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ON THE WIENER INDEX OF A GRAPH

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Abstract

A modification of the Wiener index which properly takes into account the symmetry of a graph is proposed. The explicit formulae for the modified Wiener index of path, cycle, complete bipartite, cube and lattice graphs are derived and compared with their standard Wiener index.

1. Introduction

Chemists employ structural formulae in communicating information on molecules and their structure. The structural or molecular graphs are mathematical objects representing structural formulae. By manipulating such objects, the chemical structures can be characterized numerically.

A topological index is a numerical quantity derived in an unambiguous manner from the structural graph of a molecule. These indices are graph invariants. They usually reflect molecular size and shape.

The first topological index in chemistry was introduced by H. Wiener in 1947 [1,2] to study the boiling points of paraffins. Since then, the Wiener index W has been used to explain various chemical and physical properties of molecules [3] and to correlate the structure of molecules with their biological activity [4].

The Wiener index of a graph represents the sum of all distances in the graph. Various algorithms [5–7] were developed for the evaluation of the Wiener index. A number of explicit formulae were derived for the special classes of compounds: chains [1], simple cycles [2], cyclic structures with acyclic branches [8], spiro systems [9], trees [10], polycyclic compounds [11], especially benzenoids [12–13], etc.

Although the Wiener index has become part of the general scientific culture [14], it is still the subject of intensive research [15]. Here, we propose a version of the Wiener index which properly takes into account the symmetry of a graph.

2. Definitions

Every connected graph G can be regarded as a metric space on the vertex set $V = V(G)$ in which the distance $d(u, v)$ between any two vertices is the number of edges on the shortest path from u to v.

The first "topological index" in mathematical chemistry was introduced by H. Wiener in 1947 [4]. In our notation, it can be described as follows:

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

The Wiener index of G, $W(G)$, represents the sum of all distances of G.

If A and B are two sets of vertices of G, let us introduce the following notation:

$$d(A, B) = \sum_{u \in A} \sum_{v \in B} d(u, v).$$

This means that

$$W(G) = \frac{1}{2} d(V, V).$$

Let Aut G denote the group of automorphisms of G and let $g \in \operatorname{Aut} G$ be any automorphism. Define a *distance number* $\delta(g)$ of g as

$$\delta(g) = \frac{1}{|V|} \sum_{u \in V} d(u, g(u)).$$

$\delta(g)$ represents the average distance by which g displaces a typical vertex of G. If Γ is a subgroup of Aut G, we will denote by $\delta(\Gamma)$ the average:

$$\delta(\Gamma) = \frac{1}{|\Gamma|} \sum_{g \in \Gamma} \delta(g) = \frac{1}{|\Gamma||V|} \sum_{u \in V} \sum_{g \in \Gamma} d(u, g(u)).$$

The distance number $\delta(G)$ of a graph is simply

$$\delta(G) = \delta(\operatorname{Aut} G).$$

By V_i, $1 \leq i \leq p$, we shall denote any of the p orbits of V determined by Γ. (Usually, we take $\Gamma = \operatorname{Aut} G$.) $V_i \cap V_j = \varnothing$ if $i \neq j$. The p orbits partition the vertex set V:

$$V = V_1 \cup \ldots \cup V_p.$$

Let Γ_i denote a "generic" stabilizer of a vertex v_i from V_i. It is well-known that

$$|\Gamma| = |V_i||\Gamma_i|,$$

(see, for instance, Biggs and White [16]). If Aut G has only one orbit ($p = 1$), G is said to be *vertex transitive* (see, for instance, Biggs [17]).

3. Results

In fact, our main result shows that the Wiener index of a vertex transitive graph G can be expressed in terms of the distance number of G.

THEOREM 3.1

$$|V|\delta(G) = 2\sum_{i=1}^{p}(W(V_i)/|V_i|).$$

COROLLARY 3.2

If G is a vertex transitive graph, then

$$W(G) = \frac{|V|^2\delta(G)}{2}.$$

Before we prove theorem 3.1, let us comment on some terms used in the proof. In the proof, we take $\Gamma = \mathrm{Aut}\, G$. By $n(u, v)$ we denote the number of automorphisms mapping u into v. If u is a vertex, we denote by Γ_u the stabilizer group for u. If u and v belong to the same orbit V_i, it is true that

$$n(u, v) = |\Gamma_u| = |\Gamma_v|.$$

Therefore, we may introduce a "generic" stabilizer Γ_i with $|\Gamma_i| = n(u, v)$.

