

DISTANCE-BASED TOPOLOGICAL ACHARYA POLYNOMIAL AND INDICES OF HAMILTONIAN GRAPHS

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In QSAR/QSPR study, topological indices are utilized to guess the bioactive

Abstract

Let G be a connected graph, and let $H(G)$ denote the Hamiltonian graph of G . Every complete graph with more than two vertices is a Hamiltonian graph. In this paper, a simple graph was transformed into the Hamiltonian graph structure and several topological indices based on distance for Hamiltonian graphs $H[G]$ were determined. The distance $d_{[G]}(x_i, x_j)$ between the vertices V_i and V_j of graph G is equal to the shortest path length that connects the two vertices. The number of vertex pairs of G , whose distance is l is denoted by $d(G, l)$. The distance-based topological indices based on Acharya Polynomial considered in this study are as follows: Wiener index (W), hyper-Wiener index (WW), Harary index (H), Reciprocal Terminal Wiener index (TW).

Keywords: *Acharya Polynomial, Hamiltonian graph, distance-based topological indices, molecular graph.*

Introduction

The finite and connected graphs have various applications in the engineering and medical fields especially in representing the molecular structures of various chemical components. In those closed complete graphs, the graph with Hamiltonian characteristics were of greater significance. For a graph to be Hamiltonian, all the vertices of the graph should be connected only once and it should start and terminate at the same point. So there were some basic conditions or terminologies for the graph to be Hamiltonian. They are as follows: A cycle connecting all the vertices and passing through it in a graph is Hamiltonian cycle and a graph with Hamiltonian cycle is known as Hamiltonian graph. The cyclic path was known as Hamiltonian path and a graph with Hamiltonian path is also known as traceable.

In June 2013 B. D. Acharya, defined the distance degree parameter, Acharya Index and Acharya polynomial at ICDM -2013 [1]. The topology indices based on the distance was formulated for obtaining the Wiener index, and different forms of Harary index for the double graph [2]. The Hamiltonicity of the graphs were studied with the Wiener and hyper Wiener index and Harary index. Some condition for traceable and Hamiltonian connected was determined [3].

The general Acharya index for the graph was formulated and the correlations with other existing indices were obtained [4]. Continuing the work, the Acharya polynomial for different standard graphs were formulated and validated [5]. Acharya polynomial for some standard graph transformation was performed and the expression was derived [6]. Acharya polynomial for the thorn graph was derived based on the thorn rod, thorn trees, stars and rings [7]

In the present work, the Acharya polynomial and Acharya index for the Hamiltonian graph ($H[G]$) is formulated and the different topological distance indices were derived for

(H[G]). Then based on the correlation between the Wiener index and AI for regular graphs, the obtained distance indices were expressed with respect to the AI.

Definitions

The common graph invariant based on distance is Wiener index of graphs. It is represented by $W(G)$ and defined as sum of distances of all pair of vertices in G :

$$W(G) = \sum_{u < v} d(u, v)$$

The Acharya polynomial of graph G is defined as,

$$AP(G, \lambda) = \sum_{\substack{1 \leq d \leq n-1 \\ 1 \leq k \leq p}} \mu(d, G) \lambda^k$$

where $\mu(d, G)$ denotes pair of vertices of degree d at distance k , $p = \text{diam}(G)$. It is clear that,

$$W(G) = \frac{d}{d\lambda} AP(G, \lambda) \text{ at } \lambda = 1.$$

Let $d(G, k)$ be the number of vertex pairs of G , the distance of which is equal to k . Then the Acharya polynomial can be rewritten with Wiener index as,

$$AP(G, \lambda) = \sum_{i=1}^{d(G)} \mu(G, i) \lambda^i$$

where $d(G)$ be the diameter of G and is the longest topological distance in G .

The hyper-Wiener index $WW(G)$ is defined as,

$$WW(G) = \frac{1}{2} W(G) + \frac{1}{2} \sum_{\{u, v\} \subseteq V(G)} \mu d^2(u, v)$$

Where, $d^2(u, v) = d(u, v)^2$.

