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COMPUTATION OF WIENER INDEX, RECIPROCAL WIENER INDEX AND PERIPHERAL WIENER INDEX USING ADJACENCY MATRIX

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Abstract: In this short paper, we establish formulae to compute Wiener index, reciprocal Wiener index and peripheral Wiener index of graphs using adjacency matrix. Further, we present algorithms for the same.

Keywords and Phrases: Adjacency matrix, Wiener index, peripheral Wiener index.

2020 Mathematics Subject Classification: 05C09, 05C85.

1. Introduction

For standard terminology and notion in graph theory, we follow the text-book of Harary [1]. The non-standard will be given in this paper as and when required.

Let $G = (V, E)$ be a graph (finite, simple, connected and undirected). The distance between two vertices u and v in G, denoted by $d(u, v)$ is the number of edges in a shortest path (also called a graph geodesic) connecting them. We write $u \sim v$ to denote two vertices u and v are adjacent in G.

The eccentricity of a vertex v in G is the maximum distance between v and any other vertex in G. A vertex with maximum eccentricity in G is called a peripheral vertex in G. So, vertices whose eccentricities are equal to diameter G are peripheral vertices of G. The set of all peripheral vertices of G is denoted by $PV(G)$. If $PV(G) = V(G)$, then G is called a peripheral graph. The pair $\{u, v\}$ denotes the pair of vertices u, v with $u \neq v$.

Wiener index, Reciprocal Wiener index, and peripheral Wiener index are important distance based topological indices defined for graphs having applications in Chemistry (See [2], [3], [8], [9] and [13]). For new topological indices, we suggest the reader to refer the papers [4-7], [10-12]. The Wiener index $W(G)$ of a connected graph G is defined to be the sum of distances between all vertex pairs in G:

$$W(G) = \sum_{\{u,v\} \subset V(G)} d(u, v) \tag{1}$$

The Reciprocal Wiener index $W(G)$ of a connected graph G is defined to be the sum of inverses of distances between all vertex pairs in G:

$$RW(G) = \sum_{\{u,v\} \subset V(G)} \frac{1}{d(u, v)} \tag{2}$$

The peripheral Wiener index $PW(G)$ of G is defined as the sum of the distances between all pairs of peripheral vertices of G:

$$PW(G) = \sum_{\{u,v\} \subset PV(G)} d(u, v) \tag{3}$$

The aim of this short paper is to establish formulae and present algorithms to compute Wiener index, reciprocal Wiener index and peripheral Wiener index of graphs using adjacency matrix.

2. Formulae to compute Wiener index, reciprocal Wiener index and peripheral Wiener index of graphs using adjacency matrix

Let G be a (connected) graph of diameter d with $n \geq 2$ vertices $v_1, \ldots, v_n$. Let $A = (a_{ij}^{(1)})$ be the adjacency matrix of the graph G, where

$$a_{ij}^{(1)} = \begin{cases} 1, & \text{if } v_i \sim v_j; \\ 0, & \text{otherwise.} \end{cases}$$

We consider the following powers of A: $A^2, \dots, A^d$, where d is the diameter of G. We denote the (i, j)-th element of A^t $(2 \leq t \leq d)$, by $a_{ij}^{(t)}$, where

$$a_{ij}^{(t)} = \sum_{k=1}^{n} a_{ik}^{(t-1)} a_{kj}^{(1)}.$$

We know that $a_{ij}^{(t)}$ is the number of distinct edge sequences between v_i and v_j of length t. Let $a_{ij}^{(q_{ij})}$ be the first non-zero entry in the sequence $a_{ij}^{(1)}, a_{ij}^{(2)}, \dots, a_{ij}^{(d)}$. Then it is clear that $a_{ij}^{(q_{ij})}$ is the number of geodesics between v_i and v_j of length q_{ij}. Therefore $d(v_i, v_j) = q_{ij}$. Note that the matrix (q_{ij}) is the distance matrix of G.

Therefore from (1), the Wiener index of G is given by

$$W(G) = \sum_{1 \leq i < j \leq n} q_{ij} \tag{4}$$

and the reciprocal Wiener index of G is given by

$$RW(G) = \sum_{1 \leq i < j \leq n} \frac{1}{q_{ij}} \tag{5}$$

Let us define $\phi_{ij}^{(t)}$, $(1 \leq t \leq d)$ as follows:

$$\phi_{ij}^{(t)} = \begin{cases} 1, & \text{if } a_{ij}^{(1)} = a_{ij}^{(2)} = \cdots = a_{ij}^{(t-1)} = 0 \text{ and } a_{ij}^{(t)} \neq 0; \\ 0, & \text{otherwise.} \end{cases} \tag{6}$$

