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Research Article

Geometric-arithmetic index-energy predicting the physical properties of alkanes

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Abstract: The topological indices play a crucial role in generating the weighted adjacency matrix, which exhibits significant diversity from both theoretical and application perspectives compared to the ordinary adjacency matrix. One such notable weighted matrix is the geometric-arithmetic matrix, generated from the well-known GA (geometric-arithmetic) index. Here, we focus on a comparative study of the GA index and the geometric-arithmetic energy $\mathcal{GAE}$. We establish several tight bounds on $\mathcal{GAE}$ involving various graph invariants and identify the corresponding extremal graphs. Additionally, we compare the correlation of the molecular property Bp (boiling point) with GA and $\mathcal{GAE}$. Our findings reveal that the Bp shows good correlation with $\mathcal{GAE}$ than with GA index. Furthermore, we examine the role of $\mathcal{GAE}$ in explaining different properties of drugs associated with kidney disease.

Keywords: geometric-arithmetic index, geometric-arithmetic matrix, energy, boiling point, QSPR analysis.

AMS Subject classification: 05C50, 05C90, 05C92, 15A18

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1. Introduction

We denote $G = G(V, E)$ a simple, undirected, and connected graph with vertex/node set V and edge set E. The number of elements in V is the *order* and that of in E is the *size* of G. For a, b in V, we denote their adjacency relation by $a \sim b$. For $a \in V$, the number $|\{b : b \sim a\}|$ is the *degree* of a written as d_a. The *maximum degree* (respectively *minimum degree*) is denoted by Δ (respectively δ). If each node in G have the same degree r, then G is said be r-regular graph. For undefined terminology and notation, see [6].

Mathematical descriptors associated with molecular structures, such as topological indices [28], have numerous applications in chemical studies. They play an important role in mathematical/theoretical chemistry specifically in QSAR (quantitative structure-activity relationship) and QSPR (quantitative structure-property relationship) studies. From these descriptors, a special preferences is given to topological indices. Many of them were introduced, by researchers in theoretical/mathematical part of chemistry, on the uses of molecular models involving graphs. They end up in some single numeric number related to molecular properties. During the second half of the last century and since the beginning of the present one, a multitude of such parameters were defined. Most of them knew useful applications in chemistry. For more about the topic, we refer the reader to [15, 16, 37].

The starting point of "theory" of topological indices was the pioneer research work by Wiener [40]. He proposed to use the total of all shortest paths in a molecular graph to estimate saturated hydrocarbon physical properties. Since then, the parameter is called as *Wiener index*. Randić [27] introduced another important molecular descriptor, the *Randić (connectivity) index*, defined as

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

It is the most studied molecular descriptor in mathematical chemistry. A rich literature of more than two thousand research papers and at least five textbooks considers topics related to $Ra(G)$ (see, [14, 20–23]). Other basic topological indices are the *Hosoya (1971) topological index* [19], the *Szeged index* [11], and the *revised Wiener index* (sometimes referred to as *revised Szeged index*) [29].

Motivated by the success of $Ra(G)$, Vukičević and Furtula [39] suggested the *geometric-arithmetic index* (GA index), which was defined as

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

It was observed in [39] that physico-chemical properties are somewhat better correlated with GA than with Ra. It is shown in [3] that an appropriate adjustment of GA index improves considerably its correlation with chemical compound's boiling point.

The Lower and the upper bounds on GA, over the class of trees, were established in [39], where the star S_n was proven to be the extremal tree corresponding to the lower bound, and the path P_n to the upper bound. The paper [41] provides inequalities for GA over the class of graphs (molecular) in terms of order and size. The authors in [41] identified molecular trees with the three smallest values, also second and third largest values of GA index. Inequalities concerning GA in terms of n, m, δ and Δ were established in [32]. The same paper [32] provides a list of relationships between GA and several topological indices: $Ra(G)$, sum connectivity index, first and second Zagreb indices, and harmonic index. Several other extremal results can be found in [1, 8].
The topic of finding lower bounds on GA of graphs with fixed n and δ was considered in [2, 9, 36]. A comparison of the GA index with the spectral index/radius (the largest adjacency eigenvalue) can be seen in [5]. Applications of GA in Chemistry is a topic carried out in [8, 12, 39]. For a survey and recent developments, we invite the reader to consult [2, 3, 8, 30, 38], including the references cited therein.

For a graph G, the *adjacency matrix* $A(G)$ is defined as

$$a_{ij} = \begin{cases} 1 & \text{if } \ v_i \sim v_j, \\ 0 & \text{otherwise.} \end{cases}$$

Introduced in [10] (see also [24]) to quantify the *total π-electron energy* of hydrocarbons, the *energy* of a graph G is given by $\mathcal{E}(G) = \sum\limits_{i=1}^{n} |\ell_i|$, where $\ell_i, \ i = 1, \dots, n$, are the eigenvalues of the adjacency matrix $A(G)$. The energy attracted the attention of many chemical graph theorists as shown by countless paper deal with the topic. For more about the importance/applications of the energy of G and the evolution of related research work over time with an exhaustive list of references, we refer the reader to the discussion [13].

Following the motivation of $\mathcal{E}(G)$, Rodríguez and Sigarreta introduced the geometric-arithmetic matrix ($\mathcal{GA}$ matrix) [32] and, thereafter, the corresponding energy [33]. The $\mathcal{GA}$ matrix (geometric-arithmetic matrix), denoted by $\mathcal{GA}(G)$, is defined [32] as

$$(\mathcal{GA}(G))_{ij} = \begin{cases} \dfrac{2\sqrt{d_v d_u}}{d_u + d_v} & \text{if } \ u \sim v, \\ 0 & \text{otherwise.} \end{cases}$$

We denote the eigenvalues of $\mathcal{GA}$ by $\mu_i, \ i = 1, \dots, n$, which are usually labelled such that $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$. The analysis of $\mathcal{GA}(G)$ and its connection with GA index is given in [31, 32], and other properties along with its Laplacian in [33].

Analogous to $\mathcal{E}(G)$, the geometric-arithmetic energy $\mathcal{GAE}(G)$ of graph G, is defined [33] as

$$\mathcal{GAE} = \mathcal{GAE}(G) = \sum_{i=1}^{n} |\mu_i|.$$

For a r-regular G, $A(G) = \mathcal{GA}(G)$, so it follows that $\mathcal{E}(G) = \mathcal{GAE}(G)$. $\mathcal{GAE}$ of trees was studied in [35, 42], where extremal trees were characterized. Like GA index, the spectral invariants of $\mathcal{GA}$ matrix are helpful in studying quantitative properties of alkanes. A study on correlations between $\mathcal{GAE}$ and some properties like Bp, heats of vaporization and critical temperatures can be found in [18].

In this study, we are interested in a comparison between GA and $\mathcal{GAE}$. In the next section, we give several bounds on $\mathcal{GAE}$ in terms of several invariants and identify related extremal graphs. In Section 3, we statistically compare GA index with $\mathcal{GAE}$. Namely, we compare the correlation of Bp, as a molecular entity, with each of those two topological descriptors. In order to conduct this study, we took into consideration a set of data that included the experimental Bp of saturated hydrocarbons, from [34] (also see [3, 4]). We used computational package AutoGraphiX III [7] (`https://www.gerad.ca/Gilles.Caporossi/agx/AGX/AutoGraphiX.html`) to obtain the numeric values of GA index/energy of chemical/molecular graphs.

