Research Article

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On arithmetic–geometric eigenvalues of graphs

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Abstract: In this article, we are interested in characterizing graphs with three distinct arithmetic–geometric eigenvalues. We provide the bounds on the arithmetic–geometric energy of graphs. In addition, we carry out a statistical analysis of arithmetic–geometric energy and boiling point of alkanes. We observe that arithmetic–geometric energy is better correlated with a boiling point than the arithmetic–geometric index.

Keywords: topological indices, arithmetic–geometric matrix, correlation, energy

1 Introduction

A graph $G = G(V, E)$ consists of a vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and an edge set $E(G)$. We consider only simple and undirected graphs unless otherwise stated. The number of elements in $V(G)$ is the order n, and the number of elements in $E(G)$ is the size m of G. By $u \sim v$, we mean vertex u is adjacent to vertex v, and we also denote an edge by e. The neighborhood $N(v)$ of $v \in V(G)$ is the set of vertices adjacent to v. The degree d_v of a vertex v is the number of elements in the set $N(v)$. A graph G is called r-regular if the degree of every vertex is r. For two distinct vertices u and v in a connected graph G, the distance $d(u, v)$ between them is the length of the shortest path connecting them. The largest distance between any two vertices in a connected graph is called the diameter of G. We denote the complete graph by K_n, the complete bipartite graph by $K_{a,b}$, the star $(K_{1,n-1})$ by S_n, the star plus edge $(S_n + e)$ by S_n^+, the complete t-multipartite graph by $K_{p_1,p_2,\ldots,p_t}$, and the complete split graph by $CS_{\omega,n-\omega}$. We follow the standard graph theory notation, and more graph theoretic notations are found in the study by Cvetković et al. (2010).

The adjacency matrix $A(G)$ of G is a square matrix, indexed by the vertices of G, with (i, j)-th entry equals 1, if $i \sim j$ and 0 otherwise. Clearly, $A(G)$ is a real symmetric matrix and its set of eigenvalues including multiplicities is known as the spectrum of G. Let λ_i, $i = 1,2,\ldots, n$ be the eigenvalue of $A(G)$, and we can label them such that $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. The eigenvalue λ_1 of $A(G)$ is known as the spectral radius of G, and more about this matrix can be seen in the study by Brouwer and Haemers (2010).

The energy (Gutman, 1978) of G is defined by:

$$\mathscr{E}(G) = \sum_{i=1}^{n} |\lambda_i|$$

For more about the energy of G, including the recent development, studies by Jahanbani (2018), Li et al. (2010), and Wang and Gao (2021) can be referred.

The arithmetic–geometric matrix $A_{AG}(G)$ (or AG-matrix) of a graph G, introduced by Zheng et al., (2020), is a square matrix of order n defined by:

$$A_{AG}(G) = (a_{ij})_{n\times n} = \begin{cases} \dfrac{d_u + d_v}{2\sqrt{d_u d_v}}, & \text{if } u \sim v \\ 0, & \text{otherwise} \end{cases}$$

The AG-matrix is real symmetric, so its eigenvalues are real. We denote its eigenvalues by η_i, $i = 1,2,\ldots, n$, such that $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$. The multiset of all eigenvalues of AG-matrix is known as the AG-spectrum of G, and the largest eigenvalue η_1 is called the AG-spectral radius of G. If an eigenvalue say η of AG-matrix occurs with multiplicity $\alpha \geq 2$, then we denote it by $\eta\alpha$. Zheng et al. (2020) gave several bounds for η_1 and AG-energy and provided some AG equienergetic graphs. Guo and Gao (2020) obtained sharp bounds for η_1 and AG-energy and characterized the corresponding extremal graphs. AG-energy of some specific graphs and Nordhaus–Gaddum-type relations were obtained in the study by Zheng and Jin (2021) proved that AG-spectral radius of any tree lies between the AG-spectral radius of path and the AG-spectral radius of star. In the same article, they also proved that AG-spectral radius of any unicyclic graph lies between 2 and the AG-spectral radius of S_n^+.

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The arithmetic–geometric index (shortly AG-index) of G is a topological index (Shegehall and Kanabur, 2015), defined as:

$$AG = AG(G) = \sum_{u \sim v} \frac{d_u + d_v}{2\sqrt{d_u d_v}}$$

The AG-index is used in studying the properties of chemical graphs and is considered in the QSPR/QSAR research studies. For recent developments about AG-index and some applications, we refer to studies by Rodríguez et al. (2021) and Vujošević et al. (2021), and the references cited therein. The motivation for studying the matrices based on topological indices comes from the quantitative structure–property relationships (QSPR). For instance, it was shown that the energy of topological-based matrices is better correlated with the physical properties of alkanes, especially boiling point, molar volume, surface tension, critical temperature, and other properties (Estrada, 2008; Hosamani et al., 2017; Raza et al., 2016; Rodriguez and Sigarreta, 2015; Rather and Imran, 2022).

The arithmetic–geometric energy (AG-energy, for short) of G is defined by:

$$\mathscr{E}_{\mathrm{AG}}(G) = \sum_{i=1}^{n} |\eta_i|$$

For recent work regarding the AG-energy see Guo and Gao (2020), Wang and Gao (2020), and Zheng et al. (2021), and the references cited therein.

In Section 2, we characterize graphs with two distinct AG-eigenvalues, bipartite, multipartite and uncyclic graphs with exactly three distinct AG-eigenvalues. In Section 3, we give the upper and the lower bounds on the AG-energy of graphs. In Section 4, we give a statistical analysis of AG-energy and boiling point.

2 AG-eigenvalues of graphs

A natural problem in the spectral theory of graph matrices is the following.

Problem 1. For a connected graph G of order $n \geq 2$, let $M(G)$ be a graph matrix associated with G and $k(1 \leq k \leq n)$, be a positive integer. the graphs having exactly k distinct $M(G)$-eigenvalues are characterized.

This problem has been considered for the adjacency matrix, the normalized Laplacian matrix, the distance matrix, etc., for a small value of k, see the studies by Alazemi et al. (2017), Huang and Huang (2019), Huang et al. (2018), Qi et al. (2020), Rowlinson (2017), and Pirzada et al. (2022). In fact, various articles can be found in the literature regarding this problem for the mentioned matrices when $k \leq 4$, see the studies by Chen (2018), Liu and Shiu (2015), Sun and Das (2021), and Tian and Wang (2021), and the references therein.

It is trivial that nK_1 is the only complete graph with exactly one AG-eigenvalue and its AG-spectrum is $\{0^{[n]}\}$.

The following well-known result provides a relationship between the number of distinct eigenvalues in a graph and its diameter. It can be found in Brouwer and Haemers (2010).

Theorem 2.1. *Let G be a connected graph with diameter D. Then, G has at least $D + 1$ distinct (adjacency) eigenvalues, at least $D + 1$ distinct Laplace eigenvalues, and at least $D + 1$ distinct signless Laplace eigenvalues* (Brouwer and Haemers, 2010).

The proof provided in Brouwer and Haemers (2010) *shows that the above result is true for any nonnegative symmetric matrix $M = (M_{ij})_n$ indexed by the vertices of a graph G, in which $M_{ij} > 0$ if and only if $v_i \sim v_j$. So, the next corollary follows immediately.*

Corollary 2.2. *If G is a graph of diameter D and has k distinct AG-eigenvalues, then $k \geq D + 1$.*

Another immediate consequence is next stated.

Corollary 2.3. *Let G be a connected graph of order $n \geq 2$. Then, G has exactly two distinct AG-eigenvalues if and only if $G \cong K_n$.*

Proof. The AG-matrix of K_n is its adjacency matrix. So, it is trivial that K_n has exactly two distinct AG-eigenvalues.

Conversely, if G has exactly two distinct eigenvalues, from Corollary 2.2 its diameter is 1. Therefore, G is necessarily K_n.

A set $S \subseteq V(G)$ of pairwise non-adjacent vertices is called an *independent set*. It is said to be a *clique* if every two vertices of S are adjacent to G. The cardinality of the largest possible independent set in G is called the *independence number* of G, and the cardinality of the largest possible clique in G is called the *clique number* of G. ☐

Next, we have a result that helps us in finding some AG-eigenvalues, provided G has some special structure.

