ORIGINAL PAPER

WIENER INDEX OF INTERVAL WEIGHTED GRAPHS

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Abstract. *The Wiener index is classic and well-known topological index for the characterization of molecular graphs. In this paper, we study interval weighted graphs such as graphs where the edge weights are interval or interval matrices. In this study firstly we define interval weighted graph. Later we define Wiener index of interval weighted graph. From this definition, we give algorithms for finding Wiener index of interval weighted directed and undirected graph.*
Keywords: *Wiener index; interval matrix; interval weighted graph.*

1. INTRODUCTION

The Wiener index $W(G)$ is a distance-based topological invariant much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds introduced by Harold Wiener in 1947 for predicting boiling points $b \cdot p$ of alkanes based on the formula $b \cdot p = \alpha W + \beta w(3) + \gamma$ where α, β, γ are empirical constants and $w(3)$ is called path number [1].

The Wiener index was used by chemists, decades before it attracted attention of mathematicians. In fact, it was studied long before the branch of discrete mathematics, which is now known as Graph Theory, was developed [2].

The Wiener index of a connected graph G, denoted as $W(G)$, is defined as the sum of distances between all (unordered) pairs of vertices. More precisely,

$$W(G) = \frac{1}{2}\sum\nolimits_{u,v \in V(G)} d_G(u,v)$$

where $d_G(u,v)$ is the standard shortest path distance between vertices u and v of graph G [3].

The distance matrix $D(G)$ is defined so that (i,j)-entry d_{ij}, is equal to $d_G(v_i, v_j)$ [4].

Since we study on weighted graphs in this paper, we firstly give the definition of weighted graph.

A weighted graph is a graph each edge of which has been assigned to a square matrix called the weight of the edge. All the weight matrices are assumed to be of the same order and to be positive definite [5].

Let G be a weighted graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set E. Denote by w_{ij} the positive definite weight matrix of order p of the edge ij and assume that $w_{ij} = w_{ji}$. We write $i \sim j$ if vertices i and j are adjacent. Let $w_i = \sum_{j: i \sim j} w_{ij}$ be the weight matrix of the vertex i [5].

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A vertex-weighted graph (G, w) is a graph $G = (V(G), E(G))$ together with the weight function $w: V(G) \rightarrow \mathbb{R}$. The Wiener index $W(G, w)$ of (G, w) is then defined as:

$$W(G, w) = \frac{1}{2} \sum_{u,v \in V(G)} w(u) w(v)\, d_G(u, v).$$

Note that if $w(u) = 1$ holds for all vertices $u \in V(G)$, then $W(G, w) = W(G)$. More generally, if w is a constant function, say $w \equiv m$, then $W(G, w) = m^2 W(G)$ [6].

Let us introduce some notation. An $\tilde{A}$ interval matrix is a matrix whose elements are interval numbers and defined as

$$\tilde{A} = [\underline{A}, \overline{A}] = \{A \in \mathbb{R}^{m\times n} : \underline{A} \leq A \leq \overline{A}\},$$

where $\underline{A}$, $\overline{A} \in \mathbb{R}^{m\times n}$, $\underline{A} \leq \overline{A}$ are given matrices [7].

The arithmetic operations on interval matrices are as follows [8].

If $\tilde{A}, \tilde{B} \in \mathbb{R}^{m\times n}$, $\tilde{x} \in \mathbb{R}^n$ ve $\tilde{\propto} \in \mathbb{R}$, then

i. $\tilde{\propto} \tilde{A} = (\tilde{\propto} \tilde{a}_{ij})_{m\times n}$; $(1 \leq i \leq m), (1 \leq j \leq n)$

ii. $\tilde{A} + \tilde{B} = (\tilde{a}_{ij} + \tilde{b}_{ij})_{m\times n}$; $(1 \leq i \leq m), (1 \leq j \leq n)$

iii. $\tilde{A} - \tilde{B} = \begin{cases} (\tilde{a}_{ij} - \tilde{b}_{ij})_{m\times n} & ; \ if\ \tilde{A} \neq \tilde{B} \\ \tilde{0} = 0 & ; \ if\ \tilde{A} = \tilde{B} \end{cases}$

iv. If $\tilde{A} \in \mathbb{R}^{m\times n}$, $\tilde{B} \in \mathbb{R}^{n\times p}$, then

$\tilde{A} \cdot \tilde{B} = \left(\sum_{k=1}^{n} \tilde{a}_{ik} \tilde{b}_{kj}\right)_{m\times p}$; $(1 \leq i \leq m), (1 \leq j \leq p)$

v. $\tilde{A} \cdot \tilde{x} = \left(\sum_{j=1}^{n} \tilde{a}_{ij} \tilde{x}\right)_{m\times 1}$; $(1 \leq i \leq m)$

Example 1.