2. Bounds on $\mathcal{GAE}$

The *Frobenius norm* of real $m \times n$-matrix M, denoted $\|M\|_F$, is defined as

$$\|M\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n}|m_{ij}|^2} = \sqrt{Tr(M^T M)} = \sqrt{\sum_{i=1}^{\min\{m,n\}} \eta_i^2(M)},$$

where $\eta_i(M)$'s are the *singular values* of M, $Tr(\cdot)$ denotes the trace of a matrix, and M^T is the transpose of M. If M is real symmetric, $\eta_i = |\ell_i|$ and $\|M\|_F^2 = \sum_{i=1}^{n} \ell_i(M)^2 = Tr(M^2)$, where ℓ_i's are the eigenvalues of M, see [25].

First, we recall a result, from [33], that will be utilized later in the paper.

Lemma 1 ([33]). *For $Tr(\mathcal{GA})$ of $\mathcal{GA}$ matrix, we have*

$$\|\mathcal{GA}(G)\|_F^2 = Tr(\mathcal{GA}^2) = 2\sum_{uv\in E(G)} \frac{4d_u d_v}{(d_u + d_v)^2}.$$

We will also use a result from [17].

Lemma 2 ([17]). *For G with spectral radius ℓ_1 and first Zagreb index M_1. Then*

$$\ell_1 \geq \sqrt{\frac{M_1}{n}}.$$

The equality occurs iff (if and only if) G is either regular or semiregular bipartite.

The following result [26] states that the complete graph K_n is the only connected graph with two distinct $\mathcal{GA}$-eigenvalues.

Lemma 3 ([26]). *For a connected G with $n \geq 3$, then $\mathcal{GA}$ has two distinct eigenvalue iff $G \cong K_n$.*

The next lemma is also useful.

Lemma 4 ([26]). *Let G be a connected bipartite graph of order $n \geq 4$. Then G has three distinct $\mathcal{GA}$ eigenvalues iff G is the complete bipartite graph.*

The following result [6], well-known as interlacing theorem, relates the eigenvalues of a real symmetric matrix with its principal submatrices.

Theorem 1 ([6]). *Let M be a real symmetric $\alpha \times \alpha$-matrix and M' its principal submatrix of order β, $(\beta \leq \alpha)$. Then*

$$\ell_{i+\alpha-\beta}(M) \leq \ell_i(N) \leq \ell_i(M), \qquad 1 \leq i \leq \beta.$$

In our proofs, we will use the following function

$$f(y) = y - 1 - \ln y. \tag{2.1}$$

Clearly, $f(y)$ is an increasing function on $[1, \infty)$ and decreasing on $(0, 1]$. Similarly, for $\alpha \geq 2$, the function

$$g(y) = y + \alpha - 1 + \log(|\det(M)|) - \log y \tag{2.2}$$

is increasing on $[1, n]$, where M is any real symmetric matrix and $\log = \log_e = \ln$ is natural log.
A graph is called $\mathcal{GA}$ singular if it has at least one $\mathcal{GA}$ eigenvalue zero, otherwise it is called $\mathcal{GA}$ non-singular. The multiplicity of the $\mathcal{GA}$ eigenvalue zero is the nullity of $\mathcal{GA}$ matrix.

Theorem 2. *Given a connected graph G with $n \geq 2$ and geometric-arithmetic energy $\mathcal{GAE}$. Then following holds*

(i) *If G is $\mathcal{GA}$ non-singular graph, then*

$$\mathcal{GAE} \geq \frac{2\sqrt{\delta\Delta}}{\delta+\Delta}\ell_1 + n - 1 + \log|\det(\mathcal{GA})| - \log\left(\frac{2\sqrt{\delta\Delta}}{\delta+\Delta}\ell_1\right),$$

where ℓ_1 is the spectral index of $A(G)$. The above inequality is an equality iff $G \cong K_n$.

(ii) *If the nullity of $\mathcal{GA}$ matrix is η, then*

$$\mathcal{GAE} \geq \mu_1 + n - \eta - 1 + \log\Big|\prod_{j=2}^{\eta} \mu_i\Big|.$$

with equality iff all the non-zero $\mathcal{GA}$ eigenvalues have modulus 1, except possibly for the $\mathcal{GA}$ spectral radius μ_1.

Proof. As $\mathcal{GA}$ non-singular matrix, so $|\mu_i|$ are positive for $i = 1, \ldots, n$. By Equation (2.1), $f(y) \geq f(1) = 0$ implies that $y \geq 1 + \log y$, with $y > 0$ and equality holds iff $y = 1$. Therefore, with this observation, we have

$$\begin{aligned} \mathcal{GAE} = \mu_1 + \sum_{i=2}^{n} |\mu_i| \geq & \mu_1 + n - 1 + \sum_{i=2}^{n} \log|\mu_i| \\ = & \mu_1 + n - 1 + \log\Big(\prod_{i=2}^{n} |\mu_i|\Big) \\ = & \mu_1 + n - 1 + \log\big|\det(\mathcal{GA})\big| - \log\mu_1. \end{aligned} \tag{2.3}$$

Since, $\mu_1 \geq \frac{2\sqrt{\delta\Delta}}{\delta+\Delta}\ell_1$ (see [33]), with equality iff G is regular. Therefore, $\mathcal{GAE}$ is given by

$$\mathcal{GAE} \geq \frac{2\sqrt{\delta\Delta}}{\delta+\Delta}\ell_1 + n - 1 + \log|\det(\mathcal{GA})| - \log\Big(\frac{2\sqrt{\delta\Delta}}{\delta+\Delta}\ell_1\Big). \tag{2.4}$$

Suppose equality occurs in (2.4). Then by (2.3), $|\mu_2| = |\mu_3| = \cdots = |\mu_n| = 1$. So G has at most three distinct $\mathcal{GA}$ eigenvalues and by Lemma 4, G cannot be cannot be $K_{a,n-a}$ (neither $K_{\underbrace{a,a,a,\ldots,a}_{t}}$, $t \geq 3$) as these graphs are singular. Also G cannot be C_5, since its $\mathcal{GA}$ eigenvalues are

$$\{2, 0.618034, 0.618034, -1.61803, -1.61803\}$$

and they are not of unit modulus (excluding the spectral radius). Thus the only case is that G is regular and has 2 distinct $\mathcal{GA}$ eigenvalues. By Lemma 3, we see that $|\mu_2| = |\mu_3| = \cdots = |\mu_n| = 1$. Hence equality for $G \cong K_n$. Other way, it is easy to verify the equality case for $G \cong K_n$. That proves part **(i)**.
(ii) Let G be $\mathcal{GA}$ singular and let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-\eta}$ be the non-zero $\mathcal{GA}$ eigenvalues of G. Then proceeding as in part **(i)** and applying (2.3), we have

$$\mathcal{GAE} = \mu_1 + \sum_{j=2}^{n-\eta} |\mu_i| \geq \mu_1 + n - \eta - 1 + \sum_{i=2}^{n-\eta} \log|\mu_i| = \mu_1 + n - \eta - 1 + \log\Big|\prod_{j=2}^{n-\eta} \mu_i\Big|,$$

with equality iff $|\mu_2| = |\mu_3| = \cdots = |\mu_{n-\eta}| = 1$. □
The following is a consequence of **(i)** and Lemma 2

Corollary 1. *Let G be a connected graph of order n with geometric-arithmetic energy $\mathcal{GAE}$. Then following holds*

$$\mathcal{GAE} \geq \frac{2\sqrt{\delta\Delta}}{\delta+\Delta}\sqrt{\frac{M_1(G)}{n}} + n - 1 + \log|\det(GA)| - \log\left(\frac{2\sqrt{\delta\Delta}}{\delta+\Delta}\sqrt{\frac{M_1(G)}{n}}\right),$$

with equality iff $G \cong K_n$.

