

Doubly-Connected Dominating Energy of Graphs

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Abstract

A connected dominating set D is said to be doubly-connected dominating set if the subgraph induced by the set $V - D$ is connected. In this paper, we have defined a matrix called the doubly connected dominating matrix and obtained the the corresponding spectra and energy. Further, we have obtained the chemical applicability of the doubly connected energy followed by the mathematical properties.

Keywords: Dominating set, Energy, Dominating energy, doubly-Dominating energy.

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1 Introduction

All graphs considered in this paper are finite, simple and undirected. In particular, these graphs do not have loops. Let $G = (V, E)$ be a graph with the vertex set $V(G) = \{v_1, v_2, v_3, \dots, v_n\}$ and the edge set $E(G) = \{e_1, e_2, e_3, \dots, e_m\}$, that is $|V(G)| = n$ and $|E(G)| = m$. The vertex u and v are adjacent if $uv \in E(G)$. The open(closed) neighborhood of a vertex $v \in V(G)$ is $N(v) = \{u : uv \in E(G)\}$ and $N[v] = N(v) \cup \{v\}$ respectively. The degree of a vertex $v \in V(G)$ is denoted by $d_G(v)$ and is defined as $d_G(v) = |N(v)|$. A vertex $v \in V(G)$ is pendant if $|N(v)| = 1$ and is called supporting vertex if it is adjacent to pendant vertex. Any vertex $v \in V(G)$ with $|N(v)| > 1$ is called internal vertex. If $d_G(v) = r$ for every vertex $v \in V(G)$, where $r \in \mathbb{Z}^+$ then G is called r -regular. If $r = 2$ then it is called cycle graph C_n and for $r = 3$ it is called the cubic graph. A graph G is unicyclic if $|V| = |E|$. A graph G is called a block graph, if every block in G is a complete graph. For undefined terminologies we refer the reader to [16].

A subset $D \subseteq V(G)$ is called dominating set if $N[D] = V(G)$. The minimum cardinality of such a set D is called the domination number $\gamma(G)$ of G . A dominating set D is connected if the subgraph induced by D is connected. The minimum cardinality of connected dominating set D is called the connected dominating number $\gamma_c(G)$ of G . A connected dominating set D is said to be doubly-connected dominating set if the subgraph induced by the set $V - D$ is connected. The minimum cardinality of such set is called the doubly connected domination number. It is denoted by $\gamma_{cc}(G)$. [27].

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 [13] and having a clear connection to chemical problems [15], has in newer times attracted much attention of mathematicians and mathematical chemists [3,8–12,20,22–24,28,30,31].

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 [15], distance [17], incidence [18], minimum covering energy [1] etc. Recall that a great variety of matrices has so far been associated with graphs [4,5,10,29].

Recently in [25] the authors have studied the dominating matrix which is defined as : Let $G = (V, E)$ be a graph with $V(G) = \{v_1, v_2, \dots, v_n\}$ and let $D \subseteq V(G)$ be a minimum dominating set of G . The minimum dominating matrix of G is the $n \times n$ matrix defined by $A_D(G) = (a_{ij})$, where $a_{ij} = 1$ if $v_i v_j \in E(G)$ or $v_i = v_j \in D$, and $a_{ij} = 0$ if $v_i v_j \notin E(G)$.

The characteristic polynomial of $A_D(G)$ is denoted by $f_n(G, \mu) := \det(\mu I - A_D(G))$.

The minimum dominating eigenvalues of a graph G are the eigenvalues of $A_D(G)$. Since $A_D(G)$ 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 minimum dominating energy of G is then defined as

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

Motivated by dominating matrix, here we define the minimum doubly-connected dominating matrix abbreviated as (c-dominating matrix). The c-dominating matrix of G is the $n \times n$ matrix defined by $A_{D_c}(G) = (a_{ij})$, where

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

The characteristic polynomial of $A_{D_{cc}}(G)$ is denoted by $f_n(G, \lambda) := \det(\lambda I - A_{D_{cc}}(G))$.

The doubly-connected-dominating eigenvalues of a graph G are the eigenvalues of $A_{D_{cc}}(G)$. Since $A_{D_{cc}}(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The doubly-connected-dominating energy of G is then defined as

$$E_{D_{cc}}(G) = \sum_{i=1}^n |\lambda_i|.$$

To illustrate this, consider the following examples:

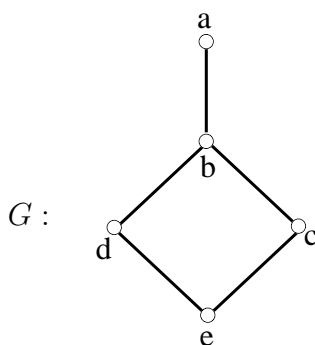


Figure 1.