Theorem 2.4. *Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and let $S = \{v_1, v_2, \ldots, v_I\}$ be a subset of G such that $N(v_i) - v_j = N(v_j) - v_i$, for all $i, j \in \{1, 2, \ldots, I\}$. Then, the following statements hold:*

1. if S is a clique of G, then -1 is the AG-eigenvalue of G with multiplicity at least $I-1$,
2. *if S is an independent set of G, then 0 is the AG-eigenvalue of G with multiplicity at least $I-1$.*

Proof. We prove point 1 in Theorem 2.4, and then point 2 in Theorem 2.4 can be proved similarly. Suppose that vertices of S form a clique. As vertices of S share the same neighborhood, it follows that $d_1 = d_2 = \cdots = d_I$. We first index the vertices of S, so that the AG-matrix of G can be put as:

$$AG(G) = \begin{pmatrix} 0 & 1 & \cdots & 1 & \\ 1 & 0 & \cdots & 1 & M_{I\times(n-I)} \\ \vdots & \vdots & \ddots & \vdots & \\ 1 & 1 & \cdots & 0 & \\ & & (M_{I\times(n-I)})^T & & C_{(n-I)\times(n-I)} \end{pmatrix}$$

For $i = 2, 3, \ldots, I$, let $X_{i-1} = (-1, x_{i2}, x_{i3}, \ldots, x_{iI}, \underbrace{0, 0, 0, \ldots, 0}_{n-I})^T$ be the vector in R^n such that $x_{ij} = 1$ if $i = j$ and 0 otherwise. Clearly, $X_1, X_2, \ldots, X_{I-1}$ are linearly independent vectors.

Noting that the rows of M are identical, we see that:

$$AG(G)X_1 = (1, -1, 0, \ldots, 0, 0, \ldots, 0)^T = -1X_1$$

Similarly, we can easily see that $X_2, X_3, \ldots, X_{I-1}$ are eigenvectors of $AG(G)$ corresponding to the eigenvalue -1. This proves point 1 in Theorem 2.4.

Next, if S forms an independent set, then with the same set of vectors, we can see that 0 is the AG-eigenvalues of G with multiplicity $I-1$.

Theorem 2.4 helps us to obtain the AG-eigenvalues of some well-known families of graphs. In the following result, we mention some of these families. ☐

Proposition 2.5. *Let G be a connected graph of order n. Then, the following statements hold:*

1. The AG-spectrum of $K_{p,q}$, with $n = p + q$ and $p, q \geq 1$, is:

$$\left\{0^{[n-2]}, \pm\frac{n}{2}\right\}$$

2. *The AG-spectrum of the complete split graph $CS_{\omega,n-\omega}$, with clique number ω and independence number $n-\omega$ is:*

$$\left\{0^{[n-\omega-1]}, (-1)^{[\omega-1]}, \frac{(\omega^2-\omega)(n-1) \pm D}{2\omega(n-1)}\right\}$$

where $D = (1 - 3n + 4n^2 - 3n^3 + n^4)\omega^2 + (-1 + 3n - 3n^2 + n^3)\omega^3 + (-1 + n)\omega^4 + (1 - n)\omega^5$.

3. *The AG-spectrum of $K_n - e$, where e is an edge, is:*

$$\left\{0, (-1)^{[n-2]}, \frac{n^3 - 6n^2 + 11n - 6 \pm \sqrt{-36 + 108n - 121n^2 + 58n^3 - 6n^4 - 4n^5 + n^6}}{2(n^2 - 3n + 2)}\right\}$$

4. *The AG-spectrum of S_n^+ consists of the simple eigenvalues -1, the eigenvalue 0 with multiplicity $n-4$ and the zeros $z_1 \geq z_2 \geq z_3$ of the following polynomial:*

$$p(x) = x^3 - x^2 - \frac{n^3 - 2n^2 + 2n + 1}{4(n-1)}x + \frac{n^3 - 3n^2}{4(n-1)}$$

Proof.

1. As $K_{p,q}$ consists of two independent sets of cardinalities p and q, where any two vertices from the same independent set share the same neighborhood. So, 0 is the AG-eigenvalue of $K_{p,q}$ with multiplicity $p + q - 2$. The other two eigenvalues are the eigenvalues of the following quotient matrix:

$$\begin{pmatrix} 0 & \frac{q(p+q)}{2\sqrt{pq}} \\ \frac{p(p+q)}{2\sqrt{pq}} & 0 \end{pmatrix}$$

which are $-\frac{p+q}{2}$ and $\frac{p+q}{2}$.

2. As ω vertices of $CS_{\omega,n-\omega}$ form a clique in which any two vertices satisfy the condition in Theorem 2.4-(1), it follows that -1 is an AG-eigenvalue of $CS_{\omega,n-\omega}$ with multiplicity $\omega - 1$. Also, the graph $CS_{\omega,n-\omega}$ has an independent set on $n - \omega$ vertices sharing the same neighborhood. It follows that 0 is an AG-eigenvalue of $CS_{\omega,n-\omega}$ with *multiplicity* $n - \omega - 1$. The other two AG-eigenvalues of $CS_{\omega,n-\omega}$ are the eigenvalues of the following quotient matrix:

$$\begin{pmatrix} \omega - 1 & \frac{(n-\omega)(n+\omega-1)}{2\sqrt{(n-1)\omega}} \\ \frac{p(p+q)}{2\sqrt{pq}} \frac{w(n+\omega-1)}{2\sqrt{(n-1)\omega}} & 0 \end{pmatrix}$$

3. It follows from (ii), with $\omega = n - 2$.
4. As above, we can verify that 0 is an AG-eigenvalue with multiplicity $n-4$ and -1 is a simple AG-eigenvalue of S_n^+ corresponding to an independent set of cardinality $n-3$ and clique of size 2.

The other three AG-eigenvalues of S_n^+ are the eigenvalues of the following equitable quotient matrix:

$$\begin{pmatrix} 1 & \frac{n+1}{2\sqrt{2(n-1)}} & 0 \\ \frac{n+1}{\sqrt{2(n-1)}} & 0 & \frac{n(n-3)}{2\sqrt{(n-1)}} \\ 0 & \frac{n}{2\sqrt{n-1}} & 1 \end{pmatrix} \quad (1)$$

The characteristic polynomial of the above matrix is:

$$p(x) = x^3 - x^2 - \frac{n^3 - 2n^2 + 2n + 1}{4(n-1)}x + \frac{n^3 - 3n^2}{4(n-1)}$$

For $n \geq 4$, it can be easily seen that:

$$p\left(-\frac{n}{2} - 1\right) = \frac{5n^3 + 20n^2 - 9n - 18}{8(n-1)} > 0$$

$$p\left(-\frac{n}{2} + 1\right) = -\frac{3n^3 - 8n^2 + n - 2}{8(n-1)} < 0$$

$$p(0) = -\frac{(n-3)n^2}{4(n-1)} < 0$$

$$p(1) = \frac{(n+1)^2}{4(n-1)} > 0$$

$$p\left(\frac{n}{2} - 1\right) = \frac{3n^3 - 16n^2 + 33n - 18}{8(n-1)} > 0$$

$$p\left(\frac{n}{2} + 1\right) = -\frac{5n^3 - 4n^2 - 9n - 2}{8(n-1)} < 0$$

From the above calculations and by intermediate value theorem, it follows that the matrix in Eq. 1 has three distinct eigenvalues.

From point 1 in Proposition 2.5, we can state the following observation. □

Remark 2.6. All complete bipartite graphs on the same order n share the same spectrum:

$$\left\{\frac{n}{2}, 0^{[n-2]}, -\frac{n}{2}\right\}$$

We observe that the AG-matrix of the bipartite graph G can be written as:

$$\begin{pmatrix} \mathbf{0} & B \\ B^T & \mathbf{0} \end{pmatrix}$$

If η is an eigenvalue of $AG(G)$ with associated eigenvector $X = (x_1, x_2)^T$, then it is clear that $AG(G)X = \eta X$. Also, it is easy to see that $AG(G)X' = -\eta X'$, where $X' = (x_1, -x_2)^T$.

This implies that AG-eigenvalues of a bipartite graph are symmetric about the origin.

The next result (Liu and Shiu, 2015) states the distinct eigenvalues of irreducible non-negative symmetric real matrix.

Theorem 2.7. *Let M be an $n \times n$ irreducible non-negative symmetric matrix with real entries and let a_1 be the maximum eigenvalue of M with its corresponding unit Perron–Frobenius eigenvector X. Then, M has $k(2 \leq k \leq n)$ distinct eigenvalues if and only if there exit $k-1$ real numbers $a_2, a_3, \ldots, a_n$ $(a_1 > a_2 > \ldots > a_n)$ such that:*

$$\prod_{i=2}^{k}(M - a_i I_n) = \prod_{i=2}^{k}(a_1 - a_i)XX^T$$

Further, $a_1 > a_2 > \ldots > a_k$ are precisely the k distinct eigenvalues of M.