Theorem 3. *Given a connected graph G of order n with geometric-arithmetic energy $\mathcal{GAE}$, and let $\|\mathcal{GA}(G)\|_F^2$ be the Frobenius norm of $\mathcal{GA}(G)$. Then*

$$\mathcal{GAE} \geq \sqrt{\|\mathcal{GA}(G)\|_F^2 + 2\binom{n}{2}\Big(\det(\mathcal{GA})\Big)^{\frac{2}{n}}}.$$

Proof. By using arithmetic and geometric mean inequality and Lemma 1, we get

$$\begin{aligned}\Big(\sum_{i=1}^{n}|\mu_i|\Big)^2 &= \sum_{i=1}^{n}\mu_i^2 + \sum_{i\neq j, 1\leq i,j\leq n}|\mu_i||\mu_j| \\ &= \|\mathcal{GA}(G)\|_F^2 + n(n-1)\Big(\prod_{i\neq j,1\leq i,j\leq n}|\mu_i||\mu_j|\Big)^{\frac{1}{n(n-1)}} \\ &= \|\mathcal{GA}(G)\|_F^2 + 2\binom{n}{2}\Big(\prod_{i\neq j,1\leq i,j\leq n}|\mu_i||\mu_j|\Big)^{\frac{1}{n(n-1)}} \\ &= \|\mathcal{GA}(G)\|_F^2 + 2\binom{n}{2}\Big(\prod_{i=1}^{n}(\mu_i)^{2(n-1)}\Big)^{\frac{1}{n(n-1)}} \\ &= \|\mathcal{GA}(G)\|_F^2 + 2\binom{n}{2}\Big(\prod_{i=1}^{n}\mu_i\Big)^{\frac{2}{n}} \\ &= \|\mathcal{GA}(G)\|_F^2 + 2\binom{n}{2}\Big(\det(\mathcal{GA})\Big)^{\frac{1}{n(n-1)}}.\end{aligned}$$

Therefore,

$$\mathcal{GAE} \geq \sqrt{\|\mathcal{GA}(G)\|_F^2 + 2\binom{n}{2}\Big(\det(\mathcal{GA})\Big)^{\frac{2}{n}}}.$$

□

Using the fact that $\|\mathcal{GA}(G)\|_F^2 \geq \frac{4\sqrt{\delta\Delta}}{\delta+\Delta}GA(G)$ with equality iff G is either regular or (δ,Δ)-biregular, we have a consequence of above result.

Corollary 2. *Given a connected G with n nodes and geometric-arithmetic energy $\mathcal{GAE}$, let $GA(G)$ be its geometric-arithmetic index. Then*

$$\mathcal{GAE} \geq \sqrt{\frac{4\sqrt{\delta\Delta}}{\delta+\Delta}GA(G) + 2\binom{n}{2}\Big(\det(\mathcal{GA})\Big)^{\frac{2}{n}}}.$$

Next, we obtain some spectral bounds and use them in obtaining bounds for the $\mathcal{GA}$ energy of graph.
If $X \neq 0$ is any vector, then by Rayleigh principle, we have $\mu_1(\mathcal{GA}(G)) \geq \frac{X^T \mathcal{GA}(G) X}{X^T X}$, with equality iff is the eigenvector belonging to μ_1. In particular, choosing $X = \frac{1}{\sqrt{n}}(1,1,\ldots,1)^T$, we obtain

$$\mu_1 \geq \frac{1}{\sqrt{n}}\left(\sum_{1\sim j}\frac{2\sqrt{d_1 d_j}}{d_1+d_j}, \sum_{2\sim j}\frac{2\sqrt{d_2 d_j}}{d_2+d_j}, \ldots, \sum_{n\sim j}\frac{2\sqrt{d_2 d_j}}{d_2+d_j}\right)X^T = \frac{2GA(G)}{n}. \tag{2.5}$$

It is easy to prove that equality holds iff the sum of every row of $\mathcal{GA}(G)$ is equal to some constant.
Also, with $C = \frac{1}{\sqrt{n}}(1,1,\ldots,1)^T$, we can write

$$\mu_1 = \sqrt{\mu_1(\mathcal{GA}(G))^2} = \sqrt{X^T(\mathcal{GA}(G))^2 X} \geq \sqrt{C^T(\mathcal{GA}(G))^2 C},$$

which after simplification gives us

$$\mu_1 \geq \sqrt{\frac{1}{n}\sum_{i=1}^{n}\sum_{i\sim j}\frac{2\sqrt{d_i d_j}}{d_i+d_j}} = \sqrt{\frac{1}{n}\sum_{i=1}^{n} R_i}, \tag{2.6}$$

where $R_i = \sum\limits_{i\sim j}\frac{2\sqrt{d_i d_j}}{d_i+d_j}$ is the row sum of i-th row of $\mathcal{GA}(G)$. Again equality holds iff $R_1 = R_2 = \cdots = R_n$.
Inequalities (2.5) and (2.6) can also be stated as in the next theorem.
Let $\mathcal{GA}(G) = (g_{ij})_{n\times n}$ be the $\mathcal{GA}$ matrix of G. Denote by $R_i = \sum\limits_{j=1}^{n} g_{ij}$ and $S_i = R_i \sum\limits_{j=1}^{n} g_{ij}$, that is equivalent to $S_i = R_i^2$. Also, consider the sequence $\{S_i^{(1)}, S_i^{(2)}, \ldots, S_i^{(t)}, \ldots\}$ defined as follows:
$S_i^{(1)} = R_i^{\alpha}$ and $S_i^{(t)} = \sum\limits_{i\sim j}\frac{2\sqrt{d_i d_j}}{d_i+d_j}\, S_j^{(t-1)}$, where $t \geq 2$ and α is a real number.

Theorem 4. *Given a connected graph G with n nodes. Then*

$$\mu_1 \geq \sqrt{\frac{1}{\sum\limits_{i=1}^{n}(S_i^{(t)})^2}\sum_{i=1}^{n}(S_i^{t+1})^2}, \tag{2.7}$$

with equality holds iff $\frac{S_1^{(t+1)}}{S_1^{(t)}} = \frac{S_2^{(t+1)}}{S_2^{(t)}} = \cdots = \frac{S_n^{(t+1)}}{S_n^{(t)}}$.