Example 1. Let G be a graph with vertices $\{a, b, c, d, e\}$ and let its minimum doubly-connected dominating set be $D_{cc} = \{a, b, c\}$. Then

$$A_{D_{cc}}(G) = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

The characteristic polynomial of $A_{D_{cc}}(G)$ is $\lambda^5 - 3\lambda^4 - \lambda^3 + 6\lambda^2 - 2\lambda = 0$. The minimum doubly-connected dominating eigenvalues are $\lambda_1 = 2.61803$, $\lambda_2 = 1.41421$, $\lambda_3 = 0.38196$, $\lambda_4 = 0.000$ and $\lambda_5 = -1.41421$.

Therefore, the minimum doubly-connected dominating energy is $E_{D_{cc}}(G) = 5.8355$.

In this paper, we are interested in studying the mathematical aspects of the c-dominating energy of a graph. This paper has organized as follows: The section 1,

the chemical applicability of c-dominating energy for molecular graphs G . The section 3, contains the mathematical properties of c-dominating energy. In the last section, we have characterized, trees, unicyclic graphs and cubic graphs and block graphs with equal minimum dominating energy and c-dominating energy. Finally, we conclude this paper by posing an open problem.

2 Chemical Applicability of $E_{D_{cc}}(G)$

We have used the doubly-dominating energy for modeling eight representative physical properties like boiling points(bp), molar volumes(mv) at $20^{\circ}C$, molar refractions(mr) at $20^{\circ}C$, heats of vaporization (hv) at $25^{\circ}C$, critical temperatures(ct), critical pressure(cp) and surface tension (st) at $20^{\circ}C$ of the 74 alkanes from ethane to nonanes. Values for these properties were taken from <http://www.molecularDescriptors.eu/dataset.htm>. The doubly-dominating energy $E_{D_{cc}}(G)$ was correlated with each of these properties and surprisingly, we can see that the $E_{D_{cc}}$ has a good correlation with the critical temperature of alkanes with correlation coefficient $r = 0.896$.

The following structure-property relationship model has been developed for the doubly connected-dominating energy $E_{D_{cc}}(G)$.

$$ct = 135.128 + [E(D_{cc})(G)]4.317 \quad (1)$$

$$ct = 10.791[E(D_{cc})(G)]^2 - 0.0101[E(D_{cc})(G)] + 70.999 \quad (2)$$

$$ct = -53.591 + \ln[E(D_{cc})(G)]100.568 \quad (3)$$

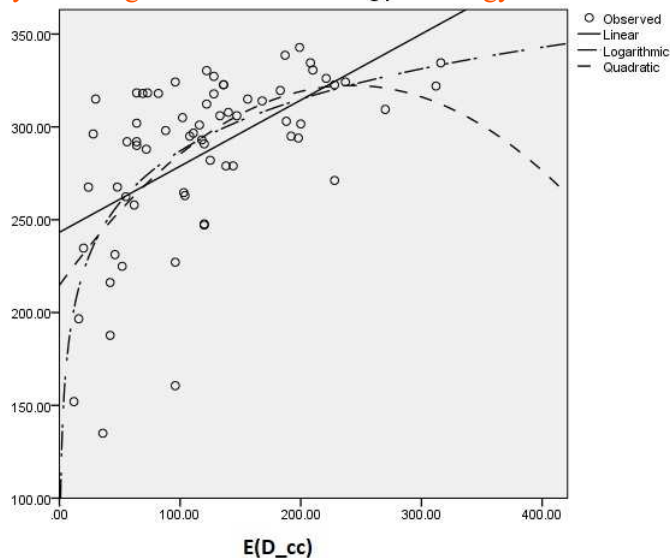


Figure 3: Correlation of $E_{D_{cc}}(G)$ with critical temperature of alkanes.

3 Mathematical Properties of Doubly Connected-Dominating Energy of Graph

We begin with the following straightforward observations.

Observation 1. Note that the trace of $A_{D_{cc}}(G) = \gamma_c c(G)$.

