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Multiplicative Geometric-Arithmetic Index

Ivan Gutman
Faculty of Science, University of Kragujevac
Kragujevac, Serbia
gutman@kg.ac.rs

Merve Ascioglu
Department of Mathematics
Faculty of Science, Engineering, Uludag
Gorukle, 16059, Bursa, Turkey
mascioglu@uludag.edu.tr

Ismail Naci Cangul
Department of Mathematics
Faculty of Science, Engineering, Uludag
Gorukle, 16059, Bursa, Turkey
cangul@uludag.edu.tr

Abstract

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. Let d_u be the degree of the vertex $u \in V(G)$. The earlier much studied geometric–arithmetic index of G is $\sum_{uv\in E(G)} \frac{2\sqrt{d_u\, d_v}}{d_u+d_v}$. We now examine its multiplicative version, namely $\prod_{uv\in E(G)} \frac{2\sqrt{d_u\, d_v}}{d_u+d_v}$ and establish some of its main properties.

Key words: Degree (of vertex), Geometric–arithmetic index, Multiplicative geometric–arithmetic index

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1 Introduction

In this paper, we are concerned with simple, undirected and connected graphs. Let G be such a graph, with vertex set $V(G)$ and edge set $E(G)$. Then $|V(G)| = n$ is the order and $|E(G)| = m$ the size of G. If two vertices $u, v \in V(G)$ are connected by an edge

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e, this situation is denoted by $e = uv$. In such a case, u and v are said to be adjacent vertices, whereas the edge $e \in E(G)$ connecting them, incident to u and v.

The degree of a vertex $u \in V(G)$ is denoted by d_u. A vertex of degree one is called a pendent vertex and the edge incident to such a vertex is called a pendent edge.

As usual, we denote by P_n , C_n , S_n , K_n , $K_{r,s}$, and $T_{r,s}$ the path, cycle, star, complete, complete bipartite, and tadpole graphs, respectively.

In the last decades, modeling of real life situations by means of graphs became a popular subject. One of the important application areas of this idea is the chemical graph theory [7, 12]. A molecule can be modeled by a graph by representing its atoms by the vertices, and the chemical bonds by the edges of the underlying graph. The advantage of this is that one can obtain information about physical and chemical properties, chemical documentation, isomer discrimination, molecular complexity, lead optimization, chirality, similarity, QSAR/QSPR studies, drug design, database selection, etc. of the given chemical compound easily by means of a mathematical analysis, instead of time and money consuming laboratory experiments. The pharmaceutical industry especially contributed towards increased interest in molecular descriptors because of the necessity to reduce the expenditure involved in synthesis, in vitro, in vivo, or clinical testing of new medicinal compounds, saving millions of dollars for each new drug.

Chemical application of graph theory often goes via so-called molecular structure descriptors, which are graph invariants reflecting some selected (and chemically relevant) property of the underlying molecule. These are usually referred to as “topological indices”. Several hundreds of such topological indices have been considered in the current literature [9, 10]. Quite a few of these are based on vertex degrees [6].

Among the vertex–degree–based topological indices, the *geometric–arithmetic index* GA was found to be of particular value in practical applications (see, for instance, [2, 4]). It is defined as [13]

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

Note that if $E(G) = \emptyset$, i.e., if G has no edges, then $GA(G) = 0$. Then, for G consisting of disconnected components $G_1, G_2, \ldots, G_p$,

$$GA(G) = \sum_{i=1}^{p} GA(G_i)\,. \tag{1}$$

The GA indices of some familiar simple graph classes are given as follows:

$$GA(G) = \begin{cases} 1 & \text{if } G = P_2 \\ 4\frac{\sqrt{2}}{3} + n - 3 & \text{if } G = P_n,\ n \geq 3 \\ n & \text{if } G = C_n,\ n \geq 3 \\ 2\frac{\sqrt{(n-1)^3}}{n} & \text{if } G = S_n,\ n \geq 2 \\ \binom{n}{2} & \text{if } G = K_n,\ n \geq 2 \\ 2\frac{rs\sqrt{rs}}{r+s} & \text{if } G = K_{r,s},\ r,s \geq 1 \\ 2\left[\frac{1}{2}(r+s-4) + 3\frac{\sqrt{6}}{5} + \frac{\sqrt{2}}{3}\right] & \text{if } G = T_{r,s},\ r \geq 3, s \geq 1\,. \end{cases}$$

