Weights on Edges of Chemical Graphs Determined by Paths§

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This paper presents two methods of assigning weights to edges of a graph. Let P (P^*) be a path (a shortest path) between a and b, and let $n(a,b)$ ($n^*(a,b)$) be the number of simple paths (shortest paths) with end points a and b. For an edge e we define the following equations: $w(e) := \sum_{P_{a,b}\ni e} 1/n(a,b)$; $w^*(e) := \sum_{P^*_{a,b}\ni e} 1/n^*(a,b)$. These weight distributions are graph invariants. Several properties of w and w^* are studied along the lines of Wiener and Lukovits. The weights w and w^* are determined for several families of graphs that are of interest in chemistry.

1. INTRODUCTION

Chemists employ structural formulas in communicating information about molecules and their structure. The *structural* or *molecular graphs* are mathematical objects representing structural formulas. These objects encode important properties of the chemical structures.

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

The first topological index in chemistry was introduced by Wiener[1] in 1947 to study boiling points of paraffins (for historical data see, for instance, ref 2). Since then, the Wiener index has been used to explain various chemical and physical properties of molecules and to correlate the structure of molecules to their biological activity.[3]

Although other indices have been proposed by various researchers (for a survey see, for instance, refs 4 and 5), the Wiener index has become part of a general scientific culture.[6] It is still a subject of intensive research.[7–12]

Here we consider a connection between certain distributions of weights on the edges of a graph and its Wiener index. For symmetric graphs this approach simplifies the computation of the Wiener index in a way that is similar to the one used in ref 8.

A *graph* $G = (V,E)$ is a combinatorial object consisting of an arbitrary set $V = V(G)$ of *vertices* and a set $E = E(G)$ of *edges*. $E(G)$ shall be considered as a set of unordered pairs $\{x,y\}$ of distinct vertices of G. With this restriction on the edge set we get undirected graphs without loops and multiple edges, i.e. *simple graphs*. Considering G as $V(G) \cup E(G)$, we sometimes write $x \in G$ for $x \in V(G)$ and $e \in G$ for $e \in E(G)$. A *simple path* from x to y is a sequence of distinct vertices $P = x_0, x_1, ..., x_l$ such that each pair x_i, x_{i+1} is connected by an edge and $x_0 = x$ and $x_l = y$. The *length* of the path is the number of edges, $l(P) = l$. For any pair of vertices x,y we define the *distance* $d(x,y)$ to be the length of the shortest path between x and y. If there is no (finite) path, we define $d(x,y) = \infty$. A graph G is *connected*, if $d(x,y) < \infty$ for any pair of vertices x,y. Here we will consider only connected graphs. The *Cartesian product* of graphs G and H is the graph $K = G\Box H$ whose vertex set $V(K)$ is the Cartesian product $V(G) \times V(H)$; i.e. each vertex of K is an ordered pair (u,v) of vertices $u \in V(G)$, $v \in V(H)$ and (u,v) is adjacent to (u',v') if and only if either u is adjacent to u' in G and $v = v'$ or $u = u'$ and v is adjacent to v' in H.

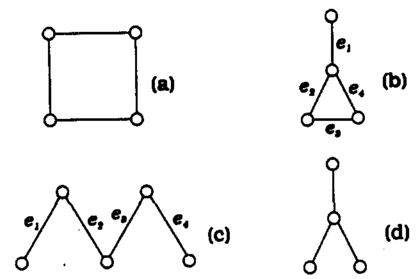

Figure 1. Four simple examples.

2. EDGE WEIGHTS AND GRAPH INDICES

Let P be a path between a and b, and let $n(a,b)$ be the number of simple paths with end points a and b. For an edge e we define

$$w(e) := \sum_{P_{a,b}\ni e} \frac{1}{n(a,b)}$$

We call $w(e)$ the *path weight* of the edge e and w the *path weight distribution*. Similarly we define $w^*(e)$, the *shortest path weight* of e. Let P^* be a shortest path between a and b, and let $n^*(a,b)$ be the number of simple shortest paths with end points a and b. For an edge e we define

$$w^*(e) := \sum_{P^*_{a,b}\ni e} \frac{1}{n^*(a,b)}$$

We call w^* the *shortest path weight distribution*. Both weight distributions are graph invariants. Essentially the same approach was taken earlier independently by Lukovits.[9,10]

Example a. $G = C_4$, the cycle of length (see Figure 1a). Let e be any edge of C_4. For every pair of distinct vertices, there are exactly two paths between them, and e is exactly on one of the two paths. Hence

$$w(e) = \sum_{e\in P} {}^1/_2 = 6\,{}^1/_2 = 3$$

On the other hand, if only the shortest paths are considered, we have

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$$w^*(e) = 1 + {}^1/_2 + {}^1/_2 + 0 + 0 + 0 = 2$$

Example b. There are four edges in the graph of Figure 1b. Obviously, there is an automorphism of the graph which maps e_2 to e_4 that implies $w(e_2) = w(e_4)$ and $w^*(e_2) = w^*(e_4)$.