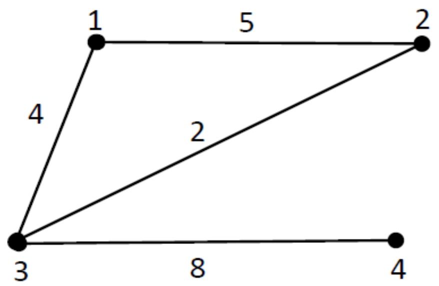

Figure 1. G Graph.

- $w(1) = 4 + 5 = 9$
- $w(2) = 5 + 2 = 7$
- $w(3) = 4 + 2 + 8 = 14$
- $w(4) = 8$
- $d_G(1,2) = d_G(2,1) = 1$
- $d_G(1,3) = d_G(3,1) = 1$
- $d_G(1,4) = d_G(4,1) = 2$

- $d_G(2,3) = d_G(3,2) = 1$
- $d_G(2,4) = d_G(4,2) = 2$
- $d_G(3,4) = d_G(4,3) = 1$

$$\begin{aligned} W(G,w) = \frac{1}{2}[&w(1)w(2)d_G(1,2) + w(1)w(3)d_G(1,3) + w(1)w(4)d_G(1,4) \\ &+ w(2)w(1)d_G(2,1) + w(2)w(3)d_G(2,3) + w(2)w(4)d_G(2,4) \\ &+ w(3)w(1)d_G(3,1) + w(3)w(2)d_G(3,2) + w(3)w(4)d_G(3,4) \\ &+ w(4)w(1)d_G(4,1) + w(4)w(2)d_G(4,2) + w(4)w(3)d_G(4,3)] \end{aligned}$$

$$\begin{aligned} W(G,w) &= \frac{1}{2}\begin{bmatrix} 9\cdot 7\cdot 1 + 9\cdot 14\cdot 1 + 9\cdot 8\cdot 2 + 7\cdot 9\cdot 1 + 7\cdot 14\cdot 1 + 7\cdot 8\cdot 2 \\ +14\cdot 9\cdot 1 + 14\cdot 7\cdot 1 + 14\cdot 8\cdot 1 + 8\cdot 9\cdot 2 + 8\cdot 7\cdot 2 + 8\cdot 14\cdot 1 \end{bmatrix} \\ &= 655 \end{aligned}$$

2. WIENER INDEX OF INTERVAL WEIGHTED GRAPHS

An interval weighted graph (interval graph) is a weighted graph in which each edge is assigned an interval or an interval square matrix. All the interval square matrices are assumed to be of the same order and to be positive definite.

Let $\tilde{G}$ be an interval graph on n vertices. Denote by $\widetilde{w}_{ij}$ the positive definite interval matrix of order p of the edge ij and assume that $\widetilde{w}_{ij} = \widetilde{w}_{ji}$. We write $i \sim j$ if vertices i and j are adjacent. Let $\widetilde{w}_i = \sum_{j:j\sim i} \widetilde{w}_{ij}$ be the weight interval matrix of the vertex i.

The distance between two vertices v_i and v_j, denoted by $d_{\tilde{G}}(v_i, v_j)$ is the length of shortest path between the vertices v_i and v_j in $\tilde{G}$. The Adjacency matrix of an interval graph $\tilde{G}$ is defined as $A(\tilde{G}) = (\tilde{a}_{ij})$, where

$$\tilde{a}_{ij} = \begin{cases} \widetilde{w}_{ij} & ; \quad i\sim j \\ [0,0] & ; \quad otherwise. \end{cases}$$

A vertex-weighted interval graph $(\tilde{G}, \widetilde{w})$ is a graph $\tilde{G}$ together with a function $\widetilde{w}: V(\tilde{G}) \to \mathbb{R}$. (Evidently, we could have chosen for vertex-weights interval or interval matrix.) The Wiener number $\widetilde{W}(\tilde{G}, \widetilde{w})$ of an interval weighted graph $(\tilde{G}, \widetilde{w})$ is defined as

$$\widetilde{W}(\tilde{G}, \widetilde{w}) = \frac{1}{2} \sum_{u,v \in V(\tilde{G})} \widetilde{w}(u)\widetilde{w}(v)\, d_{\tilde{G}}(u,v)$$

Example 2.

