

The Accurate Independent Dominating Energy of a Graph

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Abstract

Let $G = (V, E)$ be a graph. An independent dominating set $D_i \subseteq V(G)$ of G is said to be an accurate independent dominating set D_{i_a} such that no $|D_i|$ -element subset of $V(G) - D_i$ is an independent dominating set. In this paper, we study a new graph-energy like invariant viz., the accurate independent dominating energy(AIDE) of a graph G . As a chemical application of this new parameter, we show that the predicting power of AIDE is quite better than classical graph energy for enthalpy of vaporization for the set of octane isomers. Next, we obtain bounds for AIDE and finally concluded with some open problems.

Keywords: Accurate independent domination number, Energy, Accurate independent dominating energy.

AMS Subject Classification : 05C69, 05C90.

INTRODUCTION

Let $G = (V, E)$ be a connected, nontrivial, undirected graph without loops and multiple edges. The number of vertices of G we denote by n and the number of edges we denote by m , thus $|V(G)| = n$ and $|E(G)| = m$. By the open neighborhood of a vertex v of G we mean the set $N_G(v) = \{u \in V(G) : uv \in E(G)\}$. The degree of a vertex v , denoted by $d_G(v)$, is the cardinality of its open neighborhood. By $K_{r, s}$ we denote a complete bipartite graph with partite sets of cardinalities r and s . By a star we mean the graph $K_{1, n-1}$. For undefined terminologies in this paper, we suggest the interested reader to refer [14].

A subset $D \subseteq V(G)$ is a dominating set of G if every vertex of $V(G) \setminus D$ has a neighbor in D . The domination number of G , denoted by $\gamma(G)$, is the minimum cardinality of a dominating set of G . A dominating set D_i is an independent dominating set if $\langle D_i \rangle$ has no edges. The independent domination number $i(G)$ is the minimum cardinality of an independent dominating set. A dominating set D_a is an accurate dominating set such that no $|D|$ -element subset of $V(G) \setminus D_a$ is a dominating set of G . The accurate domination

number $\gamma_a(G)$ of G is the cardinality of a smallest accurate dominating set of G [9, 20]. An accurate dominating set is an accurate independent dominating set if $\langle D_a \rangle$ has no edges. The accurate independent domination number $i_a(G)$ is the minimum cardinality of an accurate independent dominating set of G [4]. For a comprehensive survey of domination in graphs, see [15, 16].

The energy $E(G)$ of a graph G is equal to the sum of the absolute values of the eigenvalues of the adjacency matrix of G . This quantity, introduced almost 30 years ago [11] and having a clear connection to chemical problems [13], has in newer times attracted much attention of mathematicians and mathematical chemists [6, 8, 10, 21, 23, 24, 26, 28].

In connection with energy (that is defined in terms of the eigenvalues of the adjacency matrix), energy-like quantities were considered also for the other matrices: Laplacian [13], distance [17], incidence [18], minimum covering energy [1] etc. Recall that a great variety of matrices has so far been associated with graphs [2, 3, 8, 27]. In this paper we study a new matrix, called the accurate independent dominating matrix(AIDM) of a graph, its eigenvalues and energy.

The accurate independent dominating matrix(AIDM) of G is the $n \times n$ matrix defined by $A_{i_a}(G) = (a_{ij})$, where

$$a_{ij} = \begin{cases} 1, & \text{if } v_i v_j \in E; \\ 1, & \text{if } i = j \text{ and } v_i \in D_{i_a}; \\ 0, & \text{otherwise.} \end{cases}$$

The characteristic polynomial of $A_{i_a}(G)$ is denoted by $\Phi_n(G, \mu) = \det(\mu I - A_{i_a}(G))$.

The accurate independent dominating eigenvalues of a graph G are the eigenvalues of $A_{i_a}(G)$. Since $A_{i_a}(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$. The accurate independent dominating energy of G is then defined as

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

ON CHEMICAL APPLICABILITY OF THE $E_{i_a}(G)$

The productivity of $E_{i_a}(G)$ was tested using a data set of octane isomers, found at <http://www.molecularDescriptors.eu/dataset.htm>. The octane data set consists of the following data: boiling point, melting point, heat capacities, molar refraction, acentric factor, total surface area, octanol-water partition coefficient and entropy. The $E_{i_a}(G)$ was correlated with each of these properties and surprisingly, we can see that the $E_{i_a}(G)$ has a good correlation with the enthalpy of vaporization of octane isomers.

