BOUNDS ON THE DISTANCE-DEGREE ENERGY AND DISTANCE-DEGREE SPECTRAL RADIUS OF GRAPHS

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Abstract

The study of graphs through their associated matrices have always been immensely advantageous. The most natural generalization of various types of energy, namely the distance energy, Harary energy, etc. was introduced recently using the notion of distance-degree energy which in turn is derived from the distance-degree matrix that imbibes both the degree of the vertices in a graph and the distance between them. In this paper, we obtain several analytic expressions and bounds for the distance-degree energy and distance-degree spectral radius of graphs.

Keywords: Distance-Degree Energy, Distance-Degree Spectral Radius, vertex-distance-vertex-degree matrix, bounds
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1. Introduction

In the booming era of graph theory, various concepts have gained importance due to their practical significance which has also led to the growth of mathematics in manifold ways. The study of different aspects of abstract objects and generalizing various notions have always interested mathematicians through the decades. One such generalization of the graph invariant, namely distance-degree energy was introduced by Sarah Surya et. al [8]., with the motivation to understand the behaviour of matrices associated to the graphs which in turn induces both the degree of the vertices and the distance between them.

The various types of topological indices are molecular descriptors which characterize different classes of graphs [3, 9, 11, 13]. Also, the parameters derived from various matrices associated to graphs have also found successful implications in several fields [10]. In this direction, it is necessary to investigate the newly introduced parameter, namely the distance-degree energy for several family of graphs.

To this end, the search for analytic expressions that interconnects the parameters derived from the distance-degree matrix was established. We denote the distance-degree matrix of a graph G by $DD(G)$, the distance-degree energy of G by $DDE(G)$ and assume that all the graphs considered in this article are finite, undirected, simple and connected.

The motivation for this article comes from our interest to obtain several lower and upper bounds for the newly defined variant of energy, namely, the distance-degree energy of a graph. The combinations of the notions of degree and distance in a graph to obtain a graph invariant of energy has been initiated recently by the definition of distance-degree energy to look up to what the society can advantageously benefit. The natural question one can ask is that if this new variant of energy inherit any of the properties of its forefathers, namely the energy or distance energy? At the same time, it is also worthy to note that various results on energy and distance energy of graphs can be found in [2, 6, 12]. In this connection, we have studied the distance-degree matrix and acquired some bounds for the parameters arising from it, that is, the distance-degree energy and distance-degree spectral radius.
Further, we have also derived different bounds for the distance-degree spectral radius and produced some interesting results for the behaviour of these parameters in regular graphs of diameter 2 due to its practical significance.

2. Preliminaries

The vertex-distance-vertex-degree matrix, which we call as the distance-degree matrix of G, was introduced by O. Ivanciuc in his subsequent papers in 1999 and 2000 [4, 5] and formally defined as follows:

Definition 1. [4, 5] For a simple graph G with V number of vertices, the vertex-distance-vertex-degree matrix $DD(G)$, is defined as a $V \times V$ matrix with the condition that

$$DD(G)_{ij} = \begin{cases} l^p(ij)d^q(i)d^r(j), & \text{if } i \neq j \\ 0, & \text{otherwise} \end{cases}$$

where $l(ij)$ is the length of the shortest path between the vertices i and j and $d(i)$, $d(j)$ denote the degrees of the vertices i and j respectively. The parameters p, q and r are natural numbers.

Definition 2. [8] Distance-Degree Energy of a graph, denoted by $DDE(G)$, is defined as the absolute sum of the eigenvalues of its vertex-distance-vertex-degree matrix.

Definition 3. The largest eigenvalue obtained from the distance-degree matrix of a graph G is called as its distance-degree spectral radius, denoted by $\lambda_1(G)$.

Definition 4. [7] If A is a real $n \times n$ symmetric matrix, then the Rayleigh quotient is defined as $r(x) = \frac{x^T A x}{x^T x}$, for any n-dimensional real vector $x \neq 0$.

3. Bounds on Distance-Degree Energy

This section contains some bounds on the distance-degree energy of graphs and the determinant of their distance-degree matrices.