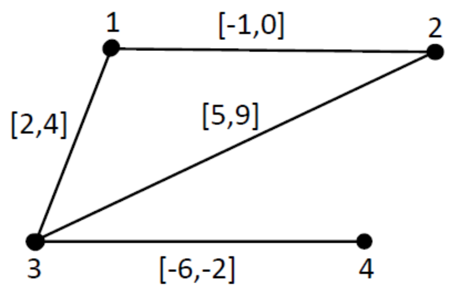

Figure 2. $\widetilde{G}$ Interval Weighted Graph.

- $\widetilde{w}(1) = [-1,0] + [2,4] = [1,4]$
- $\widetilde{w}(2) = [-1,0] + [5,9] = [4,9]$
- $\widetilde{w}(3) = [2,4] + [5,9] + [-6,-2] = [1,11]$
- $\widetilde{w}(4) = [-6,-2]$
- $d_{\tilde{G}}(1,2) = d_{\tilde{G}}(2,1) = [1,1]$
- $d_{\tilde{G}}(1,3) = d_{\tilde{G}}(3,1) = [1,1]$
- $d_{\tilde{G}}(1,4) = d_{\tilde{G}}(4,1) = [2,2]$
- $d_{\tilde{G}}(2,3) = d_{\tilde{G}}(3,2) = [1,1]$
- $d_{\tilde{G}}(2,4) = d_{\tilde{G}}(4,2) = [2,2]$
- $d_{\tilde{G}}(3,4) = d_{\tilde{G}}(4,3) = [1,1]$

$$\begin{aligned}\widetilde{W}(\tilde{G},\widetilde{w}) = \frac{1}{2}[\, & \widetilde{w}(1)\ \widetilde{w}(2)\, d_{\tilde{G}}(1,2) + \widetilde{w}(1)\widetilde{w}(3) d_{\tilde{G}}(1,3) + \widetilde{w}(1)\widetilde{w}(4)\, d_{\tilde{G}}(1,4) \\ & + \widetilde{w}(2)\ \widetilde{w}(1)\, d_{\tilde{G}}(2,1) + \widetilde{w}(2)\, \widetilde{w}(3)\, d_{\tilde{G}}(2,3) + \widetilde{w}(2)\, \widetilde{w}(4)\, d_{\tilde{G}}(2,4) \\ & + \widetilde{w}(3)\, \widetilde{w}(1)\, d_{\tilde{G}}(3,1) + \widetilde{w}(3)\ \widetilde{w}(2)\, d_{\tilde{G}}(3,2) + \widetilde{w}(3)\ \widetilde{w}(4)\, d_{\tilde{G}}(3,4) \\ & + \widetilde{w}(4)\ \widetilde{w}(1)\, d_{\tilde{G}}(4,1) + \widetilde{w}(4)\ \widetilde{w}(2)\, d_{\tilde{G}}(4,2) + +\widetilde{w}(4)\, \widetilde{w}(3)\, d_{\tilde{G}}(4,3)]\end{aligned}$$

$$\begin{aligned}\widetilde{W}(\tilde{G},\widetilde{w}) &= \frac{1}{2}\big[[1,4]\,[4,9][1,1] + [1,4][1,11][1,1] + [1,4][-6,-2][2,2] + [4,9][1,4][1,1] \\ &\quad + [4,9][1,11][1,1] + [4,9][-6,-2][2,2] + [1,11][1,4][1,1] \\ &\quad + [1,11][4,9][1,1] + [1,11][-6,-2][1,1] + [-6,-2][1,4][2,2] \\ &\quad + [-6,-2][4,9][2,2] + [-6,-2][1,11][1,1]\big] \\ &= [-213,157]\end{aligned}$$

3. ALGORITHM FOR FINDING WIENER INDEX OF VERTEX-WEIGHTED INTERVAL GRAPH

Let $\tilde{G}$ be a given connected, interval weighted graph with n vertices.