Corollary 2.8. *Let G be a connected graph of order $n \geq 3$, and let X be the unit eigenvector corresponding to the AG-spectral radius η_1. Then, G has k, $(2 \leq k \leq n)$ distinct AG-eigenvalues if and only if there exist $k-1$ real numbers $l_2, l_3, \ldots, l_k$ with $\eta_1 > l_2 > l_3 > \ldots > l_k$ such that:*

$$\prod_{i=2}^{k}(AG(G) - l_i I_n) = \prod_{i=2}^{k}(\eta_1 - l_i)XX^T$$

Further, $\eta_1, l_2, l_3, \ldots, l_k$ are precisely the k distinct AG-eigenvalues of G.

Proof. Since $AG(G)$ is an irreducible non-negative symmetric real matrix, by applying Theorem 2.7 to $AG(G)$, the result follows.

Corollary 2.2 plays the fundamental role in characterizing graphs with distinct eigenvalues and helps in solving Problem 1 for $k = 3$. □

Corollary 2.9. *Let G be a connected graph of order $n \geq 3$. Let η_1 be the AG-spectral radius of G with its associated unit eigenvector $X = (x_1, x_2, \ldots, x_n)^T$. Then G has three distinct AG-eigenvalues $\eta_1 > \eta_2 > \eta_3$ if and only if the following three conditions hold:*

1. $\sum_{v_j \in N(v_i)} \frac{(d_i + d_j)^2}{4d_i d_j} = -\eta_2\eta_3 + (\eta_1 - \eta_2)(\eta_1 - \eta_3)x_i^2$, *for every vertex v_i.*
2. $\sum_{v_k \in N(v_i) \cap N(v_j)} \left(\frac{d_i + d_k}{2\sqrt{d_i d_k}}\right)\left(\frac{d_j + d_k}{2\sqrt{d_j d_k}}\right) = (\eta_2 + \eta_3)\left(\frac{d_i + d_j}{2\sqrt{d_i d_j}}\right) + (\eta_1 - \eta_2)(\eta_1 - \eta_3)x_i x_j$, *for every pair of adjacent vertex v_i and v_j.*
3. $\sum_{v_k \in N(v_i) \cap N(v_j)} \left(\frac{d_i + d_k}{2\sqrt{d_i d_k}}\right)\left(\frac{d_j + d_k}{2\sqrt{d_j d_k}}\right) = (\eta_1 - \eta_2)(\eta_1 - \eta_3)x_i x_j$, *for every pair of non-adjacent vertex v_i and v_j.*

Proof. By Corollary 2.8, G has three distinct AG-eigenvalues if and only if the following equation holds:

$$(AG(G))^2 - AG(G)(\eta_2 + \eta_3) + \eta_2\eta_3 I_n = (\eta_1 - \eta_2)(\eta_1 - \eta_3)XX^T$$

Now, comparing the diagonal entries and the off-diagonal entries of the above equation, we get the desired result. □

Suppose we have a matrix M in some block form and we form a new matrix Q known as the *quotient matrix*, whose entries are the average of the rows (columns) of the blocks of the original matrix M. In general, the eigenvalues of Q interlace the eigenvalues of M, while if the row sums of every block of the original matrix is some constant, then each eigenvalue of Q is an eigenvalue of

M, and in such case, Q is known as the regular (equitable) quotient matrix (see Brouwer and Haemers, 2010).

For graphs with diameters greater or equal to three, Corollary 2.2 confirms that G has more than three distinct AG-eigenvalues. For the graphs of diameter at most two, we have the following result.

Proposition 2.10. *Let G be a graph of order $n \geq 4$. Then, the following holds:*
1. *if G is bipartite, then G has three distinct AG-eigenvalues if and only if G is the complete bipartite graph.*
2. *if G is the complete multipartite graphs $K_{p_1,p_2,\ldots,p_t}$, then G has three distinct AG-eigenvalues if and only if $p_1 = p_2 = \ldots = p_t$, where $p \geq 2$.*
3. *if G is unicyclic, then it has three distinct AG-eigenvalues if and only if $G \cong C_4$ or $G \cong C_5$.*

Proof. Assume that G has 3 distinct AG-eigenvalues. We note that any two non-adjacent vertices of G must have the same neighbor; otherwise, if a vertex u has neighbor w not adjacent to v, then w along with uv-path induces the path P_4 subgraph, which is a contradiction to the fact that the diameter of G is 2 and has more than three distinct AG-eigenvalues. Therefore, it follows that any two non-adjacent vertices in G share the common neighbor, and it implies that G is the complete bipartite graph.

Conversely, if $G \cong K_{p,q}$ with $n = p + q$, then by point 1 of Proposition 2.5, G has exactly three distinct AG-eigenvalues, and the result holds in this case.

Next, G is the complete multipartite graph $K_{p_1,p_2,\ldots,p_t}$ with $n = \sum_{i=1}^{t} p_i$ and $p_1 \geq p_2 \geq \ldots \geq p_t \geq 2$, $t \geq 3$. We will show that G has exactly three distinct AG-eigenvalues if and only if $p_1 = p_2 = \ldots = p_t$. First, we consider the tripartite case: for the tripartite graph, $G \cong K_{p_1,p_2,p_3}$ with $n = p_1 + p_2 + p_3$, by Theorem 2.4, gives that 0 is the AG-eigenvalue with multiplicity $n - 3$. The other three AG-eigenvalues of K_{p_1,p_2,p_3} are the eigenvalues of the following equitable quotient matrix:

$$\begin{pmatrix} 0 & \frac{p_2(p_1+p_2+2p_3)}{2\sqrt{(p_1+p_3)(p_2+p_3)}} & \frac{p_3(p_1+2p_2+p_3)}{2\sqrt{(p_1+p_2)(p_2+p_3)}} \\ \frac{p_1(p_1+p_2+2p_3)}{2\sqrt{(p_1+p_3)(p_2+p_3)}} & 0 & \frac{p_3(2p_1+p_2+p_3)}{2\sqrt{(p_1+p_3)(p_1+p_2)}} \\ \frac{p_1(p_1+2p_2+p_3)}{2\sqrt{(p_1+p_3)(p_2+p_3)}} & \frac{p_2(2p_1+p_2+2p_3)}{2\sqrt{(p_1+p_3)(p_1+p_2)}} & 0 \end{pmatrix} \quad (2)$$

If $p_1 = p_2 = p_3 = p$, then the eigenvalues of (2) are $\{2p, (-p)^{[2]}\}$, and there are three distinct AG-eigenvalues. If $p_1 = p_2 = p$ and $p_3 = q \neq p$, then in this case, the characteristic polynomial of Eq. 2 is:

$$x^3 - x\left(\frac{4p^3 + 13p^2q + 6pq^2 + q^3}{4(p+q)}\right) - \frac{pq(3p+q)^2}{4(p+q)} \quad (3)$$

Noting that the polynomial

$$x^3 + l_1x + l_2$$

has three distinct real zeros if and only if the discriminant $D = -4l_1^3 - 27l_2^2$ is positive. Now, from Eq. 3, we see that:

$$D = \frac{(-8p^3 + p^2q + 6pq^2 + q^3)^2(p^3 + 10p^2q + 6pq^2 + q^3)}{16(p+q)^3} > 0$$

and it proves that Eq. 2 has three distinct AG-eigenvalues, which implies that $K_{p,p,q}$, $p \neq q$ has more than three distinct AG-eigenvalues. For the case $p_1 \neq p_2 \neq p_3$, the characteristic polynomial of Eq. 2 is:

$$x^3 - x\left(\frac{p_2p_3(2p_1+p_2+p_3)^2}{4(p_1+p_2)(p_1+p_3)} + \frac{p_1p_3(p_1+2p_2+p_3)^2}{4(p_1+p_2)(p_2+p_3)} + \frac{p_1p_2(p_1+p_2+2p_3)^2}{4(p_1+p_3)(p_2+p_3)}\right) - \frac{p_1p_2p_3(2p_1+p_2+p_3)(p_1+2p_2+p_3)(p_1+p_2+2p_3)}{4(p_1+p_2)(p_1+p_3(p_2+p_3))}$$

It can be easily verified that the above expression has a positive determinant, which gives us that K_{p_1,p_2,p_3} has more than three distinct AG-eigenvalues. Thus, we observe that by taking distinct cardinalities of the complete tripartite graph, the number of distance AG-eigenvalues increases.