Theorem 1. $|\det(DD(G))| \leq |\lambda_1|^n$.
Proof. The result can be derived from the fact that $|\det(DD(G))| \leq |\lambda_1||\lambda_2| \cdots |\lambda_n|$ □

Theorem 2. For any connected graph G, $DDE(G) \geq n$.
Proof. Using the relation that the arithmetic mean of a set of numbers is always greater than or equal to its harmonic mean, we see that,

$$\frac{\lambda_1 + \lambda_2 + \cdots + \lambda_n}{n} \geq \frac{n}{\frac{1}{\lambda_1} + \frac{1}{\lambda_2} + \cdots + \frac{1}{\lambda_n}}$$

$$\frac{DDE(G)}{n} \geq \frac{n \times \lambda_1 \lambda_2 \cdots \lambda_n}{\lambda_2 \lambda_3 \cdots \lambda_n + \lambda_1 \lambda_3 \cdots \lambda_n + \cdots + \lambda_1 \lambda_2 \cdots \lambda_{n-1}}$$

$$\frac{DDE(G)}{n} \geq \frac{n det(DD(G))}{n(\lambda_1 \lambda_2 \cdots \lambda_n)}$$

and hence the result follows. □

Theorem 3. $DDE(G) \geq n\left[\det\left(DD(G)\right)\right]^{2/n}$, for any connected graph G.
Proof. We know that the arithmetic mean A, geometric mean G and the harmonic mean H of any set of numbers are connected by the relation $G^2 = AH$

Thus, $(\lambda_1 \lambda_2 \cdots \lambda_n)^{2/n} = \frac{\lambda_1 + \lambda_2 + \cdots + \lambda_n}{n} \times \frac{n}{\frac{1}{\lambda_1} + \frac{1}{\lambda_2} + \cdots + \frac{1}{\lambda_n}}$

$$(\lambda_1 \lambda_2 \cdots \lambda_n)^{2/n} = DDE(G) \times \frac{\lambda_1 \lambda_2 \cdots \lambda_n}{n(\lambda_1 \lambda_2 \cdots \lambda_n)}$$

$$DDE(G) \geq n(\lambda_1 \lambda_2 \cdots \lambda_n)^{2/n}$$

$$DDE(G) \geq n\left[\det\left(DD(G)\right)\right]^{2/n}$$

□

4. Bounds on Distance-Degree Spectral Radius

In this section, we obtain several lower bounds and upper bounds for the distance-degree spectral radius of graphs in terms of their distance-degree energy, number of vertices and determinant of their distance-degree matrices.

Theorem 4. For any graph G, $|\lambda_1| \geq |\det(DD(G))|^{1/n}$.
Proof. By means of using the relation that the arithmetic mean of a set of numbers is greater than or equal to its geometric mean, we see that,

$$\frac{|\lambda_1| + |\lambda_2| + \cdots + |\lambda_n|}{n} \geq |\lambda_1 \lambda_2 \cdots \lambda_n|^{1/n}$$

$$\frac{n|\lambda_1|}{n} \geq |\det(DD(G))|^{1/n}$$

from which the result follows. □

Theorem 5. For any connected graph G, $\lambda_1(G) \geq \frac{1}{n}$.

Proof. The following can be obtained by employing the fact that the geometric mean of a set of numbers is greater than or equal to its harmonic mean.

$$(\lambda_1\lambda_2 \cdots \lambda_n)^{1/n} \geq \frac{n}{\frac{1}{\lambda_1} + \frac{1}{\lambda_2} + \cdots + \frac{1}{\lambda_n}}$$

$$(n\lambda_1)^{1/n} \geq \frac{n}{\frac{\lambda_2\lambda_3 \cdots \lambda_n + \lambda_1\lambda_3 \cdots \lambda_n + \cdots + \lambda_1\lambda_2 \cdots \lambda_{n-1}}{\lambda_1\lambda_2 \cdots \lambda_n}}$$

$$(n\lambda_1)^{1/n} \geq \frac{n \det(DD(G))}{n[\lambda_1\lambda_2 \cdots \lambda_n]}$$

$$(n\lambda_1)^{1/n} \geq 1$$

$$\lambda_1^{1/n} \geq \frac{1}{n^{1/n}}$$

and hence the result follows. □

Theorem 6. For any connected graph G, $\lambda_1 \geq \frac{(1-\frac{1}{n})^{1-\frac{1}{n}}}{[\det(DD(G))]^{1/n}}$.

