Wiener and Szeged indices of Regular Tessellations

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Abstract. The Wiener index, or the Wiener number, also known as the "sum of distances" of a connected graph, is one of the quantities associated with a molecular graph that correlates nicely to physical and chemical properties, and has been studied in depth in the literature. In this paper we develop a method to compute the Wiener index of molecular graphs and thereby obtain the Wiener index of all classes of regular plane tessellations composed of the same kind of regular polygons namely triangular, square, and hexagonal. Further we study the Szeged index of regular tessellations.

Keywords: wiener index, szeged index, embedding, congestion, wirelength, regular tessellations.

1. Introduction

A graph G is an ordered pair of two sets, V and E, $V = V(G)$ being a finite non-empty set and $E = E(G)$ a binary relation defined on V. A graph can be visualized by representing the elements of V by vertices and joining pairs of vertices (x, y) by an edge if and only if $(x, y) \in E(G)$. A graph is said connected if any two vertices, x and y, are the endpoints of a path; otherwise it is disconnected. The vertex degree is the number of edges incident in that vertex. If all the vertices in G show the same degree, the graph is called regular graph.

A molecular graph is a collection of vertices representing the atoms in the molecule and a set of edges representing the covalent bonds. Graph representation of molecular structures is widely used in computational chemistry [29]. Quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR) represent attempts to correlate activities or properties with structural descriptors of compounds. To correlate and predict physical, chemical and biological activity/property from molecular structure is a very important and an unsolved problem in theoretical and computational chemistry [28]. The most important step in QSAR/QSPR is to numerically code the chemical structures of various molecules so as to build a correlation model between the chemical structures of various chemical compounds and the corresponding chemical and biological activities/properties. Thus, how to exactly transfer the chemical formula (or molecular graph) into numerical format has been a major task in QSAR/QSPR researches. There are many methods to quantify the molecular structures, of which the topological index is the most popular since it can be obtained directly from molecular structures and rapidly computed for large number of molecules [1, 4, 22, 33].

Topological indices are designed basically by transforming a molecular graph into a number. The first use of a topological index was made in 1947 by the chemist Harold Wiener [31]. The Wiener index is used to study the relation between molecular structure and physical and chemical properties of certain hydrocarbon compounds. It is defined as the sum of the distances between every pair of vertices of G. In the initial applications, the Wiener index is employed to predict physical parameters such as boiling points, heats of vaporization, molar volumes and molar refractions of alkanes [5, 8]. The study of Wiener index is one of the current areas of research in mathematical chemistry [3]. Researchers made some attempts to devise

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techniques for finding the Wiener index of chemical compounds [3, 5, 8, 11, 12, 14, 17, 26, 27] and also used brute force method based on distance matrix to compute the same [23]. In theoretical computer science, Wiener index is considered as one of the basic descriptors of fixed interconnection networks because it provides the average distance between any two nodes of the network [9, 32].

2. Wiener Index

The Wiener index was first used by Wiener for approximating the boiling points of alkanes b.p.$\approx \alpha\ W\ (G)$ + $\beta\ \omega_3 + \gamma$ where α, β and γ are empirical constants, and ω_3 is the number of vertex pairs that are at distance 3 from each other in the molecular graph, called the "path number" by Wiener. In general, the Wiener index measures how compact a molecule is for its given weight. It therefore has predictive value and chemists and physics have found many such uses for the Wiener index. For a graph G, let $d_G\ (u, v)$ be the number of edges on any shortest path joining vertex u to vertex v. The Wiener index is defined as

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

where the sum runs over all ordered pairs of vertices. If the vertex set is linearly ordered, we can write

$$W(G) = \sum_{u<v, u,v \in V(G)} d_G(u,v).$$

In this section, we use embedding as a tool to devise an elegant and simple technique for computing the Wiener index of graphs. We begin with certain definitions of the embedding problem. Graph embedding has been known as a powerful tool for implementation of parallel algorithms or simulation of different interconnection networks. A graph embedding [2] of a guest graph G into a host graph H is defined by an injective function $f : V (G) \to V (H)$ together with a mapping P_f which assigns to each edge (u, v) of G a path $P_f ((u, v))$ between $f (u)$ and $f (v)$ in H.

The edge congestion of an embedding f of G into H is the maximum number of edges of the graph G that are embedded on any single edge of H. Let $EC_f (e)$ denote the number of edges (u, v) of G such that e is in the path $P_f ((u, v))$ between $f (u)$ and $f (v)$ in H. The wirelength [24] of an embedding f of G into H is given by $WL_f (G, H) = \text{Sum}(EC_f (e))$ over e in $E(H)$. The wirelength of G into H is defined as $WL(G, H) = min\ WL_f$ (G, H) where the minimum is taken over all embeddings f of G into H. It is interesting to note that the wirelength of embedding the complete graph K_n on n vertices into the graph G on n vertices is equal to the Wiener index of G.

This motivates the following result.

Theorem 1 (*k*-Division Method) Let G be a graph on n vertices. Let $E^k(G)$ denote a collection of edges of G with each edge in G repeated exactly k times. Let $\{S_1, S_2,…,S_m\}$ be a partition of $E^k(G)$ such that each S_i is an edge cut of G and the removal of edges of S_i leaves G into 2 components G_i and $G_i^{'}$. Also each S_i satisfies the following conditions:

(i) For any two vertices $u, v \in G_i$, a shortest path between u and v has no edges in S_i.

(ii) For any two vertices $u, v \in G_i^{'}$, a shortest path between u and v has no edges in S_i.