The following structure-property relationship model has been developed for the $E_{i_a}(G)$.

$$HVAP = [23.010(\pm 1.973) - 1.640(\pm 0.311)]E_{i_n} \quad (1)$$

The correlation coefficient of Accurate independent dominating energy is $r = 0.896$ whereas the correlation coefficient with classical graph energy is $r = 0.287$.

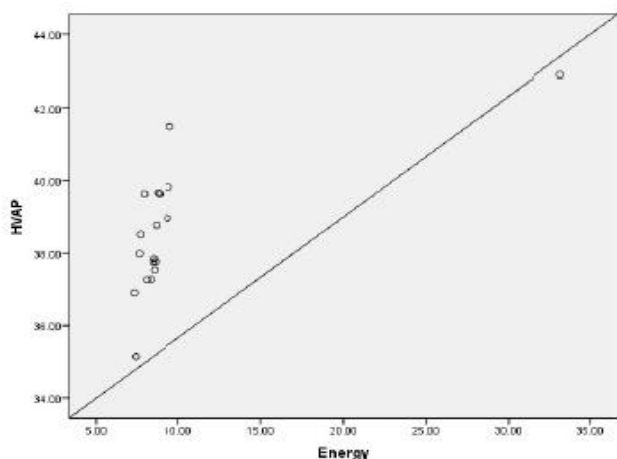
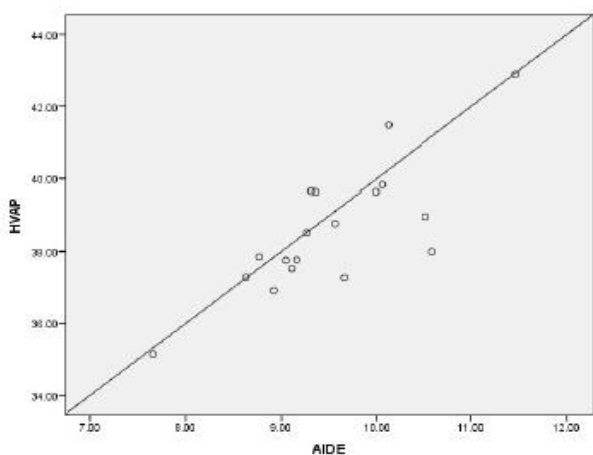


Figure 1. Correlation of AIDE with enthalpy of vaporization of octane isomers and correlation of E(G) with enthalpy of vaporization of octane isomers

RESULTS

We begin with the following straightforward observations.

Observation 1. 1 Trace of $A_{i_a}(G) = i_a(G)$.

Observation 2. 2 Suppose $a_0\mu^n + a_1\mu^{n-1} + \dots + a_n$ be the characteristic polynomial of an AIDM of G . Then

- (i) $a_0 = 1$
- (ii) $a_1 = -i_a(G)$
- (iii) $a_2 = -(m - i_a(G))$
- (iv) $a_n = \det(A_{i_a}(G))$

Observation 3. 3 Suppose $\mu_1 \geq \mu_2 \geq \mu_3 \geq \dots \geq \mu_n$ are the accurate independent eigenvalues of AIDM of G . Then

- (i) $\sum_{i=1}^n \mu_i = i_a(G)$
- (ii) $\sum_{i=1}^n \mu_i^2 = 2m + i_a(G)$

In the next successive propositions we obtain the characteristic polynomial of AIDM of the star graph $K_{1, n-1}$ and the complete bipartite graph $K_{r, s}; 2 \leq r < s$.

Proposition 4. 4 The characteristic polynomial of AIDM of $K_{1, n-1}$ is $\mu^{n-2}[\mu^2 - \mu - (n-1)]$.

Proof. Consider the star graph $K_{1, n-1}$ with the central vertex v_1 . Clearly, the accurate independent dominating set of $K_{1, n-1}$ is $D_{i_a} = \{v_1\}$. Hence the AIDM of $K_{1, n-1}$ is

$$A_{i_a}(K_{1, n-1}) = \begin{bmatrix} 1 & 1 & 1 & 1 & \dots & 1 \\ 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & \dots & 0 \end{bmatrix}$$

The characteristic polynomial of AIDM of $K_{1, n-1}$ is

$$|\mu I_n - A_{i_a}(K_{n-1})| = 0$$

$$\begin{vmatrix} \mu - 1 & -1 & -1 & -1 & \dots & -1 \\ -1 & \mu & 0 & 0 & \dots & 0 \\ -1 & 0 & \mu & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -1 & 0 & 0 & 0 & \dots & \mu \end{vmatrix} = 0.$$