Proof. Let $\mu_1(\mathcal{GA}(G))$ be the largest eigenvalue of the matrix $\mathcal{GA}(G)$ corresponding to the unit Perron eigenvector $X = (x_1, x_2, \ldots, x_n)^T$. Then, considering

$$U = \frac{1}{\sqrt{\sum\limits_{i=1}^{n}(S_i^{(t)})^2}}\left(S_1^{(t)}, S_2^{(t)}, \ldots, S_n^{(t)}\right)^T,$$

we have

$$\mu_1 \geq \sqrt{\mu_1(\mathcal{GA}(G))^2} = \sqrt{X^T(\mathcal{GA}(G))^2 X} \geq \sqrt{U^T(\mathcal{GA}(G))^2 U}.$$

Therefore, we obtain

$$\begin{aligned}\mathcal{GA}(G)U &= \frac{1}{\sqrt{\sum\limits_{i=1}^{n}(S_i^{(t)})^2}}\left(\sum_{1\sim j}\frac{2\sqrt{d_1 d_j}}{d_1+d_j}S_j^{(t)}, \sum_{2\sim j}\frac{2\sqrt{d_2 d_j}}{d_2+d_j}S_j^{(t)}, \ldots, \sum_{n\sim j}\frac{2\sqrt{d_n d_j}}{d_n+d_j}S_j^{(t)}\right)^T\\ &= \frac{1}{\sqrt{\sum\limits_{i=1}^{n}(S_i^{(t)})^2}}\left(S_1^{(t+1)}, S_2^{(t+1)}, \ldots, S_n^{(t+1)}\right)^T.\end{aligned}$$

Now, it follows that

$$\mu_1 \geq \sqrt{\frac{1}{\sum\limits_{i=1}^{n}(S_i^{(t)})^2}\sum_{i=1}^{n}(S_i^{(t+1)})^2}. \tag{2.8}$$

Suppose that equality occurs in (2.8). Then U is an eigenvector of the matrix $\mathcal{GA}(G)$ belonging to μ_1. Therefore, $\mathcal{GA}(G)U = \mu_1 U$ and it follows that $\frac{S_i^{(t+1)}}{S_i^{(t)}}$, for each $i = 1, 2, \ldots, n$. Conversely, assume that $\frac{S_1^{(t+1)}}{S_1^{(t)}} = \frac{S_2^{(t+1)}}{S_2^{(t)}} = \cdots = \frac{S_n^{(t+1)}}{S_n^{(t)}} = c$, that is $K_i^{(t+1)} = cK_i^{(t)}$ for all $i = 1, 2, \ldots, n$. Hence, $S(G)U = cU$, and so U is an eigenvector of $S(G)$ corresponding to the eigenvalue c and $\mu_1 = c$. □

For $\alpha = 1$ and $t = 1$ in the above result, we have the following consequence.

Corollary 3. *Given a connected graph G with n nodes and spectral radius μ_1, we have*

$$\mu_1 \geq \sqrt{\frac{1}{\sum\limits_{i=1}^{n}R_i^2}\sum_{i=1}^{n}S_i^2}, \tag{2.9}$$

with equality holding iff $\frac{S_1}{R_1} = \frac{S_2}{R_2} = \cdots = \frac{S_n}{R_n}$.

The spectral $\mathcal{GA}$ radius bound given by (2.7) is better than bounds (2.5), (2.6) and (2.9) and can be seen as below.

$$\mu_1 \geq \sqrt{\frac{1}{\sum_{i=1}^{n}(S_i^{(t)})^2}\sum_{i=1}^{n}(S_i^{t+1})^2} \geq \sqrt{\frac{1}{\sum_{i=1}^{n}R_i^2}\sum_{i=1}^{n}S_i^2}.$$

Now, using Cauchy-Schrawz inequality and the fact that $S_i = R_i^2$, we have

$$\sqrt{\frac{1}{\sum_{i=1}^{n}R_i^2}\sum_{i=1}^{n}S_i^2} \geq \sqrt{\frac{1}{n\sum_{i=1}^{n}R_i^2}\Big(\sum_{i=1}^{n}S_i\Big)^2} = \sqrt{\frac{1}{n\sum_{i=1}^{n}R_i^2}\Big(\sum_{i=1}^{n}R_i^2\Big)^2}$$
$$= \sqrt{\frac{1}{n}\sum_{i=1}^{n}R_i^2} \geq \sqrt{\frac{1}{n^2}\Big(\sum_{i=1}^{n}R_i\Big)^2} = \frac{2GA(G)}{n}.$$

Theorem 5. *Given a connected graph G with $n \geq 3$ nodes and geometric-arithmetic energy $\mathcal{GAE}$. Then*

$$\mathcal{GAE} \leq \sqrt{\frac{1}{\sum_{i=1}^{n}\left(S_i^{(t)}\right)^2}\sum_{i=1}^{n}\left(S_i^{t+1}\right)^2} + \sqrt{(n-1)\left(\|\mathcal{GA}(G)\|_F^2 - \frac{1}{\sum_{i=1}^{n}\left(S_i^{(t)}\right)^2}\sum_{i=1}^{n}\left(S_i^{t+1}\right)^2\right)}, \tag{2.10}$$

with equality iff either $G \cong K_n$ or G satisfies

$$\frac{S_1^{(t+1)}}{S_1^{(t)}} = \frac{S_2^{(t+1)}}{S_2^{(t)}} = \cdots = \frac{S_n^{(t+1)}}{S_n^{(t)}} = c \geq \sqrt{\frac{1}{n}\|\mathcal{GA}(G)\|_F^2}$$

and has three distinct $\mathcal{GA}$ eigenvalues c and the other two with absolute value

$$\sqrt{\frac{1}{n-1}\left(\|\mathcal{GA}(G)\|_F^2 - c^2\right)}.$$

Proof. By applying the Cauchy-Schwarz inequality to $(|\mu_2|, |\mu_3|, \ldots, |\mu_n|)$ and $(1, 1, \ldots, 1)$, we obtain

$$\sum_{i=2}^{n}|\mu_i| \leq \sqrt{(n-1)\sum_{i=2}^{n}\mu_i^2} = \sqrt{(n-1)\,[\|\mathcal{GA}(G)\|_F^2 - \mu_1^2]}.$$

From the definition of $\mathcal{GAE}$, we obtain

$$\mathcal{GAE} = \mu_1 + \sum_{i=2}^{n}|\mu_i| \leq \mu_1 + \sqrt{(n-1)\,[\|\mathcal{GA}(G)\|_F^2 - \mu_1^2]}.$$