Observation 2. Let $G = (V, E)$ be a graph with $\gamma_c c$ -set D_{cc} . Let $f_n(G, \lambda) = c_0 \lambda^n + c_1 \lambda^{n-1} + \cdots + c_n$ be the characteristic polynomial of G . Then

1. $c_0 = 1$,
2. $c_1 = -|D_{cc}| = -\gamma_c c(G)$.

Theorem 3. If $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of $A_{D_{cc}}(G)$, then

1. $\sum_{i=1}^n \lambda_i = \gamma_c c(G)$
2. $\sum_{i=1}^n \lambda_i^2 = 2m + \gamma_c c(G)$.

Proof.

1. Follows from Observation 1.

Therefore

$$\begin{aligned}\sum_{i=1}^n \lambda_i^2 &= \sum_{i=1}^n \sum_{j=1}^n a_{ij} a_{ji} \\ &= 2 \sum_{i < j} (a_{ij})^2 + \sum_{i=1}^n (a_{ii})^2 \\ &= 2m + \gamma_c c(G).\end{aligned}$$

□

We now obtain bounds for $E_{D_{cc}}(G)$ of G , similar to McClelland's inequalities [21] for graph energy.

Theorem 4. *Let G be a graph of order n and size m with $\gamma_{cc}(G) = k$. Then*

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

Proof. Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ be the eigenvalues of $A_{D_{cc}}(G)$. 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 $b_i = |\lambda_i|$, which by Theorem 3 implies

$$\begin{aligned}E_{D_{cc}}^2 &= \left(\sum_{i=1}^n |\lambda_i| \right)^2 \\ &\leq n \left(\sum_{i=1}^n |\lambda_i|^2 \right) \\ &= n \sum_{i=1}^n \lambda_i^2 \\ &= 2(2m + k).\end{aligned}$$

□

Theorem 5. *Let G be a graph of order n and size m with $\gamma_{cc}(G) = k$. Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ be a non-increasing arrangement of eigenvalues of $A_{D_{cc}}(G)$. Then*

$$E_{D_{cc}}(G) \geq \sqrt{2mn + nk - \alpha(n)(|\lambda_1| - |\lambda_n|)^2} \quad (5)$$

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

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

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

We choose $a_i := |\lambda_i|, b_i := |\lambda_i|, a = b := |\lambda_n|$ and $A = B := |\lambda_1|, i = 1, 2, \dots, n$, inequality (4) becomes

$$\left| n \sum_{i=1}^n |\lambda_i|^2 - \left(\sum_{i=1}^n |\lambda_i| \right)^2 \right| \leq \alpha(n)(|\lambda_1| - |\lambda_n|)^2. \quad (7)$$

Since $E_{G_{cc}}(G) = \sum_{i=1}^n |\lambda_i|, \sum_{i=1}^n |\lambda_i|^2 = \sum_{i=1}^n |\lambda_i|^2 = 2m + k$ and $E_{D_{cc}}(G) \leq \sqrt{n(2m + k)}$, the inequality (5) becomes

$$\begin{aligned} n(2m + k) - (E_{D_{cc}})^2 &\leq \alpha(n)(|\lambda_1| - |\lambda_n|)^2 \\ (E_{D_{cc}})^2 &\geq 2mn + nk - \alpha(n)(|\lambda_1| - |\lambda_n|)^2. \end{aligned}$$

Hence equality holds if and only if $\lambda_1 = \lambda_2 = \dots = \lambda_n$. \square

Corollary 6. Let G be a graph of order n and size m with $\gamma_{cc}(G) = k$. Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ be a non-increasing arrangement of eigenvalues of $A_{D_{cc}}(G)$. Then

$$E_{D_{cc}}(G) \geq \sqrt{2mn + nk - \frac{n^2}{4}(|\lambda_1| - |\lambda_n|)^2}. \quad (8)$$

Proof. Since $\alpha(n) = n[\frac{n}{2}](1 - \frac{1}{n}[\frac{n}{2}]) \leq \frac{n^2}{4}$, therefore by (3), result follows. \square

Theorem 7. Let G be a graph of order n and size m with $\gamma_c(G) = k$. Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ be a non-increasing arrangement of eigenvalues of $A_{D_{cc}}(G)$. Then

$$E_{G_{cc}}(G) \geq \frac{|\lambda_1||\lambda_2|n + 2m + k}{|\lambda_1| + |\lambda_n|}. \quad (9)$$

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 (see [11]).

