Complexity to Find Wiener Index of Some Graphs

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Abstract. The Wiener index is one of the oldest graph parameter which is used to study molecular-graph-based structure. This parameter was first proposed by Harold Wiener in 1947 to determining the boiling point of paraffin. The Wiener index of a molecular graph measures the compactness of the underlying molecule. This parameter is wide studied area for molecular chemistry. It is used to study the physio-chemical properties of the underlying organic compounds. The Wiener index of a connected graph is denoted by $W(G)$ and is defined as $W(G) = \frac{1}{2} \sum_{u \neq v} d(u,v)$, that is $W(G)$ is the sum of distances between all pairs (ordered) of vertices of $G$. In this paper, we give the algorithmic idea to find the Wiener index of some graphs, like cactus graphs and intersection graphs, viz. interval, circular-arc, permutation, trapezoid graphs.

Keywords: Wiener index, cactus graphs, intersection graphs, interval graphs, circular-arc graphs, permutation graphs, trapezoid graphs.

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1. Introduction
Molecular descriptor is a final result of a logic and mathematical procedure which transforms chemical information encoded with in a symbolic representation of a molecule into a useful number or the result of some standardized experiment. The Wiener index $W(G)$ is a distance-based topological invariant is also a molecular descriptor, it 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 ($\beta, \mu$) of alkanes based on the formula $b.\mu = \alpha W + \beta w(3) + \gamma$, where $\alpha, \beta, \gamma$ are empirical constants, and $w(3)$ is called path number. It is defined as the half sum of the distances between all pairs of vertices of $G[1, 12, 14]$

$$W(G) = \frac{1}{2} \sum_{u \neq v} d(u,v)$$

2. Algorithms to find Wiener index
2.1. Cactus graphs
The class of cactus graph is an important subclass of general planar graphs. Let $G = (V, E)$ be a finite, connected, undirected simple graph of $n$ vertices $m$ edges, where $V$ is the set of vertices and $E$ is the set of edges.

A vertex $u$ is called a cutvertex if removal of $u$ and all edges incident on $u$ disconnect the graph. A connected graph without a cutvertex is called a non-separable graph. A block of a graph is a maximal non-separable subgraph. A cycle is a connected graph (or subgraph) in which every vertex is of degree two. A block which is a cycle is
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called a cyclic block. A cactus graph is a connected graph in which every block is either an edge or a cycle. A weighted graph $G$ is a graph in which every edge is associates with a weight. Without loss of generality we assume that all weights are positive. A weighted cactus graph is a weighted, connected graph in which every block containing two vertices is an edge and three or more vertices is a cycle. A path of a graph $G$ is an alternating sequence of distinct vertices and edges which begins and ends with vertices in $G$. The length of a path is the sum of the weights of the edges in the path. A path from vertex $u$ to $v$ is a shortest path if there is no other path from $u$ to $v$ with lower length. The distance $d(u, v)$ between vertices $u$ and $v$ is the length of shortest path between $u$ and $v$ in $G$.

**Theorem 1.** [13] The shortest distances from a specified vertex to all other vertices of a weighted cactus graph can be computed in $O(n)$ time and the all pair shortest distance of a weighted cactus graph can be computed in $O(n^2)$ time, where $n$ represents the total number of vertices of the graph.

**Theorem 2.** The Winner index of the cactus graphs can be computed in $O(n^2)$ time, where $n$ represents the total number of vertices of the graph.

**Definition of Intersection graphs**

A graph $G = (V, E)$ is called an intersection graph for a finite family $F$ of a non-empty set if there is a one-to-one correspondence between $F$ and $V$ such that two sets in $F$ have non-empty intersection if and only if their corresponding vertices in $V$ are adjacent. We call $F$ an intersection model of $G$. For an intersection model $F$, we use $G(F)$ to denote the intersection graph for $F$.

Depending on the nature or geometric configuration of the sets $S_1, S_2, \ldots$, different types of intersection graphs are generated. The most useful intersection graphs are

- Interval graphs ($S$ is the set of intervals on a real line)
- Tolerance graphs
- Circular-arc graphs ($S$ is the set of arcs on a circle)
- Permutation graphs ($S$ is the set of line segments between two line segments)
- Trapezoid graphs ($S$ is the set of trapeziums between two line segments)
- Disk graphs ($S$ is the set of circles on a plane)
- Circle graphs ($S$ is the set of chords within a circle)
- Chordal graphs ($S$ is the set of connected subgraphs of a tree)
- String graphs ($S$ is the set of curves in a plane)
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- Graphs with boxicity $k$ ($S$ is the set of boxes of dimension $k$)
- Line graphs ($S$ is the set of edges of a graph).