Proof of theorem 3.1

$$\delta(G) = \frac{1}{|\Gamma|}\sum_{g\in\Gamma}\delta(g) = \frac{1}{|\Gamma||V|}\sum_{g\in\Gamma}\sum_{u\in V} d(u, g(u))$$

$$= \frac{1}{|\Gamma||V|}\sum_{u\in V}\sum_{v\in V} d(u, v)\cdot n(u, v) = \frac{1}{|\Gamma||V|}\sum_{i=1}^{p}\sum_{u\in V_i}\sum_{v\in V_i} d(u, v)\cdot|\Gamma_i|$$

$$= \frac{1}{|\Gamma||V|}\sum_{i=1}^{p}|\Gamma_i| d(V_i, V_i) = \frac{1}{|V|}\sum_{i=1}^{p}\frac{1}{|V_i|} d(V_i, V_i).$$

Therefore,

$$|V|\delta(G) = \sum_{i=1}^{p} \frac{1}{|V_i|} d(V_i, V_i) = \sum_{i=1}^{p} \frac{2W(V_i)}{|V_i|}$$

and

$$|V|\delta(G) = 2\sum_{i=1}^{p} W(V_i)/|V_i|. \qquad \square$$

4. Some implications

First, let us introduce some more concepts. Let us define

$$\omega(U) = \frac{1}{|U|^2} \sum_{u \in U} \sum_{v \in U} d(u,v) = \frac{1}{|U|^2} d(U,U).$$

We call $\omega(U)$ the *normalized Wiener index*. Clearly, we have

$$\omega(U) = 2W(U)/|U|^2.$$

Our theorem 3.1 has a much more interesting form in terms of ω:

$$\delta(G) = \frac{1}{|V|} \sum_{i=1}^{p} |V_i|\omega(V_i).$$

In this sense, $\delta(G)$ becomes a weighted average of normalized Wiener indices of orbits of G. Note that $\delta(G)$ depends solely on the orbit structure of G. This means that $\delta(\mathrm{Aut}\, G) = \delta(\Gamma)$ for any automorphism group Γ having the same orbit structure as $\mathrm{Aut}\, G$.

The computation of the normalized Wiener index $\omega(U)$ is somewhat simplified if U is an orbit.

PROPOSITION 4.3

If V_i is an orbit, then

$$\omega(V_i) = \frac{1}{|V_i|} d(u, V_i) \qquad \text{for each } u \in V_i .$$

Proof

$$\omega(V_i) = \frac{1}{|V_i|^2} d(V_i, V_i) = \frac{1}{|V_i|^2} \sum_{u \in V_i} d(u, V_i).$$

However, if u and v are two elements from V_i, we have $d(u, V_i) = d(v, V_i)$. Therefore,

$$\omega(V_i) = \frac{1}{|V_i|^2} |V_i| d(u, V_i). \qquad \square$$

COROLLARY 4.4

If G is a vertex transitive, then for each vertex u

$$\delta(G) = \omega(V) = \frac{1}{|V|} d(u, V).$$

The Wiener index does not consider the symmetry structure of G. In view of corollary 3.2, we may try to extend the right-hand side formula. Hereby, we introduce the *modified Wiener index* $\hat{W}(G)$ as:

$$\hat{W}(G) = \tfrac{1}{2} |V|^2 \delta(G).$$

This index can be rewritten as follows:

$$\hat{W}(G) = |V| \sum_{i=1}^{p} \frac{W(V_i)}{|V_i|}$$

and it takes into account the symmetry structure of G more appropriately than the standard Wiener index $W(G)$. This observation is the motivation for the present paper.

5. Examples

In this section, we compare $W(G)$, $\hat{W}(G)$ and $\omega(G)$ for several families of graphs.