Todeschini and Consonni [11] have suggested to study the multiplicative variants of the topological indices. Following this suggestion, in this paper we introduce the multiplicative version of the geometric–arithmetic index, denoted by $GA\Pi(G)$ and defined as

$$GA\Pi = GA\Pi(G) = \prod_{uv \in E(G)} \frac{2\sqrt{d_u\, d_v}}{d_u + d_v}\,. \tag{2}$$

If $E(G) = \emptyset$, then it is both consistent and convenient to assume that $GA\Pi(G) = 1$, in which case in parallel to Eq. (1), we have

$$GA\Pi(G) = \prod_{i=1}^{p} GA\Pi(G_i)\,.$$

Two classical vertex–degree–based graph invariants are the first and second Zagreb indices, defined respectively as

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

Details on their mathematical properties can be found in the recent surveys [1] and the references cited therein. Their multiplicative versions are [3, 5, 8]

$$\Pi_1(G) = \prod_{u \in V(G)} d_u^2 \qquad \text{and} \qquad \Pi_2(G) = \prod_{uv \in E(G)} d_u\, d_v\,. \tag{3}$$

It is well known that the first Zagreb index obeys the relation

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v) \,.$$

Based on this statement, another multiplicative version of the first Zagreb index was conceived as [3]

$$\Pi_1^*(G) = \prod_{uv \in E(G)} (d_u + d_v) \,. \tag{4}$$

Bearing in mind Eqs. (3) and (4), we immediately realize that the multiplicative GA index is related to the multiplicative Zagreb indices as

$$GA\Pi(G) = 2^m \frac{\sqrt{\Pi_2(G)}}{\Pi_1^*(G)} \tag{5}$$

where m is the number of edges of G.

In this paper, we establish the main properties of $GA\Pi$. The structure of our paper is as follows: In Section 2, some general results on $GA\Pi$, related to regularity are obtained. In Section 3, the $GA\Pi$ index of some graph classes is calculated. In Section 4, we give new inequalities on $GA\Pi$.

2 Some general results

In this section, we establish some fundamental properties of the multiplicative geometric–arithmetic index. First of all, note that as the geometric mean is always less than or equal to the arithmetic mean,

$$GA\Pi(G) \leq 1$$

for all graphs G.

Theorem 2.1. Let G be a connected graph. Then

$$GA\Pi(G) = 1$$

holds if and only if G is regular. If G is not connected, then $GA\Pi(G) = 1$ holds if every component of G is a regular graph (not necessarily of the same degree).

The following result gives an alternative way of viewing at $GA\Pi(G)$ in terms of the

$GA\Pi$'s of all edges of the graph G. Let $e = uv$ be an edge of the graph G. Define

$$GA\Pi(G,e) = \frac{2\sqrt{d_u\,d_v}}{d_u + d_v}\,.$$

Then from the multiplicativeness of $GA\Pi$, Eq. (2), we immediately get.

$$GA\Pi(G) = \prod_{e \in E(G)} GA\Pi(G,e)\,. \tag{6}$$

If G is not regular, then we may be able to reduce the calculation of $GA\Pi(G_1)$ to the calculation of $GA\Pi(G_2)$ for a simpler graph G_2 by omitting the edges with equal end-vertex degrees. We namely have

Lemma 2.2. Let $e = uv$ be an edge of G and let $d_u = d_v$. Then

$$GA\Pi(G,e) = 1\,.$$

Lemma 2.2 implies that when calculating $GA\Pi$ for a given graph G, we can omit any edge whose both end vertices have the same degree. In particular, two adjacent vertices of degree 2 may be collapsed into a single such vertex, without altering the value of $GA\Pi$. An example of such a reduction is given in in Figure 1.