$$w(e_1) = 1 + 1 + 1 = 3 \tag{1}$$

$$w(e_2) = w(e_4) = {}^1/_2 + {}^1/_2 + {}^1/_2 + {}^1/_2 + {}^1/_2 = 2.5 \tag{2}$$

$$w(e_3) = {}^1/_2 + {}^1/_2 + {}^1/_2 + {}^1/_2 + {}^1/_2 = 2.5 \tag{3}$$

$$w^*(e_1) = 1 + 1 + 1 = 3 \tag{4}$$

$$w^*(e_2) = w^*(e_4) = 1 + 1 = 2 \tag{5}$$

$$w^*(e_3) = 1 \tag{6}$$

Example c is for P_4, the path on four vertices (Figure 1c).

$$w(e_1) = w(e_4) = 4, \quad w(e_2) = w(e_3) = 6$$

$$w^*(e_i) = w(e_i)$$

Example d. The star graph $S_3 = K_{1,3}$ (Figure 1d).

$$w(e) = w^*(e) = 3$$

Note that in all the examples above (and in all examples we have computed) we found $w(e) \geq w^*(e)$. However, we have not been able to prove or disprove this in general.

Proposition 1. *For any tree T and any edge e of T we have $w(e) = w^*(e)$.*

Proof. Let T be a tree, and let e be any edge of T. Then $T\backslash e$ has exactly two connected components. Let n_1 and n_2 be the numbers of vertices in these two connected components. Now we recall the well-known properties of trees that any path in a tree is a shortest path and that there is exactly one shortest path between any pair of vertices in a tree. Hence, we have $w(e) = w^*(e) = n_1n_2$. Note that the formula $w^*(e) = n_1n_2$ was already discovered in the original paper of Wiener.[1]

Given the two distributions $w(e)$ and $w^*(e)$, with $e \in E(G)$, we can define

$$\Omega(G) = {}^1/_2 \sum_{e\in E(G)} w(e)$$

$$\Omega^*(G) = {}^1/_2 \sum_{e\in E(G)} w^*(e)$$

Let $W(G)$ denote the *Wiener index* of a graph, i.e.

$$W(G) = n\sum_{i=1}^{n}\sum_{j=i+1}^{n} d(i,j)$$

where $n = |V(G)|$ and $d(i,j)$ represents the distance between v_i and v_j. Note that the definition of $W(G)$ does not depend on the ordering of the vertices.

Now we recall some relations between $\Omega(G)$, $\Omega^*(G)$, and $W(G)$.

Proposition 2.

(*i*) *For any graph G, $\Omega^*(G)$ is equal to the Wiener index $W(G)$.*

(*ii*) *For any tree T, $\Omega(T) = \Omega^*(T)$.*

Proof. Easy consequence of the prèvious proposition and the above definitions. Note that i was applied by Lukovits. It was also known to Wiener in the case of a tree.

Theorem 1. *For any graph G, $\Omega(G) \geq \Omega^*(G)$.*

Proof. In order to prove the inequality we use the fact that the average length over all paths between two vertices is greater or equal to the minimal length, i.e. the length of a shortest path.

$$2\Omega(G) = \sum_{e\in E(G)} w(e) = \sum_{e\in E(G)} \sum_{P_{a,b}\ni e} \frac{1}{n(a,b)} =$$
$$\sum_{a\in V(G)} \sum_{b\in V(G)} \sum_{P_{a,b}} \sum_{e\in P_{a,b}} \frac{1}{n(a,b)} = \sum_{a\in V(G)} \sum_{b\in V(G)} \sum_{P_{a,b}} \frac{l(P_{a,b})}{n(a,b)} \geq$$
$$\sum_{a\in V(G)} \sum_{b\in V(G)} \sum_{P_{a,b}} \frac{d(a,b)}{n(a,b)} = \sum_{a\in V(G)} \sum_{b\in V(G)} d(a,b) =$$
$$2W(G) = 2\Omega^*(G)$$

Note that the equality holds exactly when the average length over all paths between any pair of vertices is equal to the distance between them. Graphs, for which this is true, are exactly trees. Hence $\Omega(G) = \Omega^*(G)$ if and only if G is a tree.

3. MORE EXAMPLES

In examples a–d we were able to reduce the amount of calculation by using the symmetry of the graphs. If G is a graph with the automorphism group Γ, then Γ acts as a permutation group on the vertex set $V(G)$. At the same time we may view it to act on the edge set $E(G)$. We can make a distinction by writing $(\Gamma, V(G))$ in the first case and $(\Gamma, E(G))$ in the second one. Each permutation group (Γ, X) partitions the set X into orbits. If there is only one orbit, we say that Γ is *transitive* on X. If Γ acts transitively on $V(G)$, the graph is said to be *vertex-transitive*; if the action of Γ on $E(G)$ is transitive, then the graph is said to be *edge-transitive*. For more information about graphs and permutation groups, the reader is referred to ref 13.