In order to obtain the required inequality, we consider the function

$$F(x) = x + \sqrt{(n-1)\left[\|\mathcal{GA}(G)\|_F^2 - x^2\right]},$$

with $\|\mathcal{GA}(G)\|_F^2 - x^2 \geq 0$. Clearly, $F(x)$ is non-increasing for $x \geq \sqrt{\frac{1}{n}}\|\mathcal{GA}(G)\|_F$. Furthermore, by Cauchy-Schwarz inequality, we recall that $R_i^2 = \left(\sum\limits_{j=1}^{n} g_{ij}\right)^2 \leq n \sum\limits_{i=1}^{n} g_{ij}^2$. It follows that

$$\sum_{i=1}^{n} R_i^2 \leq n \sum_{i=1}^{n}\sum_{j=1}^{n} g_{ij}^2 = 2n \sum_{v_iv_i \in E(G)} \frac{4d_id_j}{(d_i+d_j)^2} = n\|\mathcal{GA}(G)\|_F^2.$$

Also, $S_i = \sum\limits_{i=1}^{n} g_{ij}R_i \geq \sum\limits_{j=1}^{n} g_{ij}^2$ and therefore we get

$$\sum_{i=1}^{n} S_i^2 \geq \sum_{i=1}^{n}\left(\sum_{j=1}^{n} g_{ij}^2\right)^2 \geq \left(2\sum_{v_iv_i \in E(G)} \frac{4d_id_j}{(d_i+d_j)^2}\right)^2 = \left(\|\mathcal{GA}(G)\|_F^2\right)^2.$$

Thus, using the above information, we have

$$\mu_1 \geq \sqrt{\frac{1}{\sum\limits_{i=1}^{n}\left(S_i^{(t)}\right)^2}\sum_{i=1}^{n}\left(S_i^{t+1}\right)^2} \geq \sqrt{\frac{1}{\sum\limits_{i=1}^{n} R_i^2}\sum_{i=1}^{n} S_i^2} \geq \sqrt{\frac{2}{n}\|\mathcal{GA}(G)\|_F^2}.$$

Therefore,

$$SE(G) \leq F(\mu_1) \leq F\left(\sqrt{\frac{1}{\sum\limits_{i=1}^{n}\left(S_i^{(t)}\right)^2}\sum_{i=1}^{n}\left(S_i^{t+1}\right)^2}\right),$$

and Inequality (2.10) follows.
Now, assume that Inequality (2.10) is an equality. Then all the above inequalities occur as equalities. By Theorem 4, we have

$$\mu_1 = \sqrt{\frac{1}{\sum\limits_{i=1}^{n}\left(S_i^{(t)}\right)^2}\sum_{i=1}^{n}\left(S_i^{t+1}\right)^2} \quad \text{iff} \quad \frac{K_1^{(t+1)}}{K_1^{(t)}} = \frac{K_2^{(t+1)}}{K_2^{(t)}} = \cdots = \frac{K_n^{(t+1)}}{K_n^{(t)}}.$$

Also, equality holds in Cauchy-Schwarz's inequality if

$$|\mu_2| = |\mu_3| = \cdots = |\mu_n| = \sqrt{\frac{1}{n-1}\left(\|\mathcal{GA}(G)\|_F^2 - \mu_1^2\right)}.$$

In view of these observations, there are three possibilities.
(i) $\mathcal{GA}(G)$ has exactly one $\mathcal{GA}$ eigenvalue and so G must be K_1.
(ii) $\mathcal{GA}(G)$ has exactly two different $\mathcal{GA}$ eigenvalues and, using Lemma 3, G is necessarily K_n.
(iii) $\mathcal{GA}(G)$ has exactly three different $\mathcal{GA}$ eigenvalues. Thus, $\mu_1 = \sqrt{\frac{1}{\sum_{i=1}^{n}\left(S_i^{(t)}\right)^2}\sum_{i=1}^{n}\left(S_i^{t+1}\right)^2}$. Therefore, for $i = 2, \dots, n$, we have

$$|\mu_i| = \sqrt{\frac{1}{n-1}\left(\|\mathcal{GA}(G)\|_F^2 - \mu_1^2\right)}.$$

As $\frac{S_i^{(t+1)}}{S_i^{(t)}} = c$, for every $i = 1, \dots, n$, so G has three different $\mathcal{GA}$ eigenvalues, c and the other two $\mathcal{GA}$ eigenvalues are $\pm\sqrt{\frac{1}{n-1}\left(\|\mathcal{GA}(G)\|_F^2 - c^2\right)}$. □

For $\alpha = 1$ and $t = 1$ in Theorem 5, we have the following consequence.

Corollary 4. *Given a connected graph G with $n \geq 3$ nodes and geometric-arithmetic energy $\mathcal{GAE}$. Then*

$$\mathcal{GAE} \leq \sqrt{\frac{1}{\sum_{i=1}^{n} R_i^2}\sum_{i=1}^{n} S_i^2} + \sqrt{(n-1)\left(\|\mathcal{GA}(G)\|_F^2 - \sqrt{\frac{1}{\sum_{i=1}^{n} R_i^2}\sum_{i=1}^{n} S_i^2}\right)},$$

with equality as in Theorem 5.

3. Statistical Analysis

The linear regression among the Bp and GA index is shown in Figure 1, using a rounded equation.

$$Bp = 20.951 \cdot GA - 53.184.$$

The linear regression among the Bp and GA energy is displayed in Figure 2, using a rounded equation.

$$Bp = 19.554 \cdot \mathcal{GAE} - 65.45.$$

The boiling point correlation is stronger with $\mathcal{GAE}$, where $R^2 = 0.8045$, than with GA, where $R^2 = 0.7365$, according to the linear regression.