For the general case of $G \cong K_{p_1,p_2,\ldots,p_t}$, with $n = p_1 + p_2 + \ldots + p_t$. Clearly, G has t independent sets, where each vertex of every independent set shares the same neighborhood. Thus by Theorem 2.4, we get the AG-eigenvalue 0 with multiplicity $n - t$. The remaining t eigenvalues of AG-matrix of $K_{p_1,p_2,\ldots,p_t}$ are given by the following matrix:

$$\begin{pmatrix} 0 & \frac{p_2(2n-p_1-p_2)}{\sqrt[2]{(n-p_1)(n-p_2)}} & \cdots & \frac{p_t(2n-p_1-p_t)}{\sqrt[2]{(n-p_1)(n-p_t)}} \\ \frac{p_1(2n-p_1-p_2)}{\sqrt[2]{(n-p_1)(n-p_2)}} & 0 & \cdots & \frac{p_t(2n-p_2-p_t)}{\sqrt[2]{(n-p_2)(n-p_t)}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{p_1(2n-p_1-p_2)}{\sqrt[2]{(n-p_1)(n-p_2)}} & \frac{p_2(2n-p_2-p_t)}{\sqrt[2]{(n-p_2)(n-p_t)}} & \cdots & 0 \end{pmatrix}_{t\times t} \quad (4)$$

For $G \cong K_{p,p,p\ldots,p}$, $p \geq 2$, matrix (Eq. 4) takes the form:

$$\begin{pmatrix} 0 & p & \cdots & p & p \\ p & 0 & \cdots & p & p \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ p & p & \cdots & 0 & p \\ p & p & \cdots & p & 0 \end{pmatrix}_{t\times t}$$

and it is easy to see that $-p$ is its eigenvalue with multiplicity $t - 1$ and the other simple eigenvalue is $(t-1)p$.

Thus, $K_{p,p,p\ldots,p}, p \geq 2$ has exactly three distinct AG-eigenvalues. Next, in order to show that $K_{p_1,p_2,\ldots,p_t}$ have more than three distinct AG-eigenvalues, it is enough to prove that $K\_(p, p, \ldots, p, q), p \neq q$ has more than three distinct AG-eigenvalues, since we have observed in the tripartite case that the number of distinct AG-eigenvalues increase as we increase the number of distinct cardinalities of partite sets. With this assumption, the equitable quotient matrix of $K_{p,p,\ldots,p,q}$ is:

$$\begin{pmatrix} 0 & p & \cdots & p & \frac{q(2n-p-q)}{2\sqrt{(n-p)(n-q)}} \\ p & 0 & \cdots & p & \frac{q(2n-p-q)}{2\sqrt{(n-p)(n-q)}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ p & p & \cdots & 0 & \frac{q(2n-p-q)}{2\sqrt{(n-p)(n-q)}} \\ \frac{p(2n-p-q)}{2\sqrt{(n-p)(n-q)}} & \frac{p(2n-p-q)}{2\sqrt{(n-p)(n-q)}} & \cdots & \frac{p(2n-p-q)}{2\sqrt{(n-p)(n-q)}} & 0 \end{pmatrix}_{t\times t} \tag{5}$$

Consider $X_{i-1} = (-1, x_{i2}, x_{i3}, \ldots, x_{i(t-1)}, 0)$, where:

$$x_{ij} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{otherwise} \end{cases}$$

for $i = 2, 3, \ldots, t-1$. Now, we can easily verify that $X_1, \ldots, X_{t-2}$ are the eigenvectors corresponding to the AG-eigenvalue $-p$. The other two eigenvalues of Eq. 5 with the given blocks are the eigenvalues of the following equitable quotient matrix:

$$\begin{pmatrix} p(t-2) & \frac{q(2n-p-q)}{2\sqrt{(n-p)(n-q)}} \\ \frac{p(t-1)(2n-p-q)}{2\sqrt{(n-p)(n-q)}} & 0 \end{pmatrix}$$

and it is clear that it has two distinct eigenvalues. Thus the biregular complete multipartite has more than three AG-eigenvalues. Therefore it follows that $K_{p,p,\ldots,p,q}$ has more than three distinct AG-eigenvalues.

Lastly, if G is a unicyclic graph, then as above the diameter of G is exactly 2. So, G must be one of the following graphs: C_4, C_5, S_n^+. By Proposition 2.5, the graph S_n^+ has more than three distinct AG-eigenvalues. Also, the graph C_4 is bipartite and follows by point 2 in Proposition 2.10. Further, for the graph C_5, the AG-spectrum of C_5 is:

$$\{2, (0.618034)^{[2]}, (-1.61803)^{[2]}\}$$

and so the result follows in this case. □

Remark 2.11. There exists graphs, other than those characterized in Proposition 2.10 with exactly three distinct AG-eigenvalues. For example, Petersen graph H and the graph H_1 as shown in Figure 1. The AG-spectra of these graphs are:

$$\sigma(H) = \{3, 1^{[5]}, (-2)^{[4]}\}$$

$$\sigma(H_1) = \{4, 1^{[4]}, (-2)^{[4]}\}$$

Further, we see that their complements also have three distinct AG-eigenvalues.

Above remark give an insight that there can be more graphs with exactly three distinct AG-eigenvalues. Therefore, the following problem remains.

Problem 2. Characterize all graphs having exactly three distinct AG-eigenvalues.

3 *AG*-energy of graphs

Let $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_n$ be the AG-eigenvalues of G. Then it is easy to see that:

$$\sum_{i=1}^{n} \eta_i^2 = \frac{1}{2}\sum_{v_i \sim v_j}\left(\frac{d_{v_i} + d_{v_j}}{\sqrt{d_{v_i}d_{v_j}}}\right)^2 = 2B$$

where

$$B = \sum_{v_i \sim v_j}\left(\frac{d_{v_i} + d_{v_j}}{2\sqrt{d_{v_i}d_{v_j}}}\right)^2$$

Our first result gives an upper bound on the AG-energy in terms of the parameters B, the order n, and the AG-eigenvalues.

Theorem 3.1. *Let G be a graph of order n and t be the positive integer such that η_t is positive. Then:*

$$\mathcal{E}_{\mathrm{AG}} \leq \sqrt{2Bn - \frac{2n}{B}(\eta_1^2 + \eta_2^2 + \ldots + \eta_t^2 - B)^2} \tag{6}$$

Proof. Using the fact that $\eta_1^2 + \eta_2^2 + \ldots + \eta_t^2 + \eta_{t+1}^2 + \ldots + \eta_n^2 = 2B$, we have:

$$\begin{aligned} \eta_1^2 + \eta_2^2 + \ldots + \eta_t^2 - B &= \frac{1}{2}(\eta_1^2 + \eta_2^2 + \ldots + \eta_t^2 \\ &\quad - (\eta_{t+1}^2 + \ldots + \eta_n^2)) \\ &= \frac{1}{2}(\eta_1|\eta_1| + \eta_2|\eta_2| + \ldots + \eta_n|\eta_n|). \end{aligned}$$

Now, using the above information, inequality (Eq. 6) is equivalent to:

$$\begin{aligned} \frac{\mathcal{E}_{AG}^2}{n} &\leq \frac{2B^2 - 2(\eta_1^2 + \eta_2^2 + \ldots + \eta_t^2 - B)^2}{B} \\ &= \frac{2B^2 - 2\frac{1}{4}(\eta_1|\eta_1| + \eta_2|\eta_2| + \ldots + \eta_n|\eta_n|)^2}{B} \end{aligned}$$

Recall that $\sum_{i=1}^{n}\eta_i = 0$ and $\sum_{i=1}^{n}\eta_i^2 = 2B$, we have the following observation:

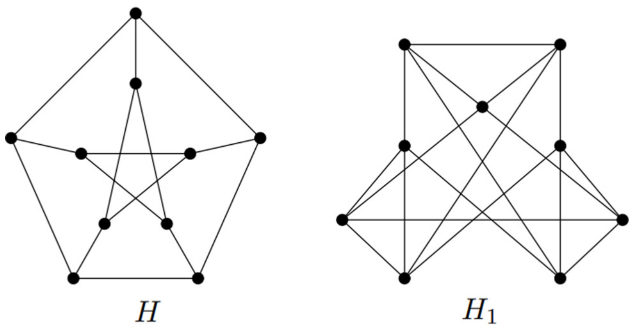


Figure 1: Graphs with three distinct AG-eigenvalues.