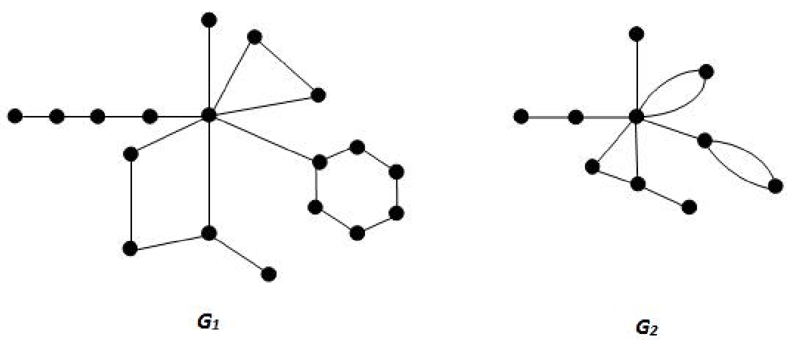

Figure 1: Both graphs have the same $GA\Pi$

3 Effect of edge addition

Theorem 3.1. Let G be a simple connected graph and let x be a vertex of G with $d_x = k > 0$. Let the vertices adjacent to x be $u_1, u_2, \dots, u_k$. Let $y \notin V(G)$. Let $G+e$ be the graph obtained by adding a new pendent edge $e = xy$ to G. Then

$$GA\Pi(G+e) = \frac{2k+2}{(k+2)\sqrt{k}} \cdot \prod_{i=1}^{k} \frac{k+d_{u_i}}{k+1+d_{u_i}} \cdot GA\Pi(G). \tag{7}$$

Proof: In view of the structure of the graph G, its multiplicative geometric–arithmetic index can be written as

$$GA\Pi(G) = \prod_{i=1}^{k} \frac{2\sqrt{k\, d_{u_i}}}{k+d_{u_i}} \cdot GA\Pi(G,*) \tag{8}$$

where, in view of Eq. (6),

$$GA\Pi(G,*) = \prod_{\substack{f \in E(G) \\ f \notin \{xu_1, xu_2, \dots, xu_k\}}} GA\Pi(G,f)\,.$$

In the graph $G+e$, the degree of the vertex x is $k+1$. Therefore,

$$GA\Pi(G+e) = \prod_{i=1}^{k} \frac{2\sqrt{(k+1)\, d_{u_i}}}{k+1+d_{u_i}} \cdot GA\Pi(G+e,xy) \cdot GA\Pi(G,*) \tag{9}$$

where because of $d_y = 1$,

$$GA\Pi(G+e,xy) = \frac{2\sqrt{(k+1)\cdot 1}}{k+1+1} = \frac{2\sqrt{k+1}}{k+2}\,.$$

Dividing (9) and (8) we get

$$\frac{GA\Pi(G+e)}{GA\Pi(G)} = \frac{\prod_{i=1}^{k} \frac{2\sqrt{(k+1)\, d_{u_i}}}{k+1+d_{u_i}} \cdot \frac{2\sqrt{k+1}}{k+2}}{\prod_{i=1}^{k} \frac{2\sqrt{k\, d_{u_i}}}{k+d_{u_i}}}$$

which after rearrangement yields Eq. (7). ∎

Note that each term $\frac{k+d_{u_i}}{k+1+d_{u_i}}$ in Eq. (7) is less than 1 and the ratio $\frac{2k+2}{(k+2)\sqrt{k}}$ is taking decreasing values between 4/3 and 0. So the product $\frac{2k+2}{(k+2)\sqrt{k}} \cdot \prod_{i=1}^{k} \frac{k+d_{v_i}}{k+1+d_{v_i}}$ is greater than 1 only for the first few values of k which means that in vast majority of the cases, $GA\Pi(G+e) \geq GA\Pi(G)$. We first study the case where $GA\Pi(G+e) = GA\Pi(G)$:

Corollary 3.2. Let G and $G+e$ be same as in Theorem 3.1. Then

$$GA\Pi(G+e) = GA\Pi(G) \iff d_x = k = 1\,.$$

Proof: $GA\Pi(G+e) = GA\Pi(G)$ means that

$$\prod_{i=1}^{k} \frac{k+d_{u_i}}{k+1+d_{u_i}} = \frac{(k+2)\sqrt{k}}{2k+2}\,.$$