1. Determine weights of vertices of an undirected graph $\tilde{G}$.
2. Determine M matrix (matrix of weights of vertices) of $\tilde{G}$.

$$M = [\widetilde{w}(v_1)\ \widetilde{w}(v_2) \ldots\ \widetilde{w}(v_n)]_{1\times n}$$

3. Determine the distance between two vertices v_i and v_j of undirected graph $\tilde{G}$.

4. Determine Distance matrix $\widetilde{D}$ of $\tilde{G}$.

$$\widetilde{D} = \begin{bmatrix} [0,0] & d_{\tilde{G}}(v_1,v_2) & \ldots & d_{\tilde{G}}(v_1,v_n) \\ d_{\tilde{G}}(v_2,v_1) & [0,0] & \ldots & d_{\tilde{G}}(v_2,v_n) \\ \vdots & \vdots & \ddots & \vdots \\ d_{\tilde{G}}(v_n,v_1) & \ldots & \ldots & [0,0] \end{bmatrix}_{n\times n}$$

5. Find Wiener index $\widetilde{W}$ of $\tilde{G}$ with the help of

$$\widetilde{W} = \left[\left(M \cdot \widetilde{D}\right) \cdot M^T\right] / 2$$

Example 3.

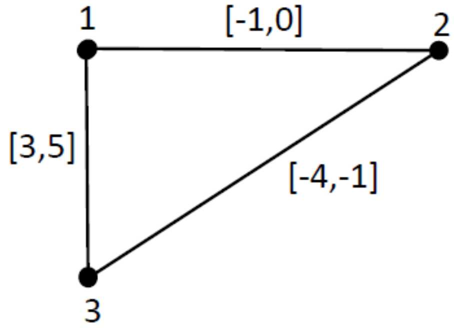

Figure 3. $\tilde{G}$ **Interval Weighted Graph.**

$\tilde{G}$ is a connected, interval weighted graph with 3 vertices.

1.
$\tilde{w}(1) = [-1,0] + [3,5] = [2,5]$
$\tilde{w}(2) = [-1,0] + [-4,-1] = [-5,-1]$
$\tilde{w}(3) = [3,5] + [-4,-1] = [-1,4]$

2.
$M = [\tilde{w}(1)\ \tilde{w}(2)\ \tilde{w}(3)\ ]_{1\times 3} = \big[[2,5]\ [-5,-1]\ [-1,4]\ \big]_{1\times 3}$

3.
$\tilde{d}(1,2) = \tilde{d}(2,1) = [1,1]$
$\tilde{d}(1,3) = \tilde{d}(3,1) = [1,1]$
$\tilde{d}(2,3) = \tilde{d}(3,2) = [1,1]$

4.
$$\tilde{D} = \begin{bmatrix} \tilde{d}(1,1) & \tilde{d}(1,2) & \tilde{d}(1,3) \\ \tilde{d}(2,1) & \tilde{d}(2,2) & \tilde{d}(2,3) \\ \tilde{d}(3,1) & \tilde{d}(3,2) & \tilde{d}(3,3) \end{bmatrix}_{3\times 3} = \begin{bmatrix} [0,0] & [1,1] & [1,1] \\ [1,1] & [0,0] & [1,1] \\ [1,1] & [1,1]] & [0,0] \end{bmatrix}_{3\times 3}$$

5.
$$\tilde{W} = \big[\big(M \cdot \tilde{D}\big) \cdot M^T\big]/2$$

$$= \left(\big[[2,5]\ [-5,-1]\ [-1,4]\ \big]_{1\times 3} \begin{bmatrix} [0,0] & [1,1] & [1,1] \\ [1,1] & [0,0] & [1,1] \\ [1,1] & [1,1]] & [0,0] \end{bmatrix}_{3\times 3_{3\times 3}} \begin{bmatrix} [2,5] \\ [-5,-1] \\ [-1,4] \end{bmatrix}_{3\times 1} \right)/2$$

$$= [-87,30]$$

4. WIENER INDEX OF INTERVAL WEIGHTED DIRECTED GRAPHS

A directed graph G is given by a set of vertices $V = V(G)$ and a set of ordered pairs of vertices $E = E(G)$ called directed edges or arcs. The number of vertices of G is denoted by n and the number of arcs is denoted by m. A directed path in G is a sequence of vertices $v_0, v_1, \dots, v_n$ such that $v_{i-1}v_i$ is an arc of G for all i. The distance $d(u, v)$ is the length of a shortest path from u to v. In digraphs, in general $d(u, v) = d(v, u)$ does not hold.