$$\frac{2B}{4B^2 - (\eta_1|\eta_1| + \eta_2|\eta_2| + \ldots + \eta_n|\eta_n|)^2}$$
$$= \sum_{i=1}^{n}\left(\frac{2B|\eta_i| - (\eta_1|\eta_1| + \eta_2|\eta_2| + \ldots + \eta_n|\eta_n|)\eta_i}{4B^2 - (\eta_1|\eta_1| + \eta_2|\eta_2| + \ldots + \eta_n|\eta_n|)^2}\right)^2$$
$$= \sum_{i=1}^{n}\frac{2B|\eta_i| - (\eta_1|\eta_1| + \eta_2|\eta_2| + \ldots + \eta_n|\eta_n|)\eta_i}{\mathcal{E}_{AG}(G)(4B^2 - (\eta_1|\eta_1| + \eta_2|\eta_2| + \ldots + \eta_n|\eta_n|)^2)}$$

Lastly, using all the above information, we have:

$$\frac{n}{\mathcal{E}_{AG}^2(G)} - \frac{2B}{4B^2 - (\eta_1|\eta_1| + \eta_2|\eta_2| + \ldots + \eta_n|\eta_n|)^2}$$
$$= \sum_{i=1}^{n}\frac{1}{\mathcal{E}_{AG}^2(G)} - \sum_{i=1}^{n}\left(\left(\frac{2B}{4B^2 - (\eta_1|\eta_1| + \eta_2|\eta_2| + \ldots + \eta_n|\eta_n|)^2}\right)\right)^2$$
$$= \sum_{i=1}^{n}\left(\frac{1}{\mathcal{E}_{\mathcal{AG}}(G)} - \frac{2B}{4B^2 - (\eta_1|\eta_1| + \eta_2|\eta_2| + \ldots + \eta_n|\eta_n|)^2}\right)^2 \geq 0$$

thus proves the result. □

The following result is the immediate consequence of Theorems 3.1 and 4.3 of Guo and Gao (2020).

Corollary 3.2. *Let G be a graph with exactly one positive AG-eigenvalue. Then:*

$$\mathcal{E}_{AG}(G) \leq 2\sqrt{B + B\sqrt{\frac{n-2}{n}}} \tag{7}$$

equality holding if and only if $G \cong K_2$.

Proof. From the proof of Theorem 4.3 of Guo and Gao (2020), we have:

$$\mathcal{E}_{AG}(G)^2 \geq \sum_{v_i \sim v_j}\left(\frac{d_{v_i} + d_{v_j}}{\sqrt{d_{v_i}d_{v_j}}}\right)^2 = 4B$$

with equality if and only if $\eta_1 = -\eta_n$ and $\eta_2 = \eta_3 = \ldots = \eta_{n-1} = 0$. Also, from Theorem 3.1, we have:

$$\mathcal{E}_{AG}(G) \leq \sqrt{2Bn - \frac{2n}{B}(\eta_1^2 - B)^2}$$

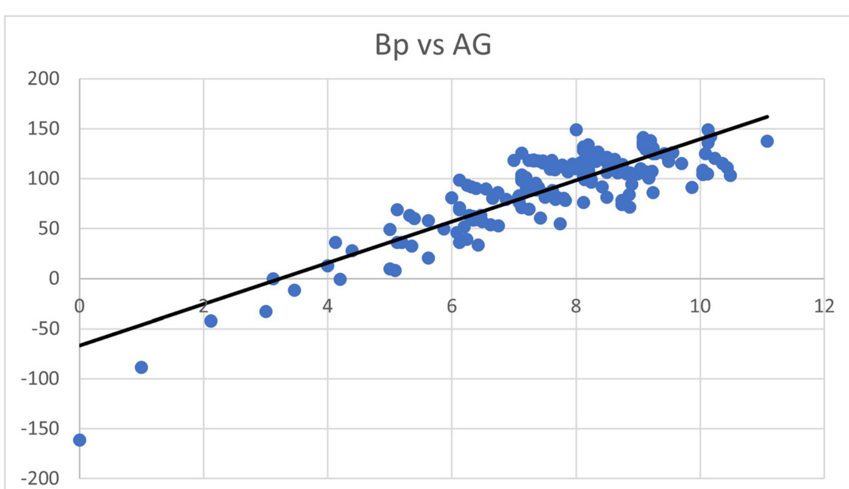
By comparing these two expressions, we obtain:

$$4B \leq 2nB - \frac{2n}{B}(\eta_1^2 - B)^2$$

which implies that:

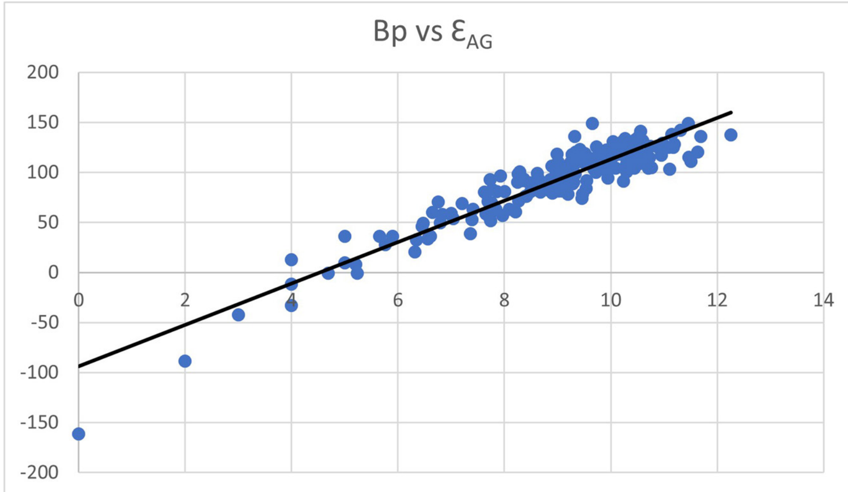
$$\eta_1 \leq \sqrt{B + B\sqrt{\frac{n-2}{2}}}$$

Therefore, by definition of AG-energy, we have:



$$Bp = 20.651\,AG - 66.819$$
$$R^2 = 0.7347$$

Figure 2: Linear regression Bp versus AG.



$$Bp = 20.694\,\mathcal{E}_{AG} - 93.887$$

$$R^2 = 0.8737$$

Figure 3: Linear regression Bp versus $\mathcal{E}_{AG}$.

$$\mathcal{E}_{AG}(G) = 2\eta_1 \le 2\sqrt{B + B\sqrt{\frac{n-2}{2}}}$$

Since, for graphs with exactly one positive AG-eigenvalue, $\mathcal{E}_{AG}(G) = 2\lambda_1$, which from above inequality is possible if $n = 2$ and $B = \lambda_1^2$, which is true if and only if G is K_2. □

Remark 3.3. From the proof of Theorem 4.1 from Guo and Gao (2020), we have:

$$\mathcal{E}_{AG}(G) \le \sqrt{\frac{n}{2}\sum_{v_iv_j}\left(\frac{d_{v_i} + d_{v_j}}{\sqrt{d_{v_i} + d_{v_j}}}\right)^2} = \sqrt{\frac{n}{2}4B} = \sqrt{2nB}$$

with equality if and only if $G \cong K_2$. Comparing it with the bound obtained in Corollary 3.2, we have:

$$4\left(B + B\sqrt{\frac{n-2}{n}}\right) \le 2nB$$

which gives us $2\sqrt{\frac{n-2}{n}} \le n - 2$, which is further equivalent to $n^2 - 2n - 4$ and true for $n \ge 4$. Thus, for graphs having exactly one positive AG-eigenvalue, the bound (Eq. 7) is better than the bounds of Guo and Gao (2020) (Theorem 4.1 therein). We say a graph is AG non singular if all its AG-eigenvalues are non zero, and by $\det(M)$ we mean the determinant of matrix M. The following result gives the lower bounds for AG-energy of graphs.

Theorem 3.4. *Let G be a non-singular graph with n vertices. Then, the following hold:*

1. $\mathcal{E}_{AG}(G) \ge \frac{2m}{n} + n - 1 + \ln(|\det(AG)|) - \ln\left(\frac{2m}{n}\right)$,
2. $\mathcal{E}_{AG}(G) \ge \sqrt{\frac{M_1(G)}{n}} + n - 1 + \ln(|\det(AG)|) - \ln\left(\sqrt{\frac{M_1(G)}{n}}\right)$, where $M_1(G) = \sum_{i=1}^{n} d_{v_i}^2$ is known as the Zagreb index of G.