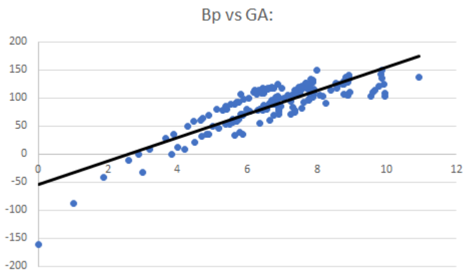
Name	Bp	GA	$\mathcal{GAE}$	Name	Bp	GA	$\mathcal{GAE}$	name	Bp	GA	$\mathcal{GAE}$
n1	-161.5	0	0	1tbc3	80.5	6.34934	7.0812	b2mc3	124	7.74822	9.5684
n2	-88.6	1	2	11ec3	88.6	6.65685	8.40648	1nepec3	106	7.2822	8.09423
n3	-42.1	1.88562	2.66667	1e23mc3	91	6.65685	7.8745	5msbc3	115.5	7.55767	9.00087
c3	-32.8	3	4	1m1ipce	81.5	6.40741	7.37491	1e2pc3	108	7.8048	9.71158
n4	-0.5	2.88562	4.26875	11m23c3	79.1	6.43495	7.41275	ib2mc3	110	7.51726	8.54567
2mn3	-11.7	2.59808	3	12m1ec3	85.2	6.46399	7.53688	11m2pc3	105.9	7.43495	8.45079
1mc3	0.7	3.82562	4.72575	1123mc3	78	6.31154	7.06364	1m12epc3	108.9	7.52057	9.16486
c4	12.6	4	4	1122mc3	76	6.08562	6.1132	11m2ipc3	94.4	7.2444	7.93836
bc110b	8	4.191918	5.04475	1pc4	100.7	6.8822	7.96021	112m2ec3	104.5	7.17124	7.89523
n5	36.0	3.88562	5.28496	1ipc4	92.7	6.69164	6.93809	11223mc3	100.5	7.04551	7.50353
2mn4	27.8	3.65466	4.75743	1e3mc4	89.5	6.70781	7.64739	1ibc4	120.1	7.65123	8.43654
22mn3	9.5	3.2	3.2	1e2mc4	94	6.74822	7.82863	p3mc4	117.4	7.70781	8.70039
1ec3	35.9	4.8822	6.26004	1ec5	103.5	6.8822	8.75056	1sbc4	123	7.74822	8.67622
12mc3	32.6	4.69164	5.4176	13mc5	91.3	6.65123	7.86973	12ec4	119	7.8048	8.97417
11mc3	20.6	4.48562	5.07019	12mc5	95.6	6.69164	7.99061	1234mc4	114.5	7.4641	8.7556
1mc4	36.4	4.82562	5.33647	11mc5	87.9	6.48562	7.57343	1133mc4	86	6.97124	6.66072
c5	49.3	5	6.47214	1mc6	101	6.82562	8.51324	1pc5	131	7.88822	9.89289
bc111p	36	5.87878	4.8	c7	118.4	7	8.98792	1ipc5	126.4	7.69164	9.27737
bc210p	46	5.191918	6.27465	dcprm	102	7.87878	9.49466	1e3mc5	121	7.70781	9.50748
s22p	39	5.77124	6.90157	bc221h	105.5	7.87878	9.49466	1e2mc5	124.7	7.74822	9.57093
mbc110b	33.5	5.63495	5.61729	bc311h	110	7.87878	8.98599	124mc5	115	7.51726	8.55538
n6	68.7	4.88562	6.78967	bc320h	110.5	7.91918	8.83441	1e1mc5	121.5	7.57124	9.32505
2mn5	60.3	4.65466	5.7233	bc410h	116	7.91918	9.56484	123mc5	117	7.55767	9.11632
3mn5	63.3	4.71124	6.44276	s33h	96.5	7.77124	7.54247	113mc5	104.5	7.31124	8.18512
23mn4	58.0	4.4641	5.2915	s24h	98.5	7.77124	8.89805	112mc5	114	7.37837	8.35116
22mn4	49.7	4.28562	5.02417	2mbc310hx	100	7.78521	9.10137	1ec6	131.8	7.8822	10.2545
1pc3	69	5.8822	7.39007	6mbc310hx	103	7.82562	9.10137	14mc6	121.8	7.65123	9.4515
1ipc3	58.3	5.69164	6.79057	mbc211hx	81.5	7.56781	8.02965	13mc6	122.3	7.65123	9.01899
1e2mc3	63	5.74822	7.04683	mbc310hx	92	7.63495	8.65877	12mc6	126.6	7.69164	9.50899
1e1mc3	57	5.57124	6.81901	13mbc111p	71.5	7.25685	6.48808	11mc6	119.5	7.82562	9.75812
123mc3	63	5.59808	6.64575	14mbc210p	74	7.37124	7.77338	1mc7	134	7.82562	9.75812
112mc3	52.6	5.37837	5.76098	11ms22p	78	7.37124	7.95577	c8	149	8	9.65685
1ec4	70.7	5.8822	6.4555	122mbcb	84	7.30209	7.51829	bcprm	129	8.87878	10.7053
13mc4	59	5.65123	6.01691	tc410024h	105	8.87878	10.0424	bc330o	137	8.91918	10.3712
12mc4	62	5.69164	6.71241	tc311024h	107	8.87878	9.37936	bcb	136	8.91918	9.19318
11mc4	53.6	5.48562	5.74727	tc221026h	106	8.87878	10.0542	bc420o	133	8.91918	10.3055
1mc5	71.8	5.82562	7.22919	tc410027h	110	8.95959	10.1976	bc510o	141	8.91918	10.3825
c6	80.7	6	8	tc410013h	107.5	8.78429	9.96783	2mbc221h	125	8.7448	10.1974
bc211hx	71	6.91918	7.43899	tec320h	108.5	9.95959	10.1954	s34o	128	8.77124	9.82054
bcpr	76	6.91918	8.18888	tec410h	104	9.95959	10.6051	7mbc221h	128	8.78521	10.5132
bc220hx	83	6.91918	7.54256	n8	125.7	6.88562	9.32136	2mbc320h	130.5	8.78521	9.48043
bc310hx	81	6.91918	8.28963	2mn7	117.6	6.65466	8.32065	s25o	125	8.77124	10.6422
s23hx	69.5	6.77124	7.32767	3mn7	118.9	6.71124	8.96041	1mbc221h	117	8.56781	9.93121
mbc210p	60.5	6.63495	7.21333	4mn7	117.7	6.71124	8.43855	7mbc410h	138	8.82562	10.574
13mbcb	55	6.37124	6.10369	25mn6	109.1	6.42369	7.74963	1mbc410h	125	8.63495	10.0242
n7	98.5	5.88562	7.86695	3en6	118.5	6.76781	9.08174	33mbc310hx	115	8.4048	9.06533
2mn6	90	5.65466	7.26758	24mn6	109.4	6.48027	7.89365	14mbc211hx	91	8.25685	8.47686
3mn6	92	5.71124	7.45753	23mn6	115.6	6.52068	7.98946	66mbc310hx	126.1	8.53908	9.53
3en5	93.5	5.76781	7.65396	34mn6	117.7	6.57726	8.65587	2244mbcb	104	8.15897	8.20168
24mn5	80.5	5.42369	6.14814	22mn6	106.8	6.28562	7.52897	1223mbcb	105	8.08562	8.08563
23mn5	89.8	5.52068	6.97099	3e2mn5	115.6	6.57726	8.15507	tc510035o	142	9.83837	10.9371
22mn5	79.2	5.28562	5.96691	234mn5	113.5	6.33013	7.49778	tc510024o	149	9.87878	11.1806
33mn5	86.1	5.37124	6.81715	33mn6	112	6.37124	7.78152	tc3210o	136	9.87878	11.3991
223mn4	80.9	5.12179	5.58344	224mn5	99.2	6.05466	6.38464	tc3300o	125	9.91918	10.9833
1bc3	98	6.8822	8.7761	3e3mn5	118.2	6.45685	8.54787	3mtc2210h	120.5	9.78521	10.9733
1sbc3	90.3	6.74822	8.47346	223mn5	109.8	6.17837	7.26012	ds2121o	103	9.54247	10.2184
1m2pc3	93	6.74822	8.10167	233mn5	114.8	6.20741	7.3741	1mtc2210h	111	9.62128	10.9733
12ec3	90	6.8048	8.57986	2233mn4	106.5	5.8	5.89237	ds2022o	115	9.65685	10.74
1m1pc3	84.9	6.57124	7.81517	1pec3	128	7.8822	9.95089	tec330o	137.5	10.9192	12.0475
1m2ipc3	81.1	6.55767	7.5725	1spec3	117.4	7.74822	9.489659				

Table 1. **Bp (Boiling point), GA index and $\mathcal{GAE}$ for alkanes up to order** 8.