From the above we get the following recurrence relation:

$$\phi_n(K_{1, n-1}, \mu) = -\mu^{n-2} + \mu\phi_{n-1}(K_{1, n-2}, \mu) \quad (2)$$

changing n to $n - 1$ in (2), we get

$$\phi_n(K_{1, n-2}, \mu) = -\mu^{n-3} + \mu\phi_{n-2}(K_{1, n-3}, \mu) \quad (3)$$

continuing this process, we obtain

$$\phi_n(K_{1, n-1}, \mu) = \mu^{n-2}[\mu^2 - \mu - (n - 1)].$$

Proposition 5.5 The characteristic polynomial of AIDM of $K_{r, s}$; $2 \leq r < s$ is

$$(\mu - 1)^{r-1} \mu^{s-1} [\mu^2 - \mu - rs]$$

Proof. Consider the complete bipartite graph $K_{r, s}$; $2 \leq r < s$ with vertex set $V = V_1 \cup V_2$ where $V_1 = \{v_1, v_2, \dots, v_r\}$ and $V_2 = \{u_1, u_2, \dots, u_s\}$. Clearly, $D_{i_a}(K_{r, s}) = V_2$. Therefore the AIDM of $K_{r, s}$ is

$$A_{i_a}(K_{r, s}) = \begin{bmatrix} O_r & J_{rs} \\ J_{sr} & I_s \end{bmatrix}$$

where J_{rs} and J_{sr} are the matrices with all entries 1 's and I_s is an identity matrix of order s .

The characteristic polynomial of AIDM of $K_{r, s}$ is

$$\begin{aligned} \phi_n(K_{r, s}, \mu) &= \begin{vmatrix} \mu I_r & -J_{rs} \\ -J_{sr} & (\mu - 1)I_s \end{vmatrix} \\ &= |(\mu - 1)I_s| |\mu I_r - J_{rs} \frac{I_r}{(\mu - 1)} J_{sr}| \\ &= (\mu - 1)^{s-r} |\mu(\mu - 1) - J_{rs} J_{sr} I_r| \\ &= (\mu - 1)^{s-r} (\mu(\mu - 1) - rs(\mu(\mu - 1)^{r-1})). \end{aligned}$$

Now we obtain bounds for $E_{i_a}(G)$ of G similar to McClelland's inequalities [22] for graph energy.

Theorem 6.6 Let G be a graph of order n and size m with accurate independent domination number $i_a(G)$. Then

$$E_{i_a}(G) \leq \sqrt{n(2m + i_a(G))}. \quad (4)$$

Proof. Let $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$ be the eigenvalues of $A_{i_a}(G)$. Bearing in mind the Cauchy-Schwarz inequality,

$$\left(\sum_{i=1}^n a_i b_i\right)^2 \leq \left(\sum_{i=1}^n a_i^2\right) \left(\sum_{i=1}^n b_i^2\right)$$

we choose $a_i = 1$ and $b_i = |\mu_i|$, which implies

$$\begin{aligned} E_{i_a}^2 &\leq \left(\sum_{i=1}^n 1\right)^2 \left(\sum_{i=1}^n |\mu_i|\right)^2 \\ &\leq n \left(\sum_{i=1}^n |\mu_i|^2\right) \\ &= n \sum_{i=1}^n \mu_i^2 \\ &= n(2m + i_a(G)) \end{aligned}$$

$$E_{i_a}(G) \leq \sqrt{n(2m + i_a(G))}.$$

Theorem 7.7 Let G be a graph of order n and size m with accurate independent domination number $i_a(G)$. Let $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$ be a non-increasing arrangement of eigenvalues of $A_{i_a}(G)$. Then

$$E_{i_a}(G) \geq \sqrt{2mn + ni_a(G) - \alpha(n)(|\mu_1| - |\mu_n|)^2} \quad (5)$$

where $\alpha(n) = n \lfloor \frac{n}{2} \rfloor (1 - \frac{1}{n} \lfloor \frac{n}{2} \rfloor)$, where $\lfloor x \rfloor$ denotes the integer part of a real number x .