Example 5.6

Let us consider the path P_n of n vertices. It is easy to see that $W(P_n) = (n^3 - n)/6$. Therefore, $\omega(P_n) = (n^2 - 1)/3n$. Also,

$$\hat{W}(P_n) = \begin{cases} \frac{n^3}{2} & \text{if } n \text{ is even,} \\ \frac{(n^3-n)}{2} & \text{if } n \text{ is odd.} \end{cases}$$

Example 5.7

The n-cycle C_n is vertex transitive. Therefore,

$$W(C_n) = \hat{W}(C_n) = \begin{cases} \frac{n^3-n}{8} & \text{if } n \text{ is odd,} \\ \frac{n^3}{8} & \text{if } n \text{ is even;} \end{cases}$$

$$\omega(C_n) = \frac{2}{n^2} W(C_n).$$

Example 5.8

The complete bipartite graph $K_{m,n}$. A simple counting argument shows that

$$W(K_{m,n}) = m^2 + mn + n^2 - m - n.$$

In the case $m = n$, we set

$$W(K_{n,n}) = 3n^2 - 2n.$$

Since $K_{n,n}$ is vertex transitive, we obtain

$$\hat{W}(K_{n,n}) = 3n^2 - 2n.$$

However, $K_{m,n}$, $m \neq n$ is not vertex transitive. Aut $K_{m,n}$ has two orbits and we obtain

$$(m \neq n) \quad \hat{W}(K_{m,n}) = (m+n)(m+n-2) = m^2 + 2mn + n^2 - 2m - 2n.$$

Note that the formula for $\hat{W}(K_{m,n})$ does *not* reduce to the formula for $\hat{W}(K_{n,n})$ by letting $m = n$. Obviously, we obtain

$$\omega(K_{m,n}) = \frac{2}{(m+n)^2} W(K_{m,n}) = \frac{2(m^2 + mn + n^2 - m - n)}{(m+n)^2}.$$

Before we proceed, let us prove a result concerning the Cartesian products of graphs. Recall the Cartesian product $G \times H$ of two graphs G and H: $V(G \times H) = V(G) \times V(H)$. The vertices (u_1, u_2) and (v_1, v_2) are adjacent if and only if either $u_1 = v_1$ and u_2 is adjacent to v_2 in H or $u_2 = v_2$ and u_1 is adjacent to v_1 in G. In the further text, we will need the following theorem:

THEOREM 5.9

$$W(G \times H) = W(G) \cdot |V(H)|^2 + W(H) \cdot |V(G)|^2.$$

Proof

If $U_1 \subseteq V(G)$ and $U_2 \subseteq V(H)$, then for $U = U_1 \times U_2$:

$$
\begin{aligned}
d(U,V) &= d(U_1\times U_2, U_1\times U_2)\\
&= \sum_{(u_1,u_2)}\sum_{(v_1,v_2)} d((u_1,u_2),(v_1,v_2))\\
&= \sum\sum (d(u_1,v_1)+d(u_2,v_2))\\
&= \sum\sum d(u_1,v_1)+\sum\sum d(u_2,v_2)\\
&= |U_2|^2\sum_{u_1}\sum_{v_1} d(u_1,v_1)+|U_1|^2\sum_{u_2}\sum_{v_2} d(u_2,v_2)\\
&= |U_1|^2 d(U_2,U_2)+|U_2|^2 d(U_1,U_1).
\end{aligned}
$$

From $d(U, U) = |U_1|^2 d(U_2, U_2) + |U_2|^2 d(U_1, U_1)$, we obtain the result from theorem 5.9 if we let $U = U_1 \times U_2 = V(G) \times V(H)$. □

COROLLARY 5.10

$$W(G^k) = kW(G)|V(G)|^{2(k-1)}.$$

Proof

By induction on k. □

Example 5.11

Take Q_n, the *n-cube graph*. Since $Q_n = K_2^n = K_2 \times K_2 \times \ldots \times K_2$ (n factors), we may conclude by corollary 5.10 that

$$W(Q_n) = n \cdot 1 \cdot 2^{2(n-1)} = n2^{2n-2}.$$

Since Q_n is vertex transitive, this gives also $\hat{W}(Q_n) = n2^{2n-2}$. Finally,

$$\omega(Q_n) = \frac{2}{2^{2n}} W(Q_n) = \frac{2}{2^{2n}} \cdot n \cdot 2^{2n-2} = \frac{n}{2}.$$

Example 5.12

The lattice graph $L_{m,n} = P_m \times P_n$. Here, we will use example 5.6 and theorem 5.9.