Role of topological indices in structure-property modelling are examined by correlating theoretical indices with experimental properties. We performed a statistical analysis to compare the relationship between the geometric-arithmetic energy $\mathcal{GAE}$ and the geometric-arithmetic index GA, on one side, and the boiling point of chemical compounds, on the other. We took into consideration the three most popular regression models: logarithmic, quadratic, and linear.
Our data, which are displayed in Table 1, include the geometric-arithmetic energy $\mathcal{GAE}$ of chemical graphs up to 8 nodes, the geometric-arithmetic index GA, and the boiling point Bp. [34] provided the boiling points; additionally, see [3, 4]. The AutoGraphiX III system was utilized to compute the values of GA and $\mathcal{GAE}$ [7].

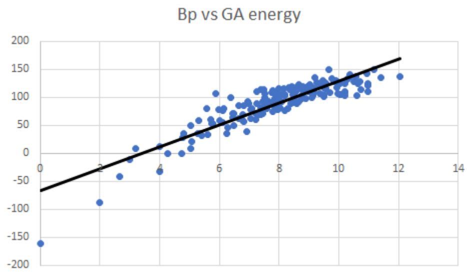
The most important finding is that, in all corresponding regressions, the boiling point Bp and the topological index GA have a stronger correlation with $\mathcal{GAE}$ energy.

The logarithmic regression among the Bp and GA index is shown in Figure 3, with a



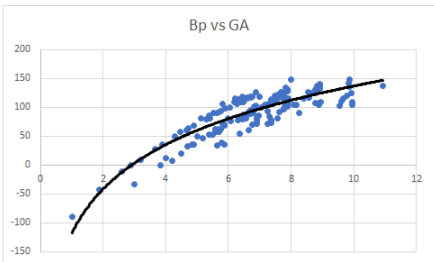
$$Bp = 20.951 \cdot GA - 53.184$$
$$R^2 = 0.7365$$

Figure 1. **Linear regression** Bp **vs** GA**.**



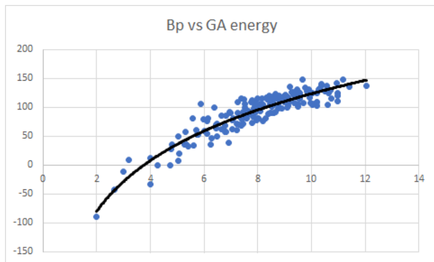
$$Bp = 19.554 \cdot \mathcal{GAE} - 65.45$$
$$R^2 = 0.8045$$

Figure 2. **Linear regression** Bp **vs** $\mathcal{GAE}$**.**



$$Bp = 110.77 \cdot \log(GA) - 117.97$$
$$R^2 = 0.7885$$

Figure 3. Logarithmic regression Bp vs GA.



$$Bp = 126.3 \cdot \log(\mathcal{GAE}) - 167.01$$
$$R^2 = 0.8499$$

Figure 4. Logarithmic regression Bp vs $\mathcal{GAE}$.

rounded equation.

$$Bp = 110.77 \cdot \log(GA) - 117.97.$$

The logarithmic regression among the Bp and GA-energy is displayed in Figure 4, with a rounded equation.

$$Bp = 126.3 \cdot \log(\mathcal{GAE}) - 167.01.$$

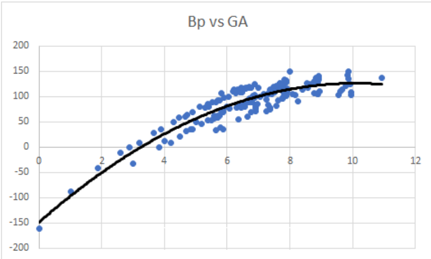
The boiling point correlation is stronger with $\mathcal{GAE}$, where $R^2 = 0.8499$, than with GA, where $R^2 = 0.7885$, according to the logarithmic regression.

The quadratic regression among the Bp and GA index is shown in Figure 5, using a rounded equation.

$$Bp = -2.7035 \cdot (GA)^2 + 54.518 \cdot GA - 148.4.$$

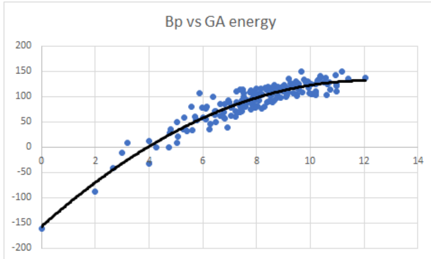
The rounded equation for the quadratic regression between the boiling point and GA-energy is displayed in Figure 6.

$$Bp = -1.9504 \cdot (\mathcal{GAE})^2 + 47.464 \cdot \mathcal{GAE} - 156.9.$$



$Bp = -2.7035 \cdot (GA)^2 + 54.518 \cdot GA - 148.4$
$R^2 = 0.8459$

Figure 5. Quadratic regression Bp vs GA.



$Bp = -1.9504 \cdot (\mathcal{GAE})^2 + 47.464 \cdot \mathcal{GAE} - 156.9$
$R^2 = 0.8836$

Figure 6. Quadratic regression Bp vs $\mathcal{GAE}$.

The boiling point correlation is stronger with $\mathcal{GAE}$, where $R^2 = 0.8836$, than with GA, where $R^2 = 0.8459$, according to the quadratic regression.

The investigation demonstrates that the geometric-arithmetic energy and the boiling point have a stronger correlation in each regression model than does the geometric-arithmetic index. The logarithmic regression provides a stronger correlation when comparing the models. Generally, the geometric-arithmetic energy and the logarithmic regression yield the best correlation with boiling point.

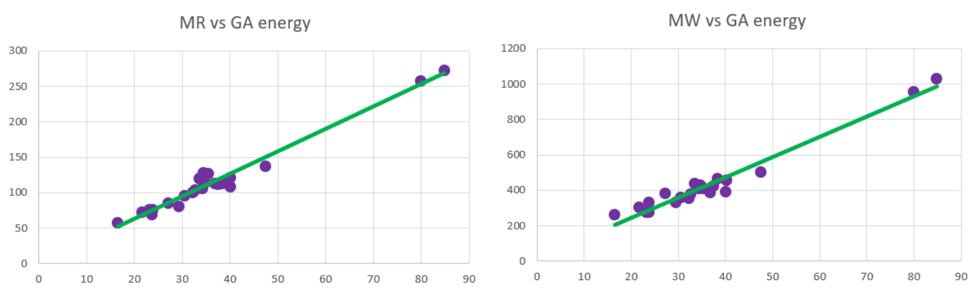
Drug name	GAE	BP	EV	MV	MR	MW
Axitinib	36.7881	668.9	98.3	284.8	113.5	386.47
Bevacizumab	23.2062	472.7	73.6	238.2	76.2	275.343
Belzutifan	27.1643	505.8	81.7	244.7	84.9	383.342
Cabozantinib	47.4417	758.1	110.4	359	137	501.506
Everolimus	79.9542	998.7	165.1	811.2	257.7	958.224
Ipilimumab	40.0186	627.2	92.8	280.9	108.6	394.302
Sorafenib	38.3283	523.3	79.7	319.5	113.1	464.825
Tivozanib	40.1330	550.4	83.1	320	120.9	454.9
Pazopanib	33.5166	728.8	106.4	310.4	120.2	437.518
Lenvatinib	37.4913	627.2	92.8	290.6	112	426.853
Temsirolimus	84.8268	1048.4	173.7	853.1	273.2	1030.3
Mitomycin	29.3781	581.8	87	213.7	80.8	334.327
Cinacalcet	32.2284	440.9	69.8	309.7	100.6	357.412
Paricalcitol	34.5075	564.8	97.5	371.4	128.6	416.63
Doxercalciferol	35.4108	538.7	93.8	404.9	127.3	412.648
Budesonide	34.7006	599.7	102.4	336.4	113.9	430.534
Finerenone	32.6529	554.7	83.6	292.8	103.7	378.424
Azathioprine	23.7418	685.7	96.9	145.4	68.9	277.263
prednisolone	30.4932	570.6	98.3	274.7	95.5	360.444
Cyclophosphamide	16.5372	336.1	57.9	195.7	58.1	261.086
Furosemide	23.7910	582.1	91.5	205.8	75.8	330.744
Ethacrynic acid	21.6127	480	78.4	224.4	72.4	303.138
Dapagliflozin	34.2446	609	95.1	303.1	105.6	408.873