Proof. Using the relation between geometric mean and harmonic mean for the $n - 1$ eigenvalues λ_2, λ_3, …, λ_n, we obtain

$$(\lambda_2\lambda_3 \cdots \lambda_n)^{1/n-1} \geq \frac{n-1}{\frac{1}{\lambda_2} + \frac{1}{\lambda_3} + \cdots + \frac{1}{\lambda_n}}$$

$$[\frac{\det(DD(G))}{\lambda_1}]^{\frac{1}{n-1}} \geq \frac{n-1}{\frac{\lambda_3\lambda_4 \cdots \lambda_n + \lambda_2\lambda_4 \cdots \lambda_n + \cdots + \lambda_2\lambda_3 \cdots \lambda_{n-1}}{\lambda_2\lambda_3 \cdots \lambda_n}}$$

$$\geq \frac{(n-1)\det(DD(G))}{n\lambda_1 \det(DD(G))}$$

$$[\det(DD(G))]^{\frac{1}{n-1}} \geq \frac{(n-1)\lambda_1^{\frac{1}{n-1}}}{n\lambda_1}$$

$$\geq \frac{(1-\frac{1}{n})}{\lambda_1^{\frac{n}{n-1}}}$$

Raising to the power of $(n - 1)$ on either sides,

$$\lambda_1 \geq \frac{(1-\frac{1}{n})^{1-\frac{1}{n}}}{[\det(DD(G))]^{\frac{1}{n}}}$$ □

Theorem 7. For any connected graph G, $\frac{n^{n-1}[\det(DD(G))]}{[DDE(G)]^{n-1}} \leq \lambda_1 \leq DDE(G) - \frac{(n-1)^2}{n}$

Proof. With the use of the relation that the arithmetic mean is always greater than or equal to the geometric mean for any set of numbers, we now consider the means for the $n - 1$ eigenvalues λ_2, λ_3, …, λ_n,

$$\frac{\lambda_2 + \lambda_3 + \cdots + \lambda_n}{n-1} \geq \frac{n-1}{\frac{1}{\lambda_2} + \frac{1}{\lambda_3} + \cdots + \frac{1}{\lambda_n}}$$

$$DDE(G) - \lambda_1 \geq \frac{(n-1)^2(\lambda_2\lambda_3 \cdots \lambda_n)}{\lambda_3\lambda_4 \cdots \lambda_n + \lambda_2\lambda_4 \cdots \lambda_n + \cdots + \lambda_2\lambda_3 \cdots \lambda_{n-1}}$$

$$\geq (n-1)^2 \frac{\frac{\det\big(DD(G)\big)}{\lambda_1}}{n\big[\det\big(DD(G)\big)\big]}$$

$$\lambda_1 \leq DDE(G) - \frac{(n-1)^2}{n}$$

Using the relation between arithmetic mean and geometric mean for the set of $n - 1$ eigenvalues $\lambda_2, \lambda_3, \ldots, \lambda_n$, we get

$$\frac{\lambda_2 + \lambda_3 + \cdots + \lambda_n}{n} \geq (\lambda_2\lambda_3 \cdots \lambda_n)^{\frac{1}{n-1}}$$

$$\frac{|\lambda_2| + |\lambda_3| + \cdots + |\lambda_n|}{n} \geq (\lambda_2\lambda_3 \cdots \lambda_n)^{\frac{1}{n-1}}$$

$$\frac{DDE(G)}{n} \geq \left[\frac{\det(DD(G))}{|\lambda_1|}\right]^{\frac{1}{n-1}}$$

$$|\lambda_1|^{\frac{1}{n-1}} \geq \frac{n\big[\det\big(DD(G)\big)\big]^{\frac{1}{n-1}}}{DDE(G)}$$

Raising to the power of $(n - 1)$ on either sides, the lower bound can be obtained. □

5. Bounds on Regular Graphs of Diameter 2

Moore and Moser [1] showed that almost all graphs are of diameter 2. In today's scenario, there is a lot of awareness and urge about more space for equitable sharing of all available resources and providing equal accessibility of all capitals for every individual on earth. As most of the real-life problems can be beneficially modeled as a graph or network to obtain optimal solutions, the study of regular graphs which have the same degrees for all its vertices becomes essential and an inevitable area of study. Hence, the results procured for the regular graphs of diameter 2 in this section are definitely going to find its use in the very near future for a special purpose. Throughout this section, we assume $p = q = r = 1$.

Theorem 8. Let G be a r-regular graph of diameter 2 on n vertices and m edges. If the eigenvalues of its distance-degree matrix are $\lambda_1, \lambda_2, \ldots, \lambda_n$, then $\sum_{i=1}^{n} \lambda_i^2 = 2r^4(2n^2 - 2n - 3m)$.

