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Another aspect of graph invariants depending on the path metric and an application in nanoscience

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ABSTRACT

The aim of this paper is to find a new expression for distance-based graph invariants of connected graphs having a decomposition into convex subgraphs. We apply this method to Schultz and Gutman indices of graphs. It can be generalized to other distance-based graph invariants. As an application, the Wiener index of the one-pentagonal nanocone is computed.

1. Introduction and notations

Throughout this paper all graphs are assumed to be simple, finite and connected. A function Top from the class of connected graphs into real numbers with the property that $\mathrm{Top}(G) = \mathrm{Top}(H)$ whenever G and H are isomorphic is known as a *topological index* in the chemical literature; see [1]. There are many examples of such functions, especially those based on distances, which are applicable in chemistry. The *Wiener index* [2], defined as the sum of all distances between pairs of vertices in a graph, is probably the first and most studied such graph invariant, both from a theoretical and a practical point of view; see for instance [3–11].

Suppose G is a graph, $x, y \in V(G)$ and λ is a non-zero real number. The distance $d(x, y)$ is the length of a shortest path connecting x and y. We also define $d_G^{\lambda}(u, v) = d_G(u, v)^{\lambda}$ and ${}^{\lambda}W(G) = \sum_{\{u,v\}\subseteq V(G)} d(u, v)^{\lambda}$. The Schultz and Gutman indices of a graph G are defined as:

$$W_+(G) = \sum_{\{u,v\}\subseteq V(G)} (\deg_G(u) + \deg_G(v))d_G(u, v),$$

$$W_*(G) = \sum_{\{u,v\}\subseteq V(G)} (\deg_G(u)\deg_G(v))d_G(u, v).$$

If G and H are graphs such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$ then H is said to be a subgraph of G, denoted by $H \le G$. If $F \subseteq V(G)$ then the subgraph $\langle F\rangle_G$ defined by $V(\langle F\rangle_G) = F$ and $E(\langle F\rangle_G) = \{e = uv | e \in E(G) \text{ and } \{u, v\} \subseteq F\}$ is called the induced subgraph of G generated by F. An isometric subgraph L of G is a subgraph in which $d_L(u, v) = d_G(u, v)$, for all

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vertices $u, v \in V(L)$. We write $L \ll G$ to show that L is an isometric subgraph of G. Clearly, $F \ll H$ and $H \ll G$ implies that $F \ll G$. Define $N_r^G(v) = \{x \in V(G) | d_G(x, v) < r\}$. By this notation, $|N_2^G(v)| = \deg_G(v) + 1$.

Throughout this paper our notation is standard and taken mainly from [12–14].

Definition 1. Suppose H is a subgraph of G and $v \in V(H)$. The vertex v is called *boundary vertex* of H in G, if $|N_2^G(v)| - |N_2^H(v)| > 0$. The set of all boundary vertices of H in G is denoted by $\partial_G(H)$.

The following simple lemma is an immediate consequence of our definition.

Lemma 1. *