In general, the weights at each edge orbit are constant. In order to compute the Wiener index, it suffices to compute the weights only once for each orbit. In the case of edge-transitive graphs, this means only one weight has to be determined. In this case the problem can be easily reversed. If the Wiener index is known, then the weights can be readily computed. If $E_1, E_2, ..., E_s$ are the edge orbits for the automorphism group of G then for each orbit E_k the weight of each edge in it is constant and the weight value can be denoted by $w^*(E_k)$. Then the Wiener index can be expressed as

$$W(G) = {}^1/_2\sum_{k=1}^{s}|E_k|w^*(E_k) \tag{7}$$

In the case of an edge-transitive graph we have

$$W(G) = {}^1/_2|E(G)|w^*(e) \tag{8}$$

Here are some useful facts that can be found in graph-theoretical literature; see, for instance, ref 14.

Proposition 3. *For any vertex-transitive graphs G and H, the Cartesian product $G\Box H$ is vertex transitive.*

Note that G and H may be both vertex- and edge-transitive and $G\Box H$ need not be edge-transitive. For instance, let $G = K_2$, $H = K_3$. The Cartesian product $K_2\Box K_3$ is vertex-transitive but has six edges in one orbit and three edges in the other.

Proposition 4. *For any vertex- and edge-transitive graph G, the nth Cartesian power G^n is (vertex- and) edge-transitive.*

In the above theorem both vertex- and edge-transitivity are needed. Note that the path on three vertices P_3 is edge-transitive but $P_3 \square P_3$ is not. Also, $K_2 \square K_3$ is vertex-transitive but $K_2 \square K_3 \square K_2 \square K_3$ is not edge-transitive.

If e is an edge of a vertex- and edge-transitive graph G, then $e^{(k)}$ will denote any edge of G^k.

Theorem 2. *For any vertex- and edge-transitive graph G of degree d, for any edge e of G, and* for any edge $e^{(k)}$ *of the nth Cartesian power G^n we have*

$$(i)\ W(G^k) = {}^1/_2|E(G^k)|w^*(e^{(k)})$$

$$(ii)\ w^*(e^{(k)}) = \frac{4W(G)}{d}|V(G)|^{k-2}$$

$$(iii)\ w^*(e^{(k)}) = w^*(e)|V(G)|^{k-1}$$

Proof. The proof follows from the definitions, from the above propositions, and from formulas 7 and 8.

The simplest examples of graphs that are vertex- and edge-transitive are K_2, cycles C_n, and regular compete r-partite graphs $K_{n,n,...,n}$. We will consider these three examples and their Cartesian powers.

Example e. The kth Cartesian power of the K_2 is the k-cube graph Q_k. Obviously we have $W(K_2) = 1, w^*(e) = 2$, and $d = 1$. Therefore by the above *theorem* 2 $w^*(e^{(k)}) = 2^k$. Note that the Wiener index of the Q_k is $W(Q_k) = k2^{2k-2}$ (see, for example, ref 8).

This can be readily generalized to the kth Cartesian power of the complete graph on n vertices, K_n. Obviously we have $W(K_n) = n(n-1)/2$, $w^*(e) = 2$, and $d = n - 1$. Therefore $w^*(e^{(k)}) = 2n^{k-1}$ and $W(K_n^k) = k(n-1)n^{2k-1}/2$.

The next example is the Cartesian power of cycles.

Example f. Using theorem 2 and the formulas

$$W(C_n) = \begin{cases} (n^2-1)n/8, & n \text{ odd} \\ n^3/8, & n \text{ even} \end{cases}$$

$$\omega^*(C_n) = \begin{cases} (n^2-1)/4, & n \\ n^2/4, & n \text{ even} \end{cases}$$

(see refs 10–12), we obtain for C_n^k

$$W(C_n^k) = \begin{cases} k(n^2-1)n^{2k-1}/8, & n \text{ odd} \\ kn^{2k+1}/8, & n \text{ even} \end{cases}$$

$$\omega^*(e^{(k)}) = \begin{cases} (n^2-1)n^{k-1}/4, & n \text{ odd} \\ n^{k+1}/4, & n \text{ even} \end{cases}$$

which, in turn, has the following asymptotical behavior:

$$w^*(e) \sim |V(G)|^{1+(2/\Delta)}$$

Example g is the complete regular r-partite graph $K_{n,n,...,n}$. The graph has rn vertices and has degree $d = (r-1)n$. It is vertex- and edge-transitive. A straightforward calculation shows that $W(K_{n,n,...,n}) = \binom{nr}{2} + r\binom{n}{2}$ and

$$w^*(e) = \frac{2(nr+n-2)}{n(r-1)}$$

This in turn gives

$$w^*(e^{(k)}) = \frac{2(nr+n-2)n^{k-2}r^{k-1}}{r-1}$$

$$W(K^k_{n,n,...,n}) = {}^1/_2k(nr+n-2)(nr)^{2k-1}$$

As a curiosity we remark that the Petersen graph is the smallest vertex- and edge-transitive graph not covered by the above examples. The Wiener index of the kth Cartesian power of the Petersen graph equals $75k(10^{2k-2})$ and the edge weight is 10^k.

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