2.2. Interval graphs
An undirected graph $G = (V, E)$ is said to be an interval graph if the vertex set $V$ can be put into one-to-one correspondence with a set $I$ of intervals on the real line such that two vertices are adjacent in $G$ if and only if their corresponding intervals have non-empty intersection. That is, there is a bijective mapping $f : V \rightarrow I$.

The set $I$ is called an interval representation of $G$ and $G$ is referred to as the interval graph of $I$ [19]. A large number of work on intersection graphs and cactus graphs have been done in [20-37].

**Theorem 3.** [7] The time complexity for finding the distances between all pair of vertices on interval graphs is $O(n^2)$.

**Theorem 4.** The Winner index of the interval graphs can be computed in $O(n^2)$ time, where $n$ represents the total number of vertices of the graph.

2.3. Circular-arc graphs
A graph is a circular-arc graph if there exists a family $A$ of arcs around a circle and a one-to-one correspondence between vertices of $G$ and arcs in $A$, such that two distinct vertices are adjacent in $G$ if and only if the corresponding arcs intersect in $A$. Such a family of arcs is called an arc representation for $G$.

A graph $G$ is a proper circular-arc (PCA) graph if there exists an arc representation for $G$ such that no arc is properly included in another.

A graph $G$ is a unit circular-arc (UCA) graph if there exists an arc representation for $G$ such that all the arcs are of the same length.

**Theorem 5.** [18] The all-pair shortest paths problem on circular-arc graph is computed in $O(n^2)$ time.

**Theorem 6.** The Winner index of the circular-arc graph is computed in $O(n^2)$ time.

2.4. Permutation graphs
An undirected graph $G = (V, E)$ with vertices $V = \{1, 2, \ldots, n\}$ is called a permutation graph if there exists a permutation $\pi$ on $N = \{1, 2, \ldots, n\}$ such that for all $i, j \in N$,

$$(i - j)(\pi^{-1}(i) - \pi^{-1}(j)) < 0$$
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if and only if \( i \) and \( j \) are joined by an edge in \( G \) [19]. Geometrically, the integers 1,2,...,\( n \) are drawn in order on a real line called as \emph{upper line} and \( \pi(1),\pi(2),...,\pi(n) \) on a line parallel to this line called as \emph{lower line} such that for each \( i \in N \), \( i \) is directly below \( \pi(i) \). Next, for each \( i \in V \), a line segment is drawn from \( i \) on the lower line to \( i \) on the upper line and it is denoted by \( l(i) \). Then from definition it follows that there is an edge \( (i, j) \) in \( G \) if and only if the line segment \( l(i) \) for \( i \) intersects the line segment \( l(j) \) for \( j \).

**Theorem 7.** [17] The all-pair shortest paths problem on permutation graphs in \( O(n^2) \) time.

**Theorem 8.** The Winner index of the permutation graphs can be computed in \( O(n^2) \) time.

### 2.5. Trapezoid graphs

A trapezoid \( T_i \) is defined by four corner points \( [a_i,b_i,c_i,d_i] \), where \( a_i < b_i \) and \( c_i < d_i \) with \( a_i,b_i \) lying on top line and \( c_i,d_i \) lying on bottom line of a rectangular channel. An undirected graph \( G = (V,E) \) with vertex set \( V = \{v_1,v_2,...,v_n\} \) and edge set \( E = \{e_1,e_2,...,e_n\} \) is called a trapezoid graph if a trapezoid representation can be obtained such that each vertex \( v_i \) in \( V \) corresponds to a trapezoid \( T_i \) and \( (v_i,v_j) \in E \) if and only if the trapezoids \( T_i \) and \( T_j \) corresponding to the vertices \( v_i \) and \( v_j \) intersect. For simplicity the vertices \( v_1,v_2,...,v_n \) are represented respectively by 1, 2, \..., \( n \). Thus the edge \( (i, j) \in E \) if and only if \( T_i \) and \( T_j \) intersect in the trapezoid representation.

**Theorem 9.** The time complexity to find all pairs shortest distances on trapezoid graphs is \( O(n^2) \).

**Theorem 10.** The time complexity to compute Winner index of a trapezoid graph is \( O(n^2) \).

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