Each term in the product on the left–hand side (LHS) is clearly less than 1, so $LHS < 1$, implying $RHS < 1$. Moreover, LHS is a rational number implying that $\sqrt{k} \in \mathbb{Z}^+$. This means that k must be an exact square. Let $k = t^2$ for $t \in \mathbb{Z}^+$. Then

$$\frac{(t^2+2)t}{2t^2+2} < 1$$

which is equivalent to

$$f(t) := t^3 - 2t^2 + 2t - 2 < 0\,.$$

As $f(t) < 0$ for $t \leq 0$, $f(t) > 0$ for $t \geq 2$, $f(1) = -1$ and $f(2) = 2$, the function $f(t)$ has its unique real root between $t = 1$ and $t = 2$. As $t \in \mathbb{Z}^+$ we conclude that $f(t) < 0$ iff $t = 1$. In this case $k = 1$. ∎

Note that by Corollary 3.2, it must be $d_{u_1} = 2$. That is, in order to have $GA\Pi(G+e) = GA\Pi(G)$ under the given conditions, the vertex u_1 (the only first neighbor of the vertex x) must be of degree 2. Note that this is in compliance with the conclusions drawn from Lemma 2.2.

We now determine the conditions for $GA\Pi(G+e) > GA\Pi(G)$. Clearly,

$$GA\Pi(G+e) > GA\Pi(G) \iff \frac{2k+2}{(k+2)\sqrt{k}} \cdot \prod_{i=1}^{k} \frac{k+d_{u_i}}{k+1+d_{u_i}} > 1\,.$$

If $k = 1$, then we have

$$\frac{1+d_{u_1}}{2+d_{u_1}} > \frac{3}{4}$$

giving $d_{u_1} > 2$.

If $k = 2$, then the required condition is

$$\frac{(1+d_{u_1})(1+d_{u_2})}{(2+d_{u_1})(2+u_{v_2})} > \frac{2\sqrt{2}}{3}\,. \tag{10}$$

If however $k \geq 3$, then

$$\prod_{i=1}^{k} \frac{1+d_{u_i}}{2+d_{u_i}} > \frac{5\sqrt{3}}{8} = 1,08\ldots$$

which means that it cannot be $GA\Pi(G+e) > GA\Pi(G)$.

In summary, $GA\Pi(G+e) > GA\Pi(G)$ holds if and only if $k = 1$ and $d_{u_1} \geq 3$ or $k = 2$ and relation (10) is satisfied.

In an analogous manner as Theorem 3.1, we can prove its extended version:

Theorem 3.3. Let G be a simple connected graph and let x and y be its two non-adjacent vertices with $d_x = k$, $d_y = \ell$. Let the vertices adjacent to x be $u_1, u_2, \ldots, u_k$. and the vertices adjacent to y be $v_1, v_2, \ldots, v_\ell$. Let $G+e$ be the graph obtained by joining the vertices x and y. Then

$$GA\Pi(G+e) = \frac{2(k+1)(\ell+1)}{(k+\ell+2)\sqrt{k\ell}} \cdot \prod_{i=1}^{k} \frac{k+1+d_{u_i}}{k+d_{u_i}} \cdot \prod_{j=1}^{\ell} \frac{\ell+1+d_{v_j}}{\ell+d_{v_j}} \cdot GA\Pi(G). \tag{11}$$

We naturally want to determine the cases where the $GA\Pi$ index stays invariant under the second type edge addition. From Eq. (11) it immediately follows:

$$GA\Pi(G+e) = GA\Pi(G) \iff \prod_{i=1}^{k} \frac{k+1+d_{u_i}}{k+d_{u_i}} \cdot \prod_{j=1}^{\ell} \frac{\ell+1+d_{v_j}}{\ell+d_{v_j}} = \frac{(k+\ell+2)\sqrt{k\ell}}{2(k+1)(\ell+1)}\,. \tag{12}$$

Corollary 3.4. If $k\ell$ is not an exact square, then $GA\Pi(G+e) \neq GA\Pi(G)$.

As both products on the right–hand side of Eq. (12) are greater than 1, we get:

Corollary 3.5. If

$$\frac{(k+\ell+2)\sqrt{k\ell}}{2(k+1)(\ell+1)} \leq 1$$

then $GA\Pi(G+e) \neq GA\Pi(G)$. In particular, if $k = \ell$, then $GA\Pi(G+e) \neq GA\Pi(G)$.