Proof. As G is non singular, so $|\eta_i|$, for $i = 1, 2, \ldots, n$ and $|\det(AG)| = \prod_{i=1}^{n}|\eta_i| > 0$.

Now, consider the function:

$$f(x) = x^2 - x - ln(x), \quad \text{for} x > 0$$

It is easy to verify that $f(x)$ is increasing on$(1, \infty)$ and decreasing on $(0,1)$. Thus, $f(x) \ge f(1)$ implies that $x \le x^2 - \ln(x)$ for $x > 0$, with equality if and only if $x = 1$. Now, using this information, we have:

$$\mathcal{E}_{AG}(G) = \eta_1 + \sum_{i=2}^{n}|\eta_i| \ge \eta_1 + n - 1 + \sum_{i=2}^{n}\ln(|\eta_i|)$$

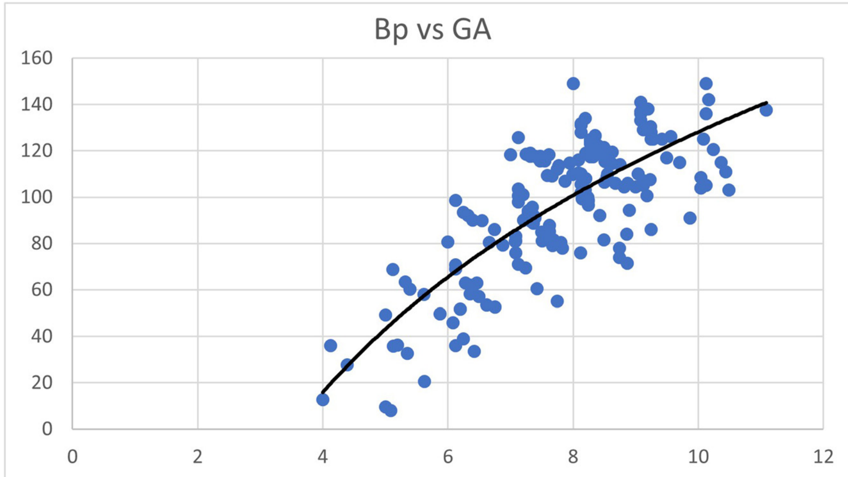
$$= \eta_1 + n - 1 + \ln\left(\prod_{i=2}^{n}|\eta_i|\right)$$

$$= \eta_1 + n - 1 + \ln(|\det(AG)|) - \ln(\eta_1). \qquad (8)$$

Recalling that $\eta_1 \ge \frac{2m}{n}$ (Lemma 6 in Wang and Gao (2020)) and noting that $g(x) = x + n - 1 + \ln(|\det(AG)|) - \ln(x)$ is an increasing function for $[1, n]$, we have:

$$g(x) \ge g\left(\frac{2m}{n}\right) = \frac{2m}{n} + n - 1 + \ln(|\det(AG)|) - \ln\left(\frac{2m}{n}\right), \quad \text{for } x \ge \frac{2m}{n}$$

Combining the above inequality with Eq. 8, we obtain the required inequality (point 1 in Theorem 3.4).



$$Bp = 122.53\ \ln(AG) - 153.98$$

$$R^2 = 0.6134$$

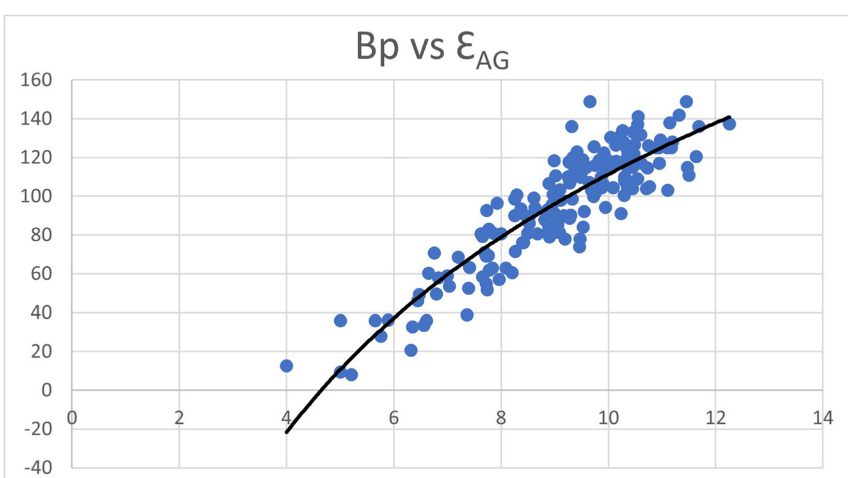
Figure 4: Logarithmic regression *Bp* versus *AG*.

For the second part, proceeding as above and using the fact that $\eta_1 \geq \sqrt{\frac{M_1(G)}{n}}$, the second lowe bound can be established. □

4 Statistical analysis

We carried out a statistical study to compare the correlation of the boiling point of chemical compounds with the arithmetic–geometric index AG, on one side, and with arithmetic-geometric energy $\mathcal{E}_{AG}$, on the other side. For the regression model, we considered the most used: linear, logarithmic, and quadratic.

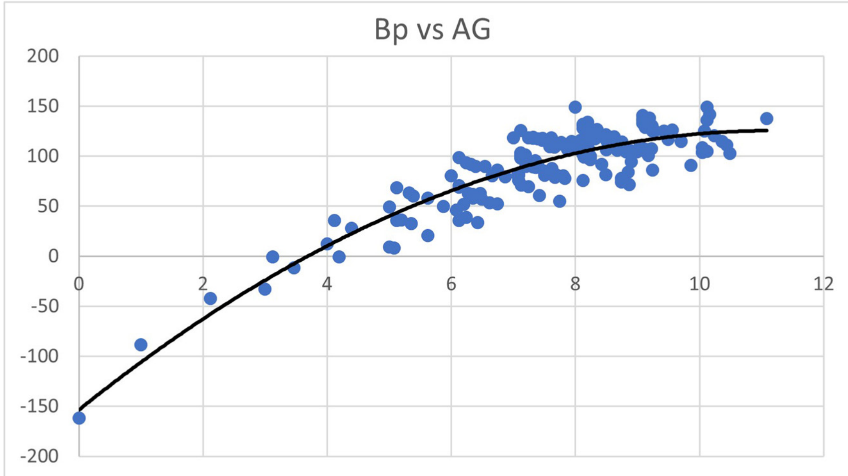
Our data, given in Table 1, consist of the boiling point Bp, the arithmetic–geometric index AG, the arithmetic–geometric energy ε_{AG} of chemical graphs up to 8 vertices. The boiling points are taken from the study by Rücker and Rücker (1999), see also Aouchiche and Ganesan (2020) and Aouchiche and Hansen (2012). The values of AG and ε_{AG} were calculated using the AutoGraphiX III system (Caporossi, 2017).



$$Bp = 145.24\ \ln(\mathcal{E}_{AG}) - 223.03$$

$$R^2 = 0.8077$$

Figure 5: Logarithmic regression *Bp* versus $\mathcal{E}_{AG}$.



$$Bp = -2.2291.(AG)^2 + 49.886.AG - 153.55$$
$$R^2 = 0.8186$$

Figure 6: Quadratic regression *Bp* versus *AG*.

The most important observation is that $\mathcal{E}_{AG}$ energy is best correlated with boiling point Bp than that of the topological index AG in all respective regressions.

Figure 2 illustrates the linear regression between the boiling point and AG index, with rounded equation:

$$Bp = 20.651 \quad AG - 66.819$$

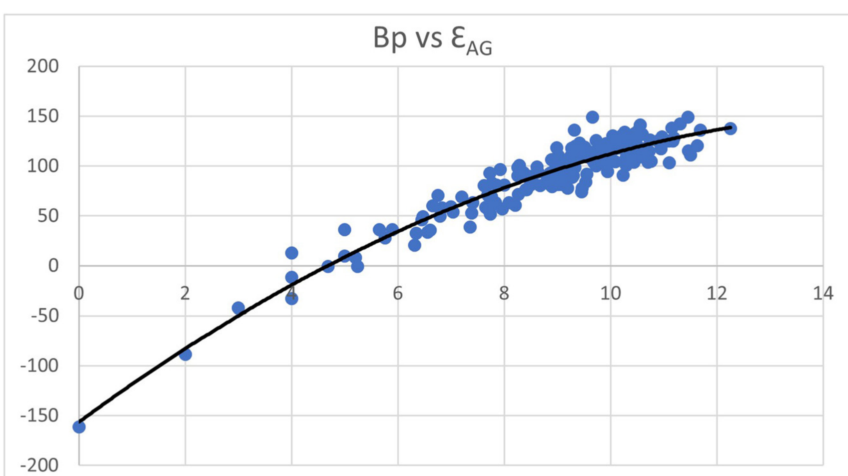
Figure 3 shows the linear regression between the boiling point and AG-energy, with rounded equation:

$$Bp = 20.694 \quad \varepsilon_{\mathrm{AG}} - 93.887.$$

The linear regression shows that the correlation of the boiling point is better with $\mathcal{E}_{AG}$, where $R^2 = 0.8737$, than with AG, where $R^2 = 0.7347$.