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

For $b_i := |\lambda_i|$, $a_i := 1$, $r := |\lambda_n|$ and $R := |\lambda_1|$, $i = 1, 2, \dots, n$ inequality (8) becomes

$$\sum_{i=1}^n |\lambda_i|^2 + |\lambda_1| |\lambda_n| \sum_{i=1}^n 1 \leq (|\lambda_1| + |\lambda_n|) \sum_{i=1}^n |\lambda_i|. \quad (11)$$

Since $\sum_{i=1}^n |\lambda_i|^2 = \sum_{i=1}^n \lambda_i^2 = 2m + k$, $\sum_{i=1}^n |\lambda_i| = E_{D_{cc}}(G)$, from inequality (9),

$$2m + k + |\lambda_1| |\lambda_n| n \leq (|\lambda_1| + |\lambda_n|) E_{D_{cc}}(G)$$

Hence the result. □

Theorem 8. Let G be a graph of order n and size m with $\gamma_{cc}(G) = k$. If $\xi = |\det A_{D_c}(G)|$, then

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

Proof.

$$\begin{aligned} (E_{D_{cc}}(G))^2 &= \left(\sum_{i=1}^n |\lambda_i| \right)^2 \\ &= \sum_{i=1}^n |\lambda_i|^2 + \sum_{i \neq j} |\lambda_i| |\lambda_j|. \end{aligned}$$

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

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

Thus,

$$\begin{aligned} (E_{D_{cc}})^2 &\geq \sum_{i=1}^n |\lambda_i|^2 + n(n-1) \left(\prod_{i \neq j} |\lambda_i| |\lambda_j| \right)^{\frac{1}{n(n-1)}} \\ &\geq \sum_{i=1}^n |\lambda_i|^2 + n(n-1) \left(\prod_{i \neq j} |\lambda_i|^{2(n-1)} \right)^{\frac{1}{n(n-1)}} \\ &= 2m + k + n(n-1)\xi^{\frac{2}{n}}. \end{aligned}$$

□

Lemma 9. If $\lambda_1(G)$ is the largest minimum doubly-connected dominating eigenvalue of $A_{D_{cc}}(G)$, then $\lambda_1 \geq \frac{2m + \gamma_{cc}(G)}{n}$.

Therefore, $\lambda_1(A_{D_c}(G)) \geq \frac{J'AJ}{J'J} = \frac{2m+\gamma_c c(G)}{n}$. \square

Next, we obtain Koolen and Moulton's [19] type inequality for $E_{D_{cc}}(G)$.

Theorem 10. *If G is a graph of order n and size m and $2m + \gamma_c c(G) \geq n$, then*

$$E_{D_{cc}}(G) \leq \frac{2m + \gamma_c c(G)}{n} + \sqrt{(n-1) \left[(2m + \gamma_c c(G)) - \left(\frac{2m + \gamma_c c(G)}{n} \right)^2 \right]}. \quad (13)$$

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 $b_i = |\lambda_i|$ then

$$\begin{aligned} \left(\sum_{i=2}^n a_i b_i \right)^2 &\leq (n-1) \left(\sum_{i=2}^n b_i \right)^2 \\ (E_{D_{cc}}(G) - \lambda_1)^2 &\leq (n-1)(2m + \gamma_c c(G) - \lambda_1^2) \\ E_{D_{cc}}(G) &\leq \lambda_1 + \sqrt{(n-1)(2m + \gamma_c c(G) - \lambda_1^2)}. \end{aligned}$$

Let

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

For decreasing function

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

Since $(2m + k) \geq n$, we have $\sqrt{\frac{2m+\gamma_{cc}(G)}{n}} \leq \frac{2m+\gamma_{cc}(G)}{n} \leq \lambda_1$. Also $f(\lambda_1) \leq f\left(\frac{2m+\gamma_{cc}(G)}{n}\right)$.

$$\begin{aligned} \text{i.e } E_{D_{cc}}(G) &\leq f(\lambda_1) \leq f\left(\frac{2m+\gamma_{cc}(G)}{n}\right). \\ \text{i.e } E_{D_{cc}}(G) &\leq f\left(\frac{2m+\gamma_{cc}(G)}{n}\right) \end{aligned}$$

Hence by (12), the result follows. \square

We conclude this paper by posing the following open problem for the researchers:

Open Problem: Construct non- cospectral graphs with unequal dominating, connected dominating and total dominating energy with respect to doubly-connected dominating energy.

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