Corollary 3.6. If

$$\frac{2(k+1)(\ell+1)}{(k+\ell+2)\sqrt{k\ell}} \geq 1$$

then $GA\Pi(G+e) > GA\Pi(G)$.

Let us now determine some values of k and ℓ for which $GA\Pi(G+e) > GA\Pi(G)$. Let $k=1$. Then in order to have $GA\Pi(G+e) > GA\Pi(G)$, it must be

$$\frac{4(\ell+1)}{(\ell+3)\sqrt{\ell}} \geq 1\,.$$

This is equivalent to

$$f(\ell) := \ell^3 - 10\ell^2 - 23\ell - 16 \leq 0\,.$$

The only real root of this cubic equation is $12,024\ldots$. We thus conclude that if $k=1$ and $1 \leq \ell \leq 12$, then $GA\Pi(G+e) > GA\Pi(G)$. Similarly, $GA\Pi(G+e) > GA\Pi(G)$ holds if $k=2$ and $1 \leq \ell \leq 11$; $k=3$ and $1 \leq \ell \leq 12$; $k=4$ and $1 \leq \ell \leq 14$; $k=5$ and $1 \leq \ell \leq 15$; $k=6$ and $1 \leq \ell \leq 16$. Of course one can interchange k and ℓ and obtain symmetric results.

4 $GA\Pi$ of some graphs

In this section, we obtain the $GA\Pi$'s of some well known graph classes. The following result follows by Theorem 2.1 using the regularity of K_n and C_n.

Lemma 4.1.

$$GA\Pi(K_n) = GA\Pi(C_n) = 1\,.$$

We now look at some non-regular graph classes:

Lemma 4.2. For $n \geq 3$,

$$GA\Pi(P_n) = \frac{8}{9}$$

and

$$GA\Pi(P_2) = 1\,.$$

Lemma 4.3.

$$GA\Pi(S_n) = \left(\frac{2\sqrt{n-1}}{n}\right)^{n-1}\,.$$

$GA\Pi(S_n)$ is decreasing. That is if $p > q$, then $GA\Pi(S_p) < GA\Pi(S_q)$.

Lemma 4.4. For a tadpole graph $T_{r,s}$,

$$GA\Pi(T_{r,s}) = \begin{cases} \frac{6\sqrt{2}}{25} & \text{if } s = 1 \\ \frac{64\sqrt{3}}{125} & \text{if } s > 1. \end{cases}$$

Lemma 4.5. For a complete bipartite graph $K_{r,s}$,

$$GA\Pi(K_{r,s}) = \left(\frac{2\sqrt{rs}}{r+s}\right)^{rs} .$$

For any fixed r, $GA\Pi(K_{r,s})$ is decreasing.

5 Bounds on $GA\Pi$

Theorem 5.1. Let G be a simple connected graph and let δ and Δ be the smallest and greatest vertex degrees of G, respectively. Then

$$\frac{\sqrt{\Pi_2(G)}}{\Delta^m} \leq GA\Pi(G) \leq \frac{\sqrt{\Pi_2(G)}}{\delta^m} .$$

Both equalities hold if and only if G is a regular graph.

Proof: By Eq. (5),

$$GA\Pi(G) = \frac{2^m \sqrt{\Pi_2(G)}}{\prod\limits_{uv \in E(G)} (d_u + d_v)} = \frac{\sqrt{\Pi_2(G)}}{\prod\limits_{uv \in E(G)} \frac{1}{2}(d_u + d_v)} .$$

Theorem 5.1 follows from $\delta \leq \frac{1}{2}(d_u + d_v) \leq \Delta$. ■

We now give upper and lower bounds for $GA\Pi(G)$ in terms of the order n, size m and the smallest vertex degree δ:

Theorem 5.2. Let G be a simple connected (n, m)-graph. Then

$$\left(\frac{\delta}{n-1}\right)^m \leq GA\Pi(G) \leq \left(\frac{n-1}{\delta}\right)^m .$$

Both equalities hold if and only if $G \cong K_n$.