(iii) For any two vertices $u \in G_i$ and $v \in G_i^{'}$, a shortest path between u and v has exactly one edge in S_i.

Then $W (G) = \dfrac{1}{k} \sum_{i=1}^{m}\ |V (G_i)|\ (n-|V (G_i)|)$.

3. Regular Plane Tessellations

Patterns covering the plane by fitting together replicas of the same basic shape have been created by Nature and Man either by accident or by design. Examples range from the simple hexagonal pattern of the bees' honeycomb or a tiled floor to the intricate decorations. These patterns are called tessellations. A regular tessellation is a pattern made by repeating a regular polygon. There are only three regular tessellations, composed of the same kind of regular polygons namely equilateral triangles, squares and hexagons. See Figure 1. These are the basis for the design of direct interconnection networks with highly competitive overall performance. Mesh connected computers and tori are based on regular square tessellations and are popular and well-known models for parallel processing. Hexagonal and honeycomb networks are based on regular triangular and hexagonal tessellations respectively. The inconsistency in the name selection (note that

a hexagonal network is not based on a hexagon, but on a triangular tessellation) is due to the duality of the two tessellations (one can be obtained from the other by joining the centres of the neighbouring polygons).
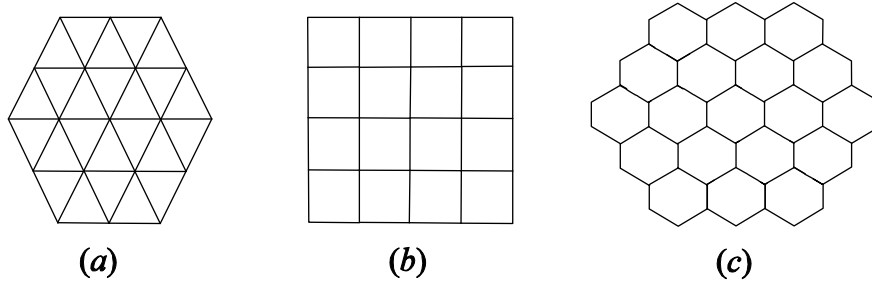

(a) (b) (c)

Fig. 1: Three regular tessellations composed of the same kind of regular polygons: (a) equilateral triangles (b) squares and (c) hexagons

Honeycomb and hexagonal networks have been studied in a variety of contexts. They have been applied in chemistry to model benzenoid hydrocarbons in image processing [30], computer graphics [21] and cellular networks [13]. Honeycomb architecture was investigated in [25], where a suitable addressing scheme, routing and broadcasting algorithms were proposed. An addressing scheme for processors and corresponding routing and broadcasting algorithms for hexagonal network are studied in [6].

A two dimensional mesh $M(m, \text{n})$ is defined as the Cartesian product $P_m \times P_n$ where P_m and P_n denote the path on m and n vertices respectively. Honeycomb networks can be built from hexagons in various ways. A hexagon is treated as a honeycomb of size one, denoted by $HC(1)$. The honeycomb $HC(2)$ of size two is obtained by adding six hexagons to the boundary edges of $HC(1)$. Inductively, honeycomb $HC(n)$ of size n is obtained from $HC(n-1)$ by adding a layer of hexagons around the boundary of $HC(n-1)$. The number of vertices and edges of $HC(n)$ are $6n^2$ and $9n^2-3n$ respectively [25]. Hexagonal networks are based on the partition of a plane into equilateral triangles. Hexagonal network $HX(n)$ of dimension n has $3n^2-3n+1$ vertices and $9n^2-15n+6$ edges, where n is the number of vertices on one side of the hexagon [6]. In this section, we obtain the Wiener number of regular tessellation using k-division method.

Lemma 1 $W(M(m,n)) = 1/6\, mn(m+n)(mn-1)$.

Lemma 2 $W(HC(n)) = 1/5\,(164n^5 - 30n^3 + n)$.

Lemma 3 $W(HX(n)) = (n/10)\,(41n^4 + 100n^2 + 9) - (n^2/4)(41n^2 + 19)$.

4. Szeged Index

Let $e = (u, v)$ be an edge of the graph G. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. In other words, $n_u(e) = |\{w : w \in V(G), d_G(u,w) < d_G(v,w)\}|$. Analogously, $n_v(e)$ is the number of vertices of G whose distance to the vertex v is smaller than the distance to the vertex u. In other words, $n_v(e) = |\{w : w \in V(G), d_G(v,w) < d_G(u,w)\}|$. Note that the vertices equidistant to u and v are not counted.

The Szeged index [19] is a molecular structure descriptor and is defined as $S_z(G) = \sum_{e \in E(G)} n_u(e) \times n_v(e)$. In the paper [15] proved that for a benzenoid graph G, $S_z(G) = \sum_{C \in C(G)} |C|\, n_1(C)\, n_2(C)$. Hence we have the following results.

Lemma 4 The Szeged index of mesh is given by $S_z(M(m, n)) = 16\, mn(2m^2n^2 - m^2 - n^2)$.

Lemma 5 The Szeged index of Honeycomb network is given by $S_z(HC(n)) = 3n^2/2\,(36n^4 - n^2 + 1)$.

It is interesting to note that the problem of devising techniques for computing the Szeged index of hexagonal network is still open.

5. Conclusion

In this paper we have formulated a new technique to compute the Wiener index of graphs. We have good reasons to believe that many more chemical graphs remain to be explored whose Wiener index can be computed applying our technique. Finally, the problem of computing the Szeged index for hexagonal network is under investigation.

6. Acknowledgements

7. References

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