Figure 4 illustrates the logarithmic regression between the boiling point and AG index, with rounded equation:

$$Bp = 122.53 \quad \ln(AG) - 153.98$$



$$Bp = -1.2306.(\mathcal{E}_{AG})^2 + 39.154.\mathcal{E}_{AG} - 156.35$$
$$R^2 = 0.9073$$

Figure 7: Quadratic regression *Bp* versus $\mathcal{E}_{AG}$.

Table 1: Boiling point, *AG* index, and $\mathcal{E}_{AG}$ energy of alkanes up to order 8

Name	Bp	AG	$\mathcal{E}_{AG}$	Name	Bp	AG	$\mathcal{E}_{AG}$	Name	Bp	AG	$\mathcal{E}_{AG}$
n1	−161.5	0	0	1tbc3	80.5	7.8016	8.67379	b2mc3	124	8.27722	10.3517
n2	−88.6	1	2	11ec3	88.6	7.36396	9.27722	1nepec3	106	8.87252	9.74915
n3	−42.1	2.12132	3	1e23mc3	91	7.39068	8.99593	5msbc3	115.5	8.50534	10.3518
c3	−32.8	3	4	1m1ipce	81.5	7.69108	9.01389	1e2pc3	108	8.2038	10.3045
n4	−0.5	3.12132	4.69042	11m23c3	79.1	7.67292	8.90465	ib2mc3	110	8.54658	9.86825
2mn3	−11.7	3.4641	4	12m1ec3	85.2	7.61766	9.05318	11m2pc3	105.9	8.67292	9.91127
1mc3	−0.7	4.19594	5.23802	1123mc3	78	7.83013	9.18966	1m12epc3	108.9	8.54425	10.5422
c4	12.6	4	4	1122mc3	76	8.12132	8.41765	11m2ipc3	94.4	8.90104	9.9405
bc110b	8	5.08248	5.20317	1pc4	100.7	7.12252	8.28829	112m2ec3	104.5	8.99262	10.0879
n5	36	4.12132	5.65685	1ipc4	92.7	7.35064	7.72793	11223mc3	100.5	9.17543	10.2962
2mn4	27.8	4.39068	5.76105	1e3mc4	89.5	7.31846	8.52598	1ibc4	120.1	8.39188	9.33738
22mn3	9.5	5	5	1e2mc4	94	7.27722	8.63449	p3mc4	117.4	8.31846	9.52741
1ec3	35.9	5.12252	6.60537	1ec5	103.5	7.12252	9.09223	1sbc4	123	8.27722	9.41768
12mc3	32.6	5.35064	6.34632	13mc5	91.3	7.39188	8.84221	12ec4	119	8.2038	9.51732
11mc2	20.6	5.62132	6.31872	12mc5	95.6	7.35064	8.94888	1234mc4	114.5	8.6188	10.7289
1mc4	36.3	5.19594	5.89327	11mc5	87.9	7.62132	8.81715	1133mc4	86	9.24264	9.05821
c5	49.3	5	6.47214	1mc6	101	7.19594	8.96625	1pc5	131	8.12252	10.2194
bc111p	36	6.12372	5	c7	118.4	7	8.98792	1ipc5	126.4	8.35064	10.134
bc210p	46	6.08248	6.44846	dcprm	102	8.12372	9.76269	1e3mc5	121	8.31846	10.3594
s22p	39	6.24264	7.3589	bc221h	105.5	8.12372	9.76269	1e2mc5	124.7	8.27722	10.3557
mbc110b	33.5	6.42292	6.56159	bc311h	110	8.12372	9.2473	124mc5	115	8.54658	9.94485
n6	68.7	5.12132	7.20036	bc320h	110.5	8.08248	9.01277	1e1mc5	121.5	8.49264	10.4653
2mn5	60.3	5.39068	6.65235	bc410h	116	8.08248	9.75124	123mc5	117	8.50534	10.6077
3mn5	63.3	5.31726	7.40948	s33h	96.5	8.24264	7.92745	113mc5	104.5	8.81726	9.8801
23mn4	58	5.6188	6.8313	s24h	98.5	8.24264	9.33053	112mc5	114	8.74634	10.0141
22mn4	49.7	5.87132	6.79126	2mbc310hx	100	8.23718	9.72558	1ec6	131.8	8.12252	10.6021
1pc3	69	6.12252	7.71721	6mbc310hx	103	8.19594	9.68638	14mc6	121.8	8.39188	10.476
1ipc3	58.3	6.35064	7.65407	mbc210hx	81.5	8.49384	9.08634	13mc6	122.3	8.39188	9.9193
1e2mc3	63	6.27722	7.83428	mbc310hx	92	8.42292	9.55002	12mc6	126.6	8.35064	10.4828
1e1mc3	57	6.49262	7.9621	13mbc111p	71.5	8.86396	8.26628	11mc6	119.5	8.62132	9.95609
123mc3	63	6.4641	8.08827	14mbc210p	74	8.74264	9.45753	1mc7	134	8.19594	10.2688
112mc3	52.6	6.74634	7.38891	11ms22p	78	8.74262	9.46973	c8	149	8	9.65685
1ec4	70.7	6.12252	6.75811	122mbcb	84	8.85201	9.5329	bcprm	129	9.12372	10.9685
13mc4	59	6.39188	6.99982	tc410024h	105	9.12372	10.349	bc330o	137	9.08248	10.5425
12mc4	62	6.35064	7.78216	tc311024h	107	9.12372	9.6418	bcb	136	9.08248	9.31797
11mc4	53.6	6.62132	7.03562	tc221026h	106	9.12372	10.3583	bc4200	133	9.08248	10.4596
1mc5	51.8	6.19594	7.74106	tc410027h	110	9.04124	10.3032	bc510o	141	9.08248	10.5556
c6	80.7	6	8	tc410013h	107.5	9.22453	10.4529	2mbc221h	125	9.27842	10.8884
bc211hx	71	7.12372	7.6929	tec320h	108.5	10.0412	10.2998	S34o	128	9.24264	10.2471
bcpr	76	7.08248	8.39864	tec410h	104	10.0412	10.7088	7mbc320h	128	9.23718	11.1892
bc220hx	83	7.08248	7.7735	n8	125.7	7.12132	9.7278	2mbc320h	130.5	9.23718	10.0441
bc310hx	81	7.08248	8.4923	2mn7	117.6	7.39068	9.27007	s25o	125	9.24264	11.0911
s23hx	69.5	7.24264	7.75831	3mn7	118.9	7.31726	9.9114	1mbc221h	117	9.49384	10.9527
mbc210p	60.5	7.42292	8.20672	4mn7	117.7	7.31726	9.26915	7mbc410h	138	9.19594	11.1487
13mbcb	55	7.74264	7.71752	25mn6	109.1	7.66004	9.31019	1mbc410h	125	9.42292	10.94
n7	98.5	6.12132	8.25402	3en6	118.5	7.24384	9.83204	33mbc310hx	115	9.7038	10.4437
2mn6	90	6.39068	8.25215	24mn6	109.4	7.58662	9.3399	14mbc211hx	91	9.86396	10.2359
3mn6	92	6.31726	8.35197	23mn6	115.6	7.54538	9.41305	66mbc310hx	126.1	9.56197	10.7436
3en5	93.5	6.24384	8.36575	34mn6	117.7	7.47196	10.106	2244mbcb	104	10.0415	10.4453
24mn5	80.5	6.66004	7.62489	22mn6	106.8	7.87132	9.27384	1223mbcb	105	10.1213	10.7638
23mn5	89.8	6.54538	8.46557	3e2mn5	115.6	7.47196	9.35947	tc510035o	142	10.165	11.3133
22mn5	79.2	6.87132	7.65211	234mn5	113.5	7.7735	9.51778	tc510024o	149	10.1237	11.4555
33mn5	86.1	6.74264	8.52444	33mn6	112	7.74264	9.40615	tc3210o	136	10.1237	11.6894
223mn4	80.9	7.06976	7.8603	224mn5	99.2	8.14068	8.61401	tc3300o	125	10.0825	11.1747
1bc3	98	7.12252	9.11395	3e3mn5	118.2	7.61396	10.1466	3mtc2210h	120.5	10.2372	11.636
1sbc3	90.3	7.27722	9.29729	223mn5	109.8	7.99634	9.48833	ds2121o	103	10.4853	11.1026