Proof. Since G is r-regular, $d(i) = r, \forall i \in V(G)$. Further, since the diameter of G is 2,

$$DD(G)_{ij} = \begin{cases} r^2 & \text{if } i \text{ is adjacent to } j \\ 2r^2 & \text{if } i \text{ is not adjacent to } j \end{cases}$$

Therefore, $\sum_{i=1}^{n} \lambda_i^2 = \sum_{i=1}^{n}\sum_{j=1}^{n} DD(G)_{ij}DD(G)_{ji} = \sum_{i=1}^{n}\sum_{j=1}^{n}\big[DD(G)_{ij}\big]^2$

$$= 2m \times (r^2)^2 + [n(n-1) - 2m] \times (2r^2)^2$$

from which the theorem follows. □

Theorem 9. If G is a graph of diameter 2 on n vertices, then $\lambda_1 = r^2(2n - r - 2)$ if and only if G is regular.

Proof. Every i^{th} row of the DD-matrix of G would contain $d(i)$ elements equal to (r^2) and $n - d(i)$ elements equal to $(2r^2)$. Then eigenvector $[1\ 1\ 1 \cdots 1]$ corresponds to the largest eigenvalue as the row sums of the DD-matrix are equal. Using the principle of Rayleigh, we can see that, $\lambda_1 = \frac{1}{n}[r \times r^2 + (n - r - 1)2r^2] = r^2(2n - r - 2)$. Conversely, the row sum of the DD-matrix of G can be equal only when the graph is regular. Hence, the proof. □

Corollary 1. If G is a r-regular graph of diameter 2 on n vertices, then $|\det(DD(G))| \leq r^{2n}(2n - r - 2)^n$.

Theorem 10. If G is a r-regular graph of diameter 2 on n vertices and m edges, then $DDE(G) \leq r^2\left[(2n-r-2)+\sqrt{4n(n-2)-nr(n-r+5)+(r+2)^2}\right]$.

Proof. From theorem 9, it follows that $\lambda_1 = r^2(2n-r-2)$. Using Cauchy-Schwarz inequality, it follows that $\left(\sum_{i=1}^{n}|\lambda_i|\right)^2 \leq (n-1)\sum_{i=1}^{n}\lambda_i^2$

$\Rightarrow DDE(G) \leq \lambda_1 + \sqrt{(n-1)[4n^2r^4 - 4nr^4 - 6mr^4 - \lambda_1^2]}$

From theorem 9, $\lambda_1 = r^2(2n-r-2)$ and since $2m = nr$, we get,

$DDE(G) \leq r^2\left[(2n-r-2)+\sqrt{4n(n-2)-nr(n-r+5)+(r+2)^2}\right]$. □

Theorem 11. For any r-regular graph of diameter 2 on n vertices, the distance-degree energy can be expressed as a function of its distance-degree spectral radius which takes values in the interval $(-r^2\sqrt{(n-1)(4n-3r-4)}, r^2\sqrt{(n-1)(4n-3r-4)})$.

Proof. Since the largest eigenvalue of a r-regular graph of diameter 2 on n vertices is $r^2(2n-r-2)$, using Cauchy-Schwarz inequality, it follows that,

$$DDE(G) \leq \lambda_1 + \sqrt{(n-1)[4n^2r^4 - 4nr^4 - 6mr^4 - \lambda_1^2]}$$

Define a function $f(x) \coloneqq x + \sqrt{(n-1)[4n^2r^4 - 4nr^4 - 6mr^4 - x^2]}$.

Hence, $DDE(G)$ can be expressed in terms of its distance-degree spectral radius which takes values in the interval $(-r^2\sqrt{(n-1)(4n-3r-4)}, r^2\sqrt{(n-1)(4n-3r-4)})$. □

Theorem 12. The spectral radius of a r-regular connected graph G of diameter 2 is bounded above by $\frac{r^4[2n-r-2]^2}{\det(DD(G))^{1/n}}$ if $DD(G)$ is non-singular.

Proof. From theorem 4, it is evident that,

$$|\lambda_1|\sum_{i=1}^{n}|\lambda_i| \geq [\det(DD(G))]^{1/n}\sum_{i=1}^{n}|\lambda_i|$$

$$|\lambda_1|^2 \geq [\det(DD(G))]^{1/n} DDE(G)$$

Using theorem 9,

$$DDE(G) \leq \frac{[r^2(2(n-1)-r)]^2}{\det(DD(G))^{1/n}}$$

$$DDE(G) \leq \frac{r^4[2n-r-2]^2}{\det(DD(G))^{1/n}}$$ □

6. Concluding Remarks and Future Scope

This paper provides an insight about how the newly defined parameters, namely, distance-degree energy and the distance-degree spectral radius assumes values for various classes of graphs. The study has also been extended in the direction to obtain bounds for any graph, in general and regular graphs of diameter 2, in particular. Investigating whether these bounds are sharp is still open.

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