1)-2m)\sqrt{(n-1-\delta)(n-1-\Delta)}}{2(n-1)-\Delta-\delta} \,. \tag{23}$$

Since

$$k \geq \sqrt{\frac{\Delta}{\delta}} \geq 1 \quad \text{and} \quad 1 - \frac{\sqrt{\delta}}{k\sqrt{\Delta}} \geq 0$$

we have

$$\left(k - \sqrt{\frac{\Delta}{\delta}}\right)\left(1 - \frac{\sqrt{\delta}}{k\sqrt{\Delta}}\right) \geq 0$$

i. e.,

$$\frac{\sqrt{\Delta\delta}}{\Delta+\delta} \geq \frac{k}{k^2+1} \,. \tag{24}$$

Again, since $k \geq \sqrt{(n-1-\delta)/(n-1-\Delta)}$, we have

$$\frac{\sqrt{(n-1-\delta)(n-1-\Delta)}}{2(n-1)-\Delta-\delta} \geq \frac{k}{k^2+1} \,. \tag{25}$$

Using (24) and (25) in (23), we get the required result (22).

By Theorem 2.3, the equality holds in (23) if and only if G is a regular graph, as G and $\overline{G}$ are connected. Moreover, all inequalities in the above argument must be equalities for regular graph. Thus the equality holds in (22) if and only if G is isomorphic to a regular graph. □

Theorem 3.2. *Let G be a connected graph on n vertices with a connected $\overline{G}$. Then*

$$GA(G) + GA(\overline{G}) \leq \binom{n}{2} - p\frac{(\sqrt{\delta_1}-1)^2}{\delta_1+1} - \overline{p}\frac{(\sqrt{\overline{\delta}_1}-1)^2}{\overline{\delta}_1+1} \tag{26}$$

where p , $\overline{p}$ *and* δ_1 , $\overline{\delta}_1$ *are the number of pendent vertices and minimum non-pendent vertex degrees in* G *and* $\overline{G}$ *, respectively. Moreover, the equality holds in (26) if and only if* G *is isomorphic to a regular graph.*

Proof: By (19), we get

$$GA(G) + GA(\overline{G}) \leq m - p + \frac{2p\sqrt{\delta_1}}{\delta_1 + 1} + \overline{m} - \overline{p} + \frac{2\overline{p}\sqrt{\overline{\delta}_1}}{\overline{\delta}_1 + 1} .$$

Since $m + \overline{m} = \binom{n}{2}$, we get the required result (26). By Corollary 2.11, the equality holds in (26) if and only if G is isomorphic to a regular graph. □

Corollary 3.3. *Let* G *be a connected graph on* n *vertices with a connected* $\overline{G}$. *Then*

$$GA(G) + GA(\overline{G}) \leq \binom{n}{2} \tag{27}$$

with equality holding in (27) if and only if G *is isomorphic to a regular graph.*

Proof: The proof follows directly from Theorem 3.2. □

Remark 3.4. *The upper bound of* $GA(G)$ *in (2) is* $\binom{n}{2}$ *, but this is our upper bound for* $GA(G) + GA(\overline{G})$.

Remark 3.5. *The lower and upper bounds given by (22) and (26), respectively, are equal when* G *is a regular graph.*

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