On Degree-Distance index of a graph

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Abstract

In this article, we give sufficient conditions for the Hamiltonian and graphical properties of graphs in the terms of degree-distance index. The degree distance index of the graph is defined as the $S(G) = \sum_{u,v \in V(G)}(d(u) + d(v))d_G(u, v)$ where $d(u)$ is the degree of the vertex in a graph and $d_G(u, v)$ is the distance between the vertices u and v in the graph G.

Keyword: Degree distance index, Topological index, Hamiltonian Properties.

1 Introduction

In this paper, we are concerned with a topological invariant of a molecular graph called the Degree distance index. Let G be a connected graph of order n and size m. Let $V(G)$ be the vertex set of G. We use $d_G(u,v)$ to denote the distance between vertices u and v of the graph G, and d(u) is used to denote the degree of the vertex u of the graph. Let K_n denote the complete graph on n vertices. Then the Degree distance index (or degree distance) of G is defined as:

$$S(G)=\sum_{u,v\in V(G)}(d(u)+d(v))d_G(u,v)=\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}(d(u)+d(v))d_G(u,v)$$

Dobrynin and Kochetova [10] and Gutman [11] independently studied the degree distance sum of a graph. The same was studied by Tomescu [22], Tomescu [22] and Bucicovschi and Cioab [7]. A related concept studied earlier for the chemical applications called " Molecular topological index " MTI by H. P. Schultz in 1989 is defined as follows [19]: Let G be a graph with labeled vertices $v_1, v_2, ..., v_n$. Then

$$MTI(G)=\sum_{i=1}^{n}[v(A+D)]_i$$

where A and D are adjacency and distance matrices of G and $v=(d(v_1), d(v_2), ..., d(v_n))$.It can be easily seen from [11] that $MTI(G)=M_1(G)+S(G)$, where $M_1(G)$ is first Zagrab index and $S(G)$ is degree distance index.

A connected graph is said to be traceable (or Hamiltonian) if it has a Hamiltonian path (or cycle). A path (or cycle) is said to be a Hamiltonian path (or cycle) if it traverses through all vertices exactly once. A graph is said to be Hamiltonian-connected if it has a Hamiltonian path between every pair of vertices. A graph is said to be k- connected if it remains connected by removing fewer than k vertices. A graph on n vertices is k-edge Hamiltonian if every path of length not exceeding k, $1\leq k\leq n-2$, is contained in a Hamiltonian cycle. The graph G is called k-path coverable if $V(G)$ can be covered by k or fewer than k vertex disjoint paths, obviously 1-path coverable is traceable. For a graph G, if $G[V\ X]$ is Hamiltonian for all $|X| \leq k$, , we call G to be k-Hamiltonian. In particular, 0-Hamiltonian is same as Hamiltonian. For other undefined graph-theoretic notations and terminology, the reader may refer to [6].

The problem of finding a Hamiltonian cycle is NP-complete as reported in [14]. In 2013, Yang [23] studied the Hamiltonian path in terms of the Wiener index and extended it to the Hamiltonian graph [18]. In the same year, Hua [12] discussed sufficient conditions for traceability in terms of the Harary index. Further, sufficient conditions for k-connected, β- deficient, and Hamiltonian cycle in terms of the first Zagreb index are studied in [2]. Also, An [3] studied graph properties based on reciprocal degree distance and An [1] discussed sufficient conditions for Hamiltonian-connectedness in terms of the first Zagreb index and reciprocal distance. In [20], the author(s) described sufficient conditions for k-edge Hamiltonian, k-path coverable, traceable, and Hamilton-connected graphs in terms of the forgotten index. In [13], author(s) studied sufficient conditions for Hamiltonicity with respect to the Wiener index, hyper-Wiener index, and Harary index. The Hamiltonian and graphical properties in terms of the eccentricity-based topological index are studied in [17, 24].

In this article, we explore sufficient conditions for the Hamiltonian path, Hamiltonian cycle, Hamiltonian-connected, and k-connected graphs in terms of the Degree distance index. The paper is organized as follows: In Section 2, we give some useful propositions which are needed in subsequent sections. In Section 3, we present the results and proofs of this paper.

2 Preliminaries

In this section, we will introduce four-degree conditions. In the following propositions, we suppose that the graph satisfies the degree sequence $\pi = (d_1 \leq d_2 \leq .... \leq d_n)$ condition.

Proposition1. [9] Let G be a graph of order $n \geq 3$ having degree sequence π. If

$$d_i \leq i - 1 \leq \frac{1}{2}(n-1) \Rightarrow d_{n-i} \geq n - i - 1$$

then G is traceable.

Proposition2. [9] Let G be a graph of order $n \geq 3$ having degree sequence π. If

$$d_i \leq i < \frac{n}{2} \Rightarrow d_{n-i} \geq n-i$$

then G is Hamiltonian.

Proposition3. [8] Let G be a graph of order $n \geq 3$ having degree sequence π. If

$$d_{i-1} \leq i \Rightarrow d_{n-i} \geq n-i+1, for 2 \leq i \leq \frac{n}{2}$$

then G is Hamiltonian connected.

Proposition4. . [4] Let G be a graph of order $n \geq 4$ having degree sequence π. If

$$d_i \leq i+k-2 \Rightarrow d_{n-k+1} \geq n-i, for 1 \leq i \leq \frac{1}{2}(n-k+1)$$

then G is k-connected.

Proposition 5. [15] Let G be a graph with degree sequence π and $n \geq 3$ and $0 \leq k \leq n-3$. If

$$d_{i-k} \leq i \Rightarrow d_{n-i} \geq n-i+k, for k+1 \leq i \leq \frac{n+k}{2}$$

then π is k-edge Hamiltonian.

Proposition 6. [9] Let G be graph with degree sequence π and $0 \leq k \leq n-3$. If

$$d_i \leq i+k \Rightarrow d_{n-i-k} \geq n-i, for 1 \leq i \leq \frac{1}{2}(n-k)$$

then G is k- Hamiltonian.

Proposition 7. $[5, 16]$ If $k \geq 1$ and the degree sequence π of G satisfies

$$d_{i+k} \leq i \rightarrow d_{n-i} \geq n-i-k, for 1 \leq i \leq \frac{1}{2}(n-k)$$

then G is k-path coverable.

Define a graph G_4as follows: A graph whose set of vertices has partition $A \bigcup B \bigcup C \bigcup D$ such that $|A| = |C| = k$ and $|B| = |D| = m-k$ and and whose edges connect each vertex

$u \in A \bigcup B$ to each vertex $v \in C \bigcup D$ except when $u \in A$ and $v \in D$.

Proposition8. [9]Let G be a bipartite graph with vertices $(u_1, u_2, ..., u_n)$ and $(v_1, v_2, ..., v_n)$ such that $d(u_1) \leq d(u_2) \leq .... \leq d(u_n)$ and $d(v_1) \leq d(v_2) \leq .... \leq d(v_n)$ and

$$d(u_k) \leq k < n \to d(v_{n-k}) \geq n - k + 1$$

Then G is either Hamiltonian or G_4.

3 Degree distance index and Hamiltonicity

This section gives sufficient conditions for a graph to be traceable, Hamiltonian, Hamiltonian-connected, k-connected graphs, k-path coverable, k-Hamiltonian,k-edge Hamiltonian in terms of Degree distance index. Further, we give sufficient condition for bipartite graph to be Hamiltonian in terms of Degree distance index.

Let G be a connected graph, and $S(G)$ denotes the Degree distance index of G:For a vertex v of G,define $D(v) = \sum_{u \in G} d_G(v, u)$ and $D'(v) = d(v)D(v)$. Then

$$\begin{aligned} S(G) &= \sum_{v \in G} D'(v) \\ &= \sum_{v \in G} d(v)D(v) \end{aligned}$$

$$\leq \sum_{v \in G} d(v)[d(v) + (n - 1 - d(v))(n - 1 - d(v))] \quad (1)$$

$$= (n-1)^2 \sum_{v \in G} d(v) - (2n - 3) \sum_{v \in G} (d(v))^2 + \sum_{v \in G} (d(v))^3$$

We now have the following:

Theorem 1. Let G be a connected graph of order $n \geq 5$ and size m. If

$$S(G) \ \geq \ 2n^4 - 12n^3 + 27n^2 - 27n + 10 - \frac{(2n-3)}{n}4m^2$$

then G is traceable.

Proof. Suppose that G is not traceable, then by Proposition 1 and Equation1, the Degree distance index of G:

$$\begin{aligned}
S(G) &\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - (2n-3)\sum_{v\in G}(d(v))^2 \\
&\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - \frac{(2n-3)}{n}\left(\sum_{v\in G} d(v)\right)^2 \\
&\leq (n-1)^2[k(k-1) + (n-2k+1)(n-k-1) + (k-1)(n-1)] \\
&+ [k(k-1)^3 + (n-2k+1)(n-k-1)^3 + (k-1)(n-1)^3]\frac{(2n-3)}{n}4m^2 \\
&= (n-1)^2[3k^2 - (2n+1)k + n^2 - n] + [3k^4 - (7n-2)k^3 + (9n^2 - 12n + 6)k^2 \\
&- (4n^3 - 4n^2 + 3)k + n^4 - 3n^3 + 3n^2 - n] - \frac{(2n-3)}{n}4m^2 \\
&= 3k^4 - (7n-2)k^3 + (12n^2 - 18n + 9)k^2 - (6n^3 - 9n^2 + 4)k \\
&+ 2n^4 - 6n^3 + 6n^2 - 2n - \frac{(2n-3)}{n}4m^2 \\
&= 2n^4 - 12n^3 + 27n^2 - 27n + 10 - \frac{(2n-3)}{n}4m^2 \\
&+ (k-1)[3k^3 - (7n-5)k^2 + (12n^2 - 25n + 14)k - 6n^3 + 21n^2 - 25n + 10]
\end{aligned}$$

Combining with the condition of the Theorem 1, we know that $(k-1)[3k^3 - (7n-5)k^2 + (12n^2 - 25n + 14)k - 6n^3 + 21n^2 - 25n + 10] \geq 0$. Since G is connected and $k \geq d_k + 1 \geq 2$. Let $q(x) = 3x^3 - (7n-5)k^2 + (12n^2 - 25n + 14)x - 6n^3 + 21n^2 - 25n + 10$. Since k is an integer we have $2 \leq k \leq \frac{n+1}{2}$ is equivalent to $k \leq \frac{n}{2}$. So what follows we assume that $k \leq \frac{n}{2}$

The first derivative of $q(x)$ is $q'(x) = 9x^2 - 2(7n-5)x + (12n^2 - 25n + 14)$ and the discriminant $\Delta$of $q'(x) = 0$ is $\Delta = 4(7n-5)^2 - 36(12n^2 - 25n + 14) = -4(59n^2 - 155n + 101) < 0 \forall n \geq 2$. Therefore $q'(x) > 0$ and $q(x)$ is strictly increasing in the interval of $[2, \frac{n}{2}]$. Hence $max(q(x))$ is obtained at the right endpoint of the interval $[2, \frac{n}{2}]$.We consider the parity of n. If n is even then

$$max(q(x)) = q(\frac{n}{2}) = -\frac{1}{8}n(n(11n-78)+144)+10 < 0, \forall n \geq 5.$$

If n is odd then

$$max(q(x)) = q(\frac{n-1}{2}) = -\frac{1}{8}(n-1)(n(11n-38)+31) < 0, \forall n \geq 3.$$

Therefore $max(q(x)) < 0 \forall n \geq 5$. Then $S(G) \leq 2n^4 - 12n^3 + 27n^2 - 27n + 10 - \frac{(2n-3)}{n}4m^2$. Thus proof is coplete □

Theorem 2. Let G be a connected graph of order $n \geq 12$ and size m. If

$$S(G) \geq 2n^4 - 18n^3 + 82n^2 - 162n + 136 - \frac{(2n-3)}{n}4m^2$$

then G is Hamiltonian.

Proof. Suppose that G is not Hamiltonian, then by Proposition 2 and Equation 1, the Degree distance index of G:

$$\begin{aligned}
S(G) &\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - (2n-3)\sum_{v\in G}(d(v))^2 \\
&\leq (n-1)^2\sum_{v\in G} d(v) + \sum_{v\in G}(d(v))^3 - \frac{(2n-3)}{n}(\sum_{v\in G}(d(v))^2 \\
&\leq (n-1)^2[k^2+(n-2k)(n-k-1)+k(n-1)] \\
&+ [k^4+(n-2k)(n-k-1)^3+k(n-1)^3]\frac{(2n-3)}{n}4m^2 \\
&= (n-1)^2[3k^2-(2n-1)k+n^2-n]+[3k^4-(7n-6)k^3+(9n^2-15n+6)k^2 \\
&- (4n^3-9n^2+6n-1)k+n^4-3n^3+3n^2-n] - \frac{(2n-3)}{n}4m^2 \\
&= 3k^4-(7n-6)k^3+(12n^2-21n+9)k^2-(6n^3-14n^2+10n-2)k \\
&+ 2n^4-6n^3+6n^2-2n-\frac{(2n-3)}{n}4m^2 \\
&= 2n^4-18n^3+82n^2-162n+136-\frac{(2n-3)}{n}4m^2 \\
&+ (k-2)[3k^3-(7n-12)k^2+(12n^2-35n+33)k-6n^3+38n^2-80n+68]
\end{aligned}$$

Combining with the condition of the Theorem 2, we know that $(k-2)[3k^3-(7n-12)k^2+(12n^2-35n+33)k-6n^3+38n^2-80n+68] \geq 0$. Since $2 \leq k < \frac{n}{2}$ is equivalent to $k \leq \frac{1}{2}(n-1)$. So what follows, we suppose $k \leq \frac{1}{2}(n-1)$. Let $q(x) = 3x^3-(7n-12)x^2+(12n^2-35n+33)x-6n^3+38n^2-80n+68$ where $2 \leq x \leq \frac{1}{2}(n-1)$. We divide the proof into following two parts.

Case1:$(k-2)q(x) = 0$, we have $k = 2$ or $q(x) = 0$, It is easy to see that $q'(x) = 9x^2-2(7n-12)x+(12n^2-35n+33)$ and the discriminant Δ of the equation $q'(x) = 0$ is $\Delta = 4(7n-12)^2-36(12n^2-35n+33) = -4(59n^2-147n+153) < 0 \forall n \geq 1$. Therefore $q'(x) > 0$ and q(x) is strictly increasing in the interval $2 \leq x < \frac{1}{2}(n-1)$. Then max(q(x)) is in the right endpoints of the domain of interval$[2, \frac{1}{2}(n-1)]$. Since k is an integer, we need to consider the parity of n. If n is even then $max(q(x)) = q(\frac{1}{2}(n-2))$. By a simple calculation, we have

$$q(\frac{1}{2}(n-2)) = -\frac{1}{8}n(n-4)(11n-86)+44 < 0, \forall n \geq 9$$

If n is odd, then $max(q(x)) = q(\frac{1}{2}(n-1))$. By a simple calculation, we have

$$q(\frac{1}{2}(n-1)) = \frac{1}{8}[-11n^3+159n^2-421n+433] < 0, \forall n \geq 12$$

In both the cases $q(x) < 0$. From the above analysis, we can see that $q(x) \neq 0$ for $2 \leq x \leq \frac{1}{2}(n-1)$ and $n \geq 12$. Hence we only need to consider the case $k = 2$. If $k = 2$ then $S(G) \leq 2n^4-18n^3+82n^2-162n+136-\frac{(2n-3)}{n}4m^2$. If equality holds then $d_1 = d_2 = 2, d_3 = ... = d_{n-2} = n-3, d_{n-1} = d_n = n-1$, which implies $G = K_2 \vee (2K_1+K_{n-4})$. But in this case the equality $\sum_{v \in V(G)} d(v)^2 = \frac{1}{n}\left(\sum_{v \in (V(G))} d(v)\right)^2$ does not holds.

Case 2: $(k-2)q(x) > 0$. In this case $k \geq 3$ and $q(x) = 3x^3-(7n-12)x^2+(12n^2-35n+33)x-6n^3+38n^2-80n+68 > 0$. By **case 1**, we know that $q(x)$ is strictly increasing and $max(q(x)) < 0$. Therefore for $3 \leq x \leq \frac{1}{2}(n-1)$, we have $3x^3-(7n-12)x^2+(12n^2-35n+33)x-6n^3+38n^2-80n+68 < 0$.A contradiction. Thus proof is complete. □

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