(*Continued*)

Table 1: (*Continued*)

Name	Bp	AG	$\mathcal{E}_{AG}$	Name	Bp	AG	$\mathcal{E}_{AG}$	Name	Bp	AG	$\mathcal{E}_{AG}$
1m2pc3	93	7.27722	8.85944	233mn5	114.8	7.94108	9.58514	1mtc2210h	111	10.4345	11.5024
12ec3	90	7.2038	9.17525	2233mn4	106.5	8.5	8.88819	ds2022o	115	10.364	11.4681
1m1pc3	84.9	7.49264	8.88115	1pec3	128	8.12252	10.2807	tec330o	137.5	11.0825	12.2547
1m2ipc3	81.1	7.50534	8.87111	1spec3	117.4	8.27722	10.2413				

Figure 5 shows the logarithmic regression between the boiling point and AG-energy, with rounded equation:

$$Bp = 145.24 \quad \ln(\varepsilon_{AG}) - 223.03$$

The logarithmic regression shows that the correlation of the boiling point is better with ε_{AG}, where $R^2 = 0.8077$, than with AG, where $R^2 = 0.6134$.

Figure 6 illustrates the quadratic regression between the boiling point and AG index, with rounded equation:

$$Bp = -2.2291 \cdot (AG)^2 + 49.886 \cdot AG - 153.55$$

Figure 7 shows the quadratic regression between the boiling point and AG-energy, with rounded equation:

$$Bp = -1.2306 \cdot (\varepsilon_{AG})^2 + 39.154 \cdot \varepsilon_{AG} - 156.35$$

The quadratic regression shows that the correlation of the boiling point is better with AG-energy, where $R^2 = 0.9073$, than with AG, where $R^2 = 0.8186$.

The study shows that in each regression model, the boiling point is better correlated with the arithmetic–geometric energy than with the arithmetic–geometric index. Comparing the models, the logarithmic regression gives a better correlation. Overall, the best correlation with boiling point is obtained with the arithmetic–geometric energy using the logarithmic regression.

5 Conclusions

The result in this article characterizes certain classes of graphs with three distinct AG-eigenvalues and gives several bunds on AG-energy. Statistical analysis of boiling point and AG-energy of chemical graphs up to eight vertices shows that AG-energy is better correlated with a boiling point than AG-index.

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References

Alazemi A., Andelić M., Koledin T., Stanić Z., Distance-regular graphs with small number of distinct distance eigenvalues, Linear Algebra Appl., 2017, 531, 83–97.

Aouchiche M., Ganesan V., Adjusting geometric-arithmetic index to estimate boiling point. Match Commun. Math. Comput. Chem., 2020, 84, 483–497.

Aouchiche M., Hansen P., The normalized revised Szeged index. Match Commun. Math. Comput. Chem., 2012, 67, 369–381.

Brouwer A.E., Haemers W.H., Spectra of graphs, Springer, New York, 2010.

Caporossi G., Variable neighborhood search for extremal vertices: The AutoGraphiX-III system. Comput. Oper. Res., 2017, 78 431–438.

Chen X., On ABC eigenvalues and ABC energy. Linear Algebra Appl. 2018, 544, 141–157.

Cvetković D.M., Rowlison P., Simić S., An introduction to theory of graph spectra. London mathematics society student text, 75, Cambridge University Press, UK, 2010.

Estrada E., Atom-bond connectivity and the energetic of branched alkanes, Chem. Phys. Lett., 2008, 463(4–6), 422–425.

Guo X., Gao Y., Arithmetic-geometric spectral radius and energy of graphs. Match Commun. Math. Comput. Chem., 2020, 83, 651–660.
Gutman I., The Energy of a graph. Ber. Math. Statist. Sekt. Forschungszenturm Graz., 1978, 103, 1–22.
Hosamani S.M., Kulkarni B.B., Boli R.G., Gadag V.M., QSPR analysis of certain graph theoretical matrices and their corresponding energy. Appl. Math. Nonlinear Sci., 2017, 2, 131–150.
Huang X., Huang Q., On graphs with three of four distinct normalized Laplacian eigenvalue. Algebra Colloquium, 2019, 26(1), 65–82.
Huang X., Huang Q., Lu L. Graphs with at most three distance eigenvalue different from −1 and −2. Graphs Combinatorics, 2018, 34, 395–414.
Jahanbani A., Lower bounds for the energy of graphs. AKCE Int. J. Graphs Combinatorics, 2018, 15(1), 88–96.
Li X., Shi Y., Gutman I., Graph energy, Springer, New York, 2010.
Liu R., Shiu W.C., General Randić matrix and general Randić incidence matrix. Discrete Appl. Math., 2015, 186, 168–175.
Pirzada S., Rather B.A., Aouchiche M., On eigenvalues and energy of geometric–arithmetic matrix of graphs. Medit. J. Math., 2022, 19, 115. doi: 10.1007/s00009-022-02035-0.
Qi L., Miao L., Zhao W., Lu L. Characterization of graphs with an eigenvalue of large multiplicity. Adv. Math. Physics, 2020, 2020. doi: 10.1155/202/3054672.
Rather B.A., Aouchiche M., Pirzada S., On the spread of the geometric-arithmetic matrix of graphs, AKCE Int. J. Graphs Comb., 2022, 19(2), 146–153. doi: 10.1080/09728600.2022.2088315.
Rather B.A., Imran M., Sharp bounds on the sombor energy of graphs. Match Commun. Math. Comput. Chem., 2022, 88(3), 605–624.
Raza Z., Bhatti A.A., Ali A., More on comparison between first geometric–arithmetic index and atom–bond connectivity index. Miskolc Math. Notes, 2016, 17, 561–570.
Rowlinson P., More on graphs with just three distinct eigenvalues. Appl. Anal. Discrete Math., 2017, 11, 74–80.
Rodríguez J.M., Sánchez J.L., Sigarreta J.M., Tourís E., Bounds on the arithmetic-geometric index. Symmetry, 2021, 13(4), 689.
Rodriguez J.M., Sigarreta J.M., Spectral study of the geometric-arithmetic index. Match Commun. Math. Comput. Chem., 2015, 74, 121–135.
Rücker G., Rücker C., On topological indices, boiling points and cycloalkanes. J. Chem. Inf. Comput. Sci., 1999, 39, 788–802.
Shegehall V.S., Kanabur R., Arithmetic-geometric indices of path graphs. J. Math. Comput. Sci.,2015, 16, 19–24.
Sun S., Das K.C., On the multiplicities of normalized Laplacian eigenvalues of graphs. Linera Algebra Appl., 2021, 609, 365–385.
Tian F., Wang Y., Full characterization of graphs having certian normalized Laplacian eigenvalues of multiplicity $n-3$. Linear Algebra Appl., 2021, 630, 69–83.
Vujošević S., Popivoda G., Vukiećević Z.K., Furtula B., Skrekovski R., Arithmetic-geometric index and its relation with arithmetic-geometrix index. Appl. Math. Comput., 2021, 391, 125706.
Wang Y., Gao Y., Nordhaus-Gaddum-type relations for the arithmetic-geometric spectral radius and energy. Math. Problems Eng., 2020, 2020, 5898735.
Wang Y., Gao Y., Bounds for the energy of graphs. Math., 2021, 9, 1687.
Zheng L., Tian G.X., Cui S.Y., On spectral radius and energy of arithmetic-geometric matrix of graphs. Match Commun. Math. Comput. Chem., 2020, 83, 635–650.
Zheng L., Tian G.X., Cui S.Y., Arithmetic-geometric energy of specific graphs. Discrete Math. Algorithms Appl., 2021, 215005, 15.
Zheng R., Jin X., Arithmetic-geometric spectral radius of trees and unicyclic graphs. 2021, Arxiv:2015.03884.