Then

$$q_{ij} = 1 \cdot \phi_{ij}^{(1)} + 2 \cdot \phi_{ij}^{(2)} + \cdots + d \cdot \phi_{ij}^{(d)} = \sum_{t=1}^{d} t \cdot \phi_{ij}^{(t)} \tag{7}$$

Using (7) in (4) and (5), we get

$$W(G) = \sum_{1 \leq i < j \leq n} \sum_{t=1}^{d} t \cdot \phi_{ij}^{(t)} \tag{8}$$

and

$$RW(G) = \sum_{1 \leq i < j \leq n} \frac{1}{\sum_{t=1}^{d} t \cdot \phi_{ij}^{(t)}} \tag{9}$$

Suppose that G has k peripheral vertices. Without loss of generality we may assume that $v_1, \ldots, v_k$ are the peripheral vertices of G (This is nothing but relabeling of vertices). Then,

$$PW(G) = \sum_{1 \le i < j \le k} \sum_{t=1}^{d} t \cdot \phi_{ij}^{(t)} \tag{10}$$

Thus we have,

Theorem 2.1. *Let G be a (connected) graph of diameter d with $n \ge 2$ vertices $v_1, \ldots, v_n$ and k peripheral vertices $v_1, \ldots, v_k$. Let $A = (a_{ij}^{(1)})$ be the adjacency matrix of G and (i,j)-th element of A^t $(2 \le t \le d)$, is denoted by $a_{ij}^{(t)}$. Then*

$$W(G) = \sum_{1 \le i < j \le n} \sum_{t=1}^{d} t \cdot \phi_{ij}^{(t)},$$

$$RW(G) = \sum_{1 \le i < j \le n} \frac{1}{\sum_{t=1}^{d} t \cdot \phi_{ij}^{(t)}}$$

and

$$PW(G) = \sum_{1 \le i < j \le k} \sum_{t=1}^{d} t \cdot \phi_{ij}^{(t)},$$

where $\phi_{ij}^{(t)}$, $(1 \le t \le d)$ is given by

$$\phi_{ij}^{(t)} = \begin{cases} 1, & \text{if } a_{ij}^{(1)} = a_{ij}^{(2)} = \cdots = a_{ij}^{(t-1)} = 0 \text{ and } a_{ij}^{(t)} \ne 0; \\ 0, & \text{otherwise.} \end{cases}$$

3. Algorithms to compute Wiener index, reciprocal Wiener index and peripheral Wiener index of graphs using adjacency matrix

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1. Algorithm to find the Wiener index

Input: Adjacency matrix of a connected graph G
Output: $W(G)$, Wiener Index of a connected graph G
Start:

Step 1: Define the adjacency matrix A of G

Step 2: Determine the distance matrix D of G

Step 3: Compute the Wiener Index

Step 3.1: [Initialize $W(G)$ to 0]

Step 3.2: Repeat for $i = 1$ to n
Repeat for $j = 1$ to n
if $(i < j)$ then
$W(G) = W(G) + D[i, j]$

Step 4: End of the algorithm

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2. Algorithm to find the Reciprocal Wiener index

Input: Adjacency matrix of a connected graph G
Output: $RW(G)$, Reciprocal Wiener Index of a connected graph G
Start:

Step 1: Define the adjacency matrix A of G

Step 2: Determine the distance matrix D of G

Step 3: Compute the Reciprocal Wiener Index

Step 3.1: [Initialize $RW(G)$ to 0]

Step 3.2: Repeat for $i = 1$ to n
Repeat for $j = 1$ to n
if $(i < j)$ then
$RW(G) = W(G) + 1/D[i, j]$

Step 4: End of the algorithm

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3. Algorithm to find the Peripheral Wiener index

Input: Adjacency matrix of a connected graph G

Output: 1. $PW(G)$, Peripheral Wiener Index of a connected graph G
2. P, Vector of Peripheral vertices

Start:

Step 1: Define the adjacency matrix A of G

Step 2: Determine the distance matrix D of G

Step 3: Determine P

Step 3.1: [Initialize k to 1]

Step 3.2: [Determine the diameter t of the graph]
$t = D[1, 1]$
Repeat for $i = 1$ to n
Repeat for $j = 1$ to n
If $i < j$ then
if $(D[i, j] > t)$ then
$t = D[i, j]$

Step 3.3: Repeat for $j = 1$ to n
If $(D[k, j] = t)$ then
$P[k] = j$
$k = k + 1$

Step 4: Compute the Peripheral Wiener Index

Step 4.1: [Initialize $PW(G)$ to 0]

Step 4.2: Repeat for $i = 1$ to k
Repeat for $j = i + 1$ to k

$$PW(G) = PW(G) + D[P[i], P[j]]$$

Step 5: End of the algorithm

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