$$W(P_m \times P_n) = m^2 W(P_n) + n^2 W(P_n) = m^2 \frac{n^3 - n}{6} + n^2 \frac{m^3 - m}{6},$$

$$W(P_m \times P_n) = \frac{mn(m+n)(mn-1)}{6}.$$

Clearly,

$$\omega(P_m \times P_n) = \frac{2}{(mn)^2} W(P_m \times P_n) = \frac{(m+n)(mn-1)}{3mn}.$$

In order to determine $\hat{W}(P_m \times P_n)$, we would need a theorem for $\hat{W}(G \times H)$. Let us assume that

$$V(G) = V_1 \cup V_2 \cup \ldots \cup V_p$$

and

$$V(H) = U_1 \cup U_2 \cup \ldots \cup U_q$$

are the orbit partitions of G and H. We will assume that $V(G \times H) = T_{11} \cup \ldots \cup T_{pq}$ is the orbit partition of $G \times H$ when $T_{ij} = V_i \times U_j$.

Under the above assumptions, we may prove the following theorem:

THEOREM 5.13

$$\hat{W}(G \times H) = |V(G)|^2 \hat{W}(H) + |V(H)|^2 \hat{W}(G).$$

Proof

$$\hat{W}(G \times H) = |V(G) \times V(H)| \sum_{i=1}^{p} \sum_{j=1}^{q} W(T_{ij})/|T_{ij}|$$

$$= |V(G)||V(H)| \sum_i \sum_j W(V_i \times U_j)/(|V_i||U_j|)$$

$$= |V(G)||V(H)| \sum_i \sum_j \frac{|V_i|^2 W(U_j) + |U_i|^2 W(V_j)}{|U_i||V_j|}$$

$$= |V(G)||V(H)| \left[\sum_i \frac{|V_i|^2}{|V_i|} \sum_j \frac{W(U_j)}{|U_j|} + \sum_j \frac{|U_j|^2}{|U_j|} \sum_i \frac{W(V_i)}{|V_i|} \right]$$

$$= |V(G)||V(H)| \left[\sum_i |V_i| \frac{\hat{W}(H)}{|V(H)|} + \sum_j |U_j| \frac{\hat{W}(H)}{|V(H)|} \right]$$

$$= |V(G)||V(H)| \left[|V(G)| \hat{W}(H)/|V(H)| + |V(H)| \hat{W}(G)/|V(G)| \right]$$

$$= |V(G)|^2 \hat{W}(H) + |V(H)|^2 \hat{W}(G). \qquad \square$$

COROLLARY 5.14

Under the assumptions, we obtain

$$\hat{W}(G^k) = k\hat{W}(G)|V(G)|^{2(k-1)}.$$

Example 5.12 (revisited)

$\hat{W}(P_m \times P_n)$ can be computed from example 5.6 and theorem 5.13. There are four cases:

$$\hat{W}(P_m \times P_n) = \begin{cases} n^2 \frac{m^3}{2} + m^2 \frac{n^3}{2} & m \text{ even, } n \text{ even,} \\ n^2 \frac{m^3-m}{2} + m^2 \frac{n^3}{2} & m \text{ odd, } n \text{ even,} \\ n^2 \frac{m^3}{2} + m^2 \frac{n^3-n}{2} & m \text{ even, } n \text{ odd,} \\ n^2 \frac{m^3-m}{2} + m^2 \frac{n^3-n}{2} & m \text{ odd, } n \text{ odd;} \end{cases}$$

$$\hat{W}(P_m \times P_n) = \begin{cases} \frac{n^2m^2}{2}(m+n) & m \text{ even, } n \text{ even,} \\ \frac{nm}{2}((m^2-1)n + (n^2m)) & m \text{ odd, } n \text{ even,} \\ \frac{nm}{2}(m^2n + (n^2-1)m) & m \text{ even, } n \text{ odd,} \\ \frac{nm}{2}((m^2-1)n + (n^2-1)m) & m \text{ odd, } n \text{ odd.} \end{cases}$$

Note that although for $m = n$ the graph $P_m \times P_n$ is "more symmetric" than for $m \neq n$, we nevertheless have the same orbit structure and the above formulae remain valid.

Correlations between the Wiener index and various chemical and physical properties of molecules have been extensively studied. Perhaps it would be of interest to extend similar studies to the modified Wiener index proposed in this paper.

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