Proof: Recall that $\delta \le d_i \le n-1$. Bearing in mind the definition (2), we get

$$\prod_{uv\in E(G)} 2\frac{\sqrt{\delta^2}}{2(n-1)} \le GA\Pi(G) \le \prod_{uv\in E(G)} 2\frac{\sqrt{(n-1)^2}}{2\delta}$$

which implies the result. ∎

Theorem 5.3. Let G be a simple connected graph with p pendent vertices and greatest vertex degree Δ. Then

$$GA\Pi(G) \ge \frac{2^n}{(\Delta+1)^p\,\Delta^{m-p}}\,.$$

Proof: If there are p pendent vertices, then there are p pendent edges and hence $m-p$ non-pendent edges. Thus,

$$\begin{aligned}
GA\Pi(G) &= 2^m \cdot \prod_{\substack{v_iv_j\in E(G)\\ d_j=1}} \frac{\sqrt{d_i}}{d_i+1} \cdot \prod_{\substack{v_iv_j\in E(G)\\ d_i,d_j>1}} \frac{\sqrt{d_i\,d_j}}{d_i+d_j} \\
&\ge 2^m \cdot \prod_{\substack{v_iv_j\in E(G)\\ d_j=1}} \frac{\sqrt{\Delta}}{\Delta+1} \cdot \prod_{\substack{v_iv_j\in E(G)\\ d_i,d_j>1}} \frac{\sqrt{d_i\,d_j}}{2\Delta} \\
&= 2^m \left(\frac{\sqrt{\Delta}}{\Delta+1}\right)^p \cdot \frac{1}{(2\Delta)^{m-p}} \cdot \sqrt{\prod_{\substack{v_iv_j\in E(G)\\ d_i,d_j>1}} d_i\,d_j} \\
&\ge \frac{2^p\Delta^{\frac{3p}{2}-m}}{(\Delta+1)^p} \cdot \sqrt{\frac{\prod_{v_i\in V(G)} d_i^{d_ia_i}}{\Delta^p}} = \frac{2^p}{(\Delta+1)^p\Delta^{m-p}} \cdot \sqrt{\prod_{v_i\in V(G)} d_i^{d_ia_i}} \\
&\ge \frac{2^p}{(\Delta+1)^p\Delta^{m-p}} \cdot \sqrt{\prod_{v_i\in V(G)} 2^{2a_i}} = \frac{2^n}{(\Delta+1)^p\Delta^{m-p}}
\end{aligned}$$

where a_i denotes the number of vertices of degree i. Here we use the fact that $a_2+a_3+\cdots+a_\Delta = n-p$. ∎

Our next result is another lower bound for $GA\Pi$ depending on the order n, size m and number of pendent vertices p:

Theorem 5.4. Let G be a simple connected graph. Then

$$GA\Pi(G) \ge \frac{1}{\sqrt{2^p}} \cdot \left(\frac{16m}{n(n+1)^2}\right)^{m/2}\,.$$

Proof:

$$
\begin{aligned}
GA\Pi(G) &= 2^m \cdot \prod_{\substack{v_iv_j\in E(G)\\ d_j=1}} \frac{\sqrt{d_i\cdot 1}}{d_i+1} \cdot \prod_{\substack{v_iv_j\in E(G)\\ d_i,d_j>1}} \frac{\sqrt{d_i\cdot d_j}}{d_i+d_j} \\
&\geq 2^m \cdot \prod_{\substack{v_iv_j\in E(G)\\ d_j=1}} \frac{\sqrt{n-1}}{n} \cdot \prod_{\substack{v_iv_j\in E(G)\\ d_i,d_j>1}} \frac{\sqrt{2(n-1)}}{n+1} \\
&= \frac{2^{\frac{3m-p}{2}}\sqrt{n-1}^{m}}{n^p\,(n+1)^{m-p}} \geq 2^{\frac{3m-p}{2}} \cdot \left(\frac{\sqrt{n-1}}{n+1}\right)^m \\
&\geq 2^{2m-\frac{p}{2}} \cdot \left(\sqrt{\frac{m}{n(n+1)^2}}\right)^m = \frac{1}{\sqrt{2^p}} \cdot \left(\sqrt{\frac{16m}{n(n+1)^2}}\right)^m .
\end{aligned}
$$

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