Proof. Let a_1, a_2, \dots, a_n and b_1, b_2, \dots, b_n be real numbers for which there exist real constants a, b, A and B , so that for each i , $i = 1, 2, \dots, n$, $a \leq a_i \leq A$ and $b \leq b_i \leq B$. Then the following inequality is valid

$$\left| n \sum_{i=1}^n a_i b_i - \sum_{i=1}^n a_i \sum_{i=1}^n b_i \right| \leq \alpha(n)(A - a)(B - b) \quad (6)$$

where $\alpha(n) = n \lfloor \frac{n}{2} \rfloor (1 - \frac{1}{n} \lfloor \frac{n}{2} \rfloor)$. Equality holds if and only if $a_1 = a_2 = \dots = a_n$ and $b_1 = b_2 = \dots = b_n$.

We choose $a_i = |\mu_i|, b_i = |\mu_i|, a = b = |\mu_n|$ and $A = B = |\mu_1|, i = 1, 2, \dots, n$, inequality (6) becomes

$$\left| n \sum_{i=1}^n |\mu_i|^2 - \left(\sum_{i=1}^n |\mu_i|\right)^2 \right| \leq \alpha(n)(|\mu_1| - |\mu_n|)^2 \quad (7)$$

Since $E_{i_a}(G) = \sum_{i=1}^n |\mu_i|, \sum_{i=1}^n |\mu_i|^2 = 2m + i_a(G)$ and

$$E_{i_a}(G) \leq \sqrt{n(2m + i_a(G))},$$

the inequality (7) becomes

$$n(2m + i_a(G)) - (E_{i_a})^2 \leq \alpha(n)(|\mu_1| - |\mu_n|)^2$$

$(E_{i_a})^2 \geq 2mn + ni_a(G) - \alpha(n)(|\mu_1| - |\mu_n|)^2$. Hence the equality holds if and only if $\mu_1 = \mu_2 = \dots = \mu_n$.

Corollary 8.8 Let G be a graph of order n and size m with accurate independent domination number $i_a(G)$. Let

$\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$ be a non-increasing arrangement of eigenvalues of $A_{i_\alpha}(G)$. Then

$$E_{i_\alpha}(G) \geq \sqrt{2mn + ni_\alpha(G) - \frac{n^2}{4}(|\mu_1| - |\mu_n|)^2} \quad (8)$$

Proof. Since $\alpha(n) = n \binom{n}{2} (1 - \frac{1}{n} \binom{n}{2}) \leq \frac{n^2}{4}$, therefore by (5), result follows.

Theorem 9.9 Let G be a graph of order n and size m with accurate independent domination number $i_\alpha(G)$. Let $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$ be a non-increasing arrangement of eigenvalues of $A_{i_\alpha}(G)$. Then

$$E_{i_\alpha}(G) \geq \frac{|\mu_1||\mu_n|n + 2m + i_\alpha(G)}{|\mu_1| + |\mu_n|} \quad (9)$$

Proof. Let a_1, a_2, \dots, a_n and b_1, b_2, \dots, b_n be real numbers for which there exist real constants r and R so that for each $i, i = 1, 2, \dots, n$ holds $ra_i \leq b_i \leq Ra_i$. Then the following inequality is valid.

$$\sum_{i=1}^n b_i^2 + rR \sum_{i=1}^n a_i^2 \leq (r + R) \sum_{i=1}^n a_i b_i. \quad (10)$$

Equality of (10) holds if and only if, for at least one $i, 1 \leq i \leq n$ holds $ra_i = b_i = Ra_i$.

For $b_i = |\mu_i|, a_i = 1, r = |\mu_n|$ and $R = |\mu_1|, i = 1, 2, \dots, n$ inequality (10) becomes

$$\sum_{i=1}^n |\mu_i|^2 + |\mu_1||\mu_n| \sum_{i=1}^n 1 \leq (|\mu_1| + |\mu_n|) \sum_{i=1}^n |\mu_i|. \quad (11)$$

Since $\sum_{i=1}^n |\mu_i|^2 = \sum_{i=1}^n \mu_i^2 = 2m + i_\alpha(G)$,

$$\sum_{i=1}^n |\mu_i| = E_{i_\alpha}(G), \text{ from inequality (11),}$$

$$2m + i_\alpha(G) + |\mu_1||\mu_n|n \leq (\mu_1 + \mu_n)E_{i_\alpha}(G)$$

Hence the result.