Let $\tilde{G}$ be a vertex-weighted directed interval graph on n vertices. Denote by $\widetilde{w}_{ij}$ the positive definite interval matrix of order p of the edge ij. We write $i \sim j$ if vertices i and j are adjacent. Let $\widetilde{w}_i{}^+ = \sum_{j:j\sim i} \widetilde{w}_{ij}$ be the weight interval matrix of the vertex i.

A vertex-weighted directed interval graph $(\tilde{G}, \widetilde{w})$ is a graph $\tilde{G}$ together with a function $\widetilde{w}: V(\tilde{G}) \to \mathbb{R}$. (Evidently, we could have chosen for vertex-weights interval or interval matrix.) The Wiener number $\widetilde{W}(\tilde{G}, \widetilde{w})$ of an interval weighted directed graph $(\tilde{G}, \widetilde{w})$ is defined as

$$\widetilde{W}(\tilde{G}, \widetilde{w}) = \sum_{\vec{p}(u,v)} \widetilde{w}^+(u)\, d_{\tilde{G}}(u, v).$$

5. ALGORITHM FOR FINDING WIENER INDEX OF VERTEX-WEIGHTED DIRECTED INTERVAL GRAPH

Let $\tilde{G}$ be a given connected, vertex-weighted directed interval graph with n vertices.

1. Determine weights of vertices of a directed graph $\tilde{G}$.
2. Determine Adjacency matrix A of $\tilde{G}$.
3. Determine Sparse matrix DG of A.
4. Determine Distance matrix DM of DG.
5. The Wiener index of $\tilde{G}$ is the sum of elements of Distance matrix DM.

Example 4.

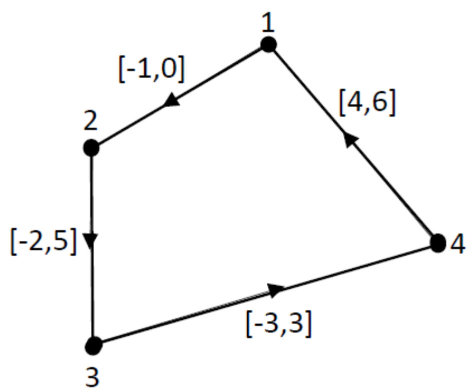

Figure 4. $\tilde{G}$ Vertex-Weighted Directed Interval Graph.

$\tilde{G}$ is a connected, interval weighted directed graph with 4 vertices.

1.
$$\widetilde{w}^{+}(1) = [-1,0]$$
$$\widetilde{w}^{+}(2) = [-2,5]$$
$$\widetilde{w}^{+}(3) = [-3,3]$$
$$\widetilde{w}^{+}(4) = [4,6]$$

2.
$$A = \begin{bmatrix} [0,0] & [-1,0] & [0,0] & [0,0] \\ [0,0] & [0,0] & [-2,5] & [0,0] \\ [0,0] & [0,0] & [0,0] & [-3,3] \\ [4,6] & [0,0] & [0,0] & [0,0] \end{bmatrix}_{4\times 4}$$

3.
$$DG = \begin{bmatrix} 1 & 2 & [-1,0] \\ 2 & 3 & [-2,5] \\ 3 & 4 & [-3,3] \\ 4 & 1 & [4,6] \end{bmatrix}_{4\times 3}$$

4.
$$DM = \begin{bmatrix} [0,0] & [-1,0] & [-3,5] & [-6,8] \\ [-1,14] & [0,0] & [-2,5] & [-5,8] \\ [1,9] & [0,9] & [0,0] & [-3,3] \\ [4,6] & [3,6] & [1,11] & [0,0] \end{bmatrix}_{4\times 4}$$

5.
$$\widetilde{W} = [-1,14] + [1,9] + [4,6] + [-1,0] + [0,9] + [3,6] + [-3,5] + [-2,5] + [1,11] + [-6,8] + [-5,8] + [-3,3]$$

$$= [-12,84]$$

6. CONCLUSION

To summarize, we have introduced interval weighted graphs, where the weights of the edges are interval or interval matrices in this paper. Then, we define Wiener index of interval weighted graph. From this definition, we give algorithms for finding Wiener index of interval weighted directed and undirected graph.

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