The hyper-Wiener Polarity Index $WW(G)$ is defined as,

$$WW(G) = W(G) + W^{\mu d^2}(G)$$

Harary index of a graph G, denoted by H(G) is defined as follows:

$$H(G) = \frac{1}{W(G)}$$

The Acharya polynomial of Terminal wiener index of a graph G is denoted by,

$$TW_p(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V_1(G)} \mu d_G(u,v)$$

Hamiltonian Graphs

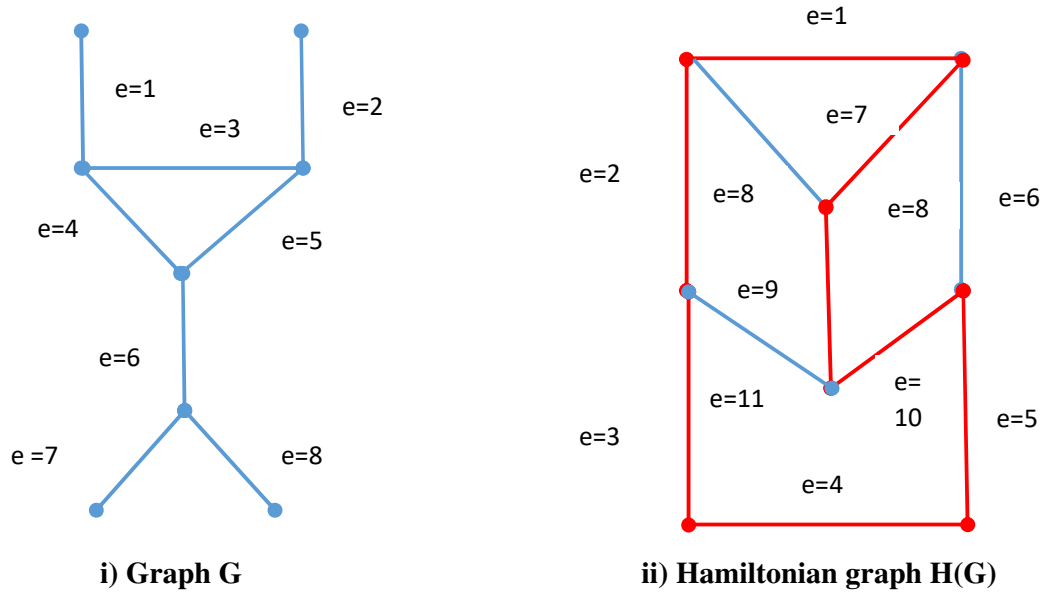


Figure 1. Transformation of simple graph into Hamiltonian graph

Let G be the simple graph with the vertices $V_i (i=1, \dots, n)$, and $H[G]$ be the Hamiltonian graph with the same number of vertices as it was the case for this graph. For determining the Acharya polynomial of the Hamiltonian graph, the graph the following Lemma were generated.

Lemma 1 the distance between vertices of the Hamiltonian graph is given as

$$d_{H[G]}(x_i, x_j) = l$$

Lemma 2 The generated Hamiltonian graph $H[G]$ as

$$d_{H(G)}(x_i, x_j) = d_G(x_i, x_j); i, j = 1, \dots, n$$

Proof:

Evidently, $G \subset H(G)$. Let $\{x_i, x_j\} \subseteq V(G) \subset V(H[G])$ then $d_{H(G)}(x_i, x_j) \leq d_H(x_i, x_j)$.

Assume, $l = d_{H(G)}(x_i, x_j) \leq d_H(x_i, x_j) = m$ and shortest path in $D(G)$ from x_i and x_j is $x_i v_1 v_2 \dots v_{l-1} x_j$. If $l=1$, then the property is apparent. Then, assume $l \geq 2$. Subsequently, $1 < m$, there exists some $v_k \in V(G_1)$. As v_{k-1} and v_{k+1} are adjacent to v_k , shows the definition of the Hamiltonian graph v_{k-1} and v_{k+1} are adjacent to x_k . Now, the obtained path is denoted as $x_i v_1 v_2 \dots x_k \dots v_{l-1} x_j$ in graph G of length l . Then, $d_{H(G)}(x_i, x_j) = d_H(x_i, x_j)$

Lemma 3 For a Hamiltonian graph

$$d_{H[G]}(x_i) = d_G(x_i)$$

Based on the above lemma the following results on the Acharya polynomial (AP), Acharya index (AI), wiener index (W), terminal wiener (TW), hyper wiener (WW) and the Harary index (H) for the Hamiltonian graph was derived.

MAIN RESULTS

Theorem 1: Based on the definition and DIRAC statement, the Acharya polynomial of a Hamiltonian graph $H[G]$ is defined as,

$$AP(H[G], \lambda) = \sum_{\substack{\frac{n}{2} \leq d \leq n-1 \\ 1 \leq k \leq p}} \mu(d, G) \lambda^k$$

Theorem 2: The Acharya index of graph $H[G]$ is defined as.

$$AI(H[G], \lambda) = \sum_{\substack{\frac{n}{2} \leq d \leq n-1 \\ 1 \leq k \leq p}} \mu(d, G) \cdot k$$

Proof:

From the statement of DIRAC:

“If G is a graph with n vertices, where $n \geq 3$ and $d(v) \geq n/2$, for every vertex v of G , then G is Hamiltonian”.