Theorem 10.10 Let G be a graph of order n and size m with accurate independent domination number $i_\alpha(G)$. Let $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$ be a non-increasing arrangement of eigenvalues of $A_{i_\alpha}(G)$. If $\xi = \det A_{i_\alpha}(G)$, then

$$E_{i_\alpha}(G) \geq \sqrt{2m + i_\alpha(G) + n(n-1)\xi^{\frac{2}{n}}}. \quad (12)$$

Proof.

$$\begin{aligned} (E_{i_\alpha}(G))^2 &= \left(\sum_{i=1}^n |\mu_i|\right)^2 \\ &= \sum_{i=1}^n |\mu_i|^2 + \sum_{i \neq j} |\mu_i||\mu_j|. \end{aligned}$$

Employing the inequality between the arithmetic and geometric means, we obtain

$$\frac{1}{n(n-1)} \sum_{i \neq j} |\mu_i||\mu_j| \geq \left(\prod_{i \neq j} |\mu_i||\mu_j|\right)^{\frac{1}{n(n-1)}}.$$

Thus,

$$\begin{aligned} (E_{i_\alpha}(G))^2 &\geq \sum_{i=1}^n \mu_i^2 + n(n-1) \left(\prod_{i \neq j} |\mu_i||\mu_j|\right)^{\frac{1}{n(n-1)}} \\ &\geq \sum_{i=1}^n \mu_i^2 + n(n-1) \left(\prod_{i \neq j} |\mu_i|^{2(n-1)}\right)^{\frac{1}{n(n-1)}} \\ &= 2m + i_\alpha(G) + n(n-1)\xi^{\frac{2}{n}}. \end{aligned}$$

Next, we obtain Koolen and Moulton's [13] type inequality for $E_{i_\alpha}(G)$.

Theorem 11.11 If G is a graph of order n and size m and $2m + i_\alpha(G) \geq n$, then

$$E_{i_\alpha}(G) \leq \frac{2m + i_\alpha(G)}{n} + \sqrt{(n-1) \left[(2m + i_\alpha(G)) - \left(\frac{2m + i_\alpha(G)}{n}\right)^2 \right]} \quad (13)$$

Proof. Bearing in mind the Cauchy-Schwarz inequality,

$$\left(\sum_{i=1}^n a_i b_i\right)^2 \leq \left(\sum_{i=1}^n a_i\right)^2 \left(\sum_{i=1}^n b_i\right)^2.$$

Put $a_i = 1$ and $b_i = |\mu_i|$ then

$$\begin{aligned} \left(\sum_{i=1}^n a_i b_i\right)^2 &\leq (n-1) \left(\sum_{i=1}^n b_i\right)^2 \\ (E_{i_\alpha}(G) - \mu_1)^2 &\leq (n-1)(2m + i_\alpha(G) - \mu_1^2) \\ E_{i_\alpha}(G) &\leq \mu_1 + \sqrt{(n-1)(2m + i_\alpha(G) - \mu_1^2)}. \end{aligned}$$

Let

$$f(x) = x + \sqrt{(n-1)(2m + i_\alpha(G) - x^2)} \quad (14)$$

For decreasing function

$$\begin{aligned} f'(x) &\leq 0 \\ \Rightarrow 1 - \frac{x(n-1)}{\sqrt{(n-1)(2m + i_\alpha(G) - x^2)}} &\leq 0 \end{aligned}$$

$$x \geq \sqrt{\frac{2m + i_\alpha(G)}{n}}.$$

Since $(2m + i_\alpha(G)) \geq n$,

we have $\sqrt{\frac{2m+i_a(G)}{n}} \leq \frac{2m+i_a(G)}{n} \leq \mu_1$.

Also $f(\mu_1) \leq f\left(\frac{2m+i_a(G)}{n}\right)$.

$$\text{i.e } E_{i_a}(G) \leq f(\mu_1) \leq f\left(\frac{2m+i_a(G)}{n}\right).$$

$$\text{i.e } E_{i_a}(G) \leq f\left(\frac{2m+i_a(G)}{n}\right)$$

Hence, the result (13) follows.

OPEN PROBLEMS

We close with the following list of open problems for further research in spectral theory of graphs:

Problem 1 Construct graphs with $E(G) = E_{i_a}(G)$.

Problem 2 Characterize graphs with equal Laplacian energy and accurate independent dominating energy.

ACKNOWLEDGEMENTS

The work was partially supported by the University Grants Commission(UGC), New Delhi, India through UGC-SAP-DRS-III, 2016-2021: F.510/3/DRS-III/2016(SAP-I).

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