Table 2. **Theoretical values of $\mathcal{GAE}$ and experimental properties of drug compounds.**

Now we examine the role of $\mathcal{GAE}$ in structure-property modelling for several well-known drug compounds. These include Belzutifan, Axitinib, Bevacizumab, Cabozantinib, Everolimus, Ipilimumab, Sorafenib, Tivozanib, Pazopanib, Lenavatinib, Temsirolimus, Mitomycin, Cinacalcet, Paricalcitol, Doxercalciferol, Budesonide, Finerenone, Azathioprine, Prednisolone, Cyclophosphamide, Furosemide, Ethacrynic Acid, and Dapagliflozin. The investigation requires both theoretical and experimental data. The theoretical indices are computed using in-house Matlab code that employs adjacency matrices, and the results are summarized in Table 2. Key properties considered for analysis include enthalpy of vaporization (EV), boiling point (BP), molar volume (MV), molar refractivity (MR), and molecular weight (MW). To evaluate the performance of these indices as structural descriptors, linear, quadratic and logarithmic regression analyses are conducted.
We have observed that the correlation coefficient of $\mathcal{GAE}$ with BP, EV, MV, MR and MW are 0.8839, 0.9151, 0.9593, 0.9849, and 0.9814, respectively. So, $\mathcal{GAE}$ is strongly correlated with MR and MW. Now we investigate linear, quadratic and logarithmic regression relations of $\mathcal{GAE}$ with MR and MW. The linear relation of $\mathcal{GAE}$ with MR and MW are reported below.

$$MR = 3.1736\,\mathcal{GAE} - 0.4991,$$
$$MW = 11.427\,\mathcal{GAE} + 17.728.$$

The linear fittings of GA energy with MR and MW are depicted in Figure 7. The coefficient of determination for this regression relations are 0.97 and 0.963, respectively. The F-statistic values are 549.348, respectively. The significance F values are 1.75×10^{-17} and 1.54×10^{-16}, respectively. The data variance and F-valuer are significantly high. The SF-values is considerably less than 0.05.



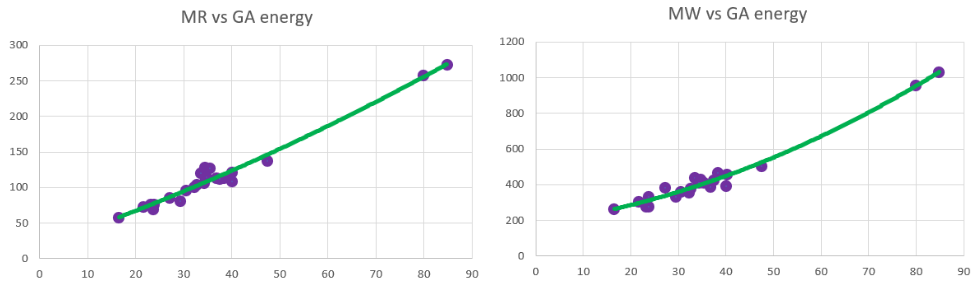
(a) (b)

Figure 7. Linear fitting of GA energy with (a) MR and (b) MW.

The quadratic relation of $\mathcal{GAE}$ with MR and MW are presented below.

$$MR = 0.0081\,\mathcal{GAE}^2 + 2.3301\mathcal{GAE} + 17.447,$$
$$MW = 0.0746\,\mathcal{GAE}^2 + 3.6656\mathcal{GAE} + 182.86.$$

The quadratic fittings of GA energy with MR and MW are depicted in Figure 8. The strong regression is clearly reflected from the Figure 8.



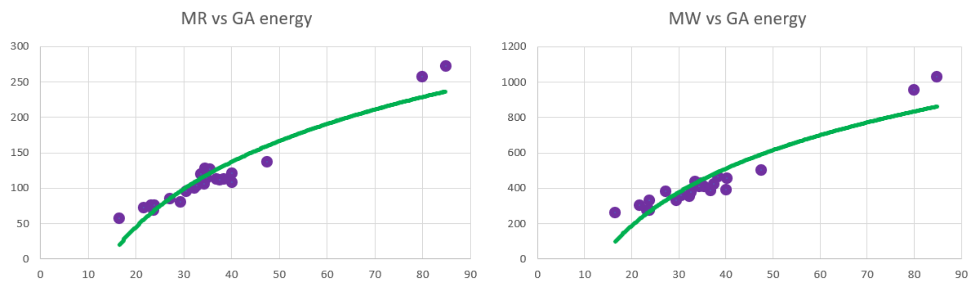
(a) (b)

Figure 8. Quadratic fitting of GA energy with (a) MR and (b) MW.

The logarithmic relation of $\mathcal{GAE}$ with MR and MW are presented below.

$$MR = 132.43\,\mathcal{GAE} - 351.56,$$
$$MW = 466.03\,\mathcal{GAE} - 1208.3.$$

The logarithmic fittings of GA energy with MR and MW are depicted in Figure 9.



(a) (b)

Figure 9. Logarithmic fitting of GA energy with (a) MR and (b) MW.

4. Concluding Remarks

We have determined some important relationships between the geometric arithmetic energy of graphs and its geometric arithmetic index. Numerous tight bounds on $\mathcal{GAE}$ have been derived in terms of various graph parameters, including spectral radius, graph order, maximum degree, minimum degree, nullity, and the first Zagreb index, along with the identification of corresponding extremal graphs. The role of $\mathcal{GAE}$ in structure-property modelling has been investigated using alkanes up to order 8 and molecular structure of some drugs. To conduct this investigation, three types of regression analysis were performed. It has been demonstrated that $\mathcal{GAE}$ effectively explains the boiling points of these chemicals, even outperforming the well-known GA index. Additionally, $\mathcal{GAE}$ has shown significant potential in modelling molar refractivity and molecular weight for certain chemicals relevant to kidney disease treatments.

Conflict of Interest: The authors declare that they have no conflict of interest.

Data Availability: Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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