Theorem 3: Let there be n vertices for the simple graph G , then the wiener index for the Hamiltonian graph $H[G]$ is given by

$$W(H[G]) = W[G] + n$$

Proof:

The wiener index of the graph $H[G]$ was given by

$$\begin{aligned} W(H[G]) &= \sum_{1 \leq i < j \leq n} d_{H[G]}(v_i, v_j) \\ &= \sum_{1 \leq i < j \leq n} d_{H[G]}(x_i, x_j) + \sum_{i=1,2,\dots,n} d_{H[G]}(x_i) \\ &= W[G] + ln \\ &= W[G] + n \quad (\text{when } l=1) \end{aligned}$$

For a regular graph the $AI(G) = W(G)$, hence

$$AI(G) + n = W(H[G])$$

$$W(H[G]) = \sum_{\substack{\frac{n}{2} \leq d \leq n-1 \\ 1 \leq k \leq p}} \mu(d, G) \cdot k + n$$

Theorem 4: The hyper wiener index for the Hamiltonian graph was given as

$$WW(H[G]) = \frac{1}{4} \{W[G](W[G] + 2n + 1) + n(n + 1)\}$$

Proof:

$$WW(H[G]) = \frac{1}{4} \{ \sum_{1 \leq i < j \leq n} (d_{H[G]}(v_i, v_j) + d_{H[G]}^2(v_i, v_j)) \}$$

$$\begin{aligned}
&= \frac{1}{4}[W[G] + n + (W[G] + n)^2] \\
&= \frac{1}{4}[W[G]^2 + n^2 + 2W[G].n + W[G] + n] \\
&= \frac{1}{4}\{W[G](W[G] + 2n + 1) + n(n + 1)\}
\end{aligned}$$

Based on the relationship between the acharya index and wiener index,

$$\begin{aligned}
&WW(H[G]) = AI(AI + 2n + 1) + n(n + 1) \\
&= \sum_{\substack{\frac{n}{2} \leq d \leq n-1 \\ 1 \leq k \leq p}} \mu(d, G).k \left(\sum_{\substack{\frac{n}{2} \leq d \leq n-1 \\ 1 \leq k \leq p}} \mu(d, G).k + 2n + 1 \right) + n(n + 1)
\end{aligned}$$

Theorem 5: The terminal wiener index for the Hamiltonian graph was given as,

$$TW(H[G]) = \frac{1}{2}(W(G) + n)$$

Proof:

$$\begin{aligned}
TW(H[G]) &= \frac{1}{2}W(H[G]) \\
&= \frac{1}{2}(W(G) + n)
\end{aligned}$$

From the relationship of acharya index and wiener index, the terminal wiener index can be given as,

$$\begin{aligned}
TW(H[G]) &= \frac{1}{2}(AI + n) \\
&= \frac{1}{2} \left(\sum_{\substack{\frac{n}{2} \leq d \leq n-1 \\ 1 \leq k \leq p}} \mu(d, G).k + n \right)
\end{aligned}$$

Theorem 6: Similarly, the Harary index for the Hamiltonian graph was given by,

$$H(H[G]) = H[G] + n$$

Proof:

The Harary index of the graph $H[G]$ was given by

$$\begin{aligned} H(H[G]) &= \sum_{1 \leq i < j \leq n} \frac{1}{d_{H[G]}(v_i, v_j)} \\ &= \sum_{1 \leq i < j \leq n} \frac{1}{d_{H[G]}(x_i, x_j)} + \sum_{i=1,2,\dots,n} \frac{1}{d_{H[G]}(x_i)} \\ &= H[G] + n \end{aligned}$$

Similar to the Wiener index, the Harary index of the Hamiltonian graph was given by

$$\begin{aligned} H(H[G]) &= \frac{1}{AI(G)} + n \\ &= \frac{1}{\sum_{\substack{2 \leq d \leq n-1 \\ 1 \leq k \leq p}} \mu(d, G) \cdot k} + n \end{aligned}$$

Conclusion

In these work the basic expression on the Acharya polynomial and index for the Hamiltonian graph was derived based on its properties. The expression for the distance based topological indices that include Wiener, terminal Wiener and the hyper Wiener along with the Harary were derived for the Hamiltonian graph. The derived topologies were employed with AI based on the correlating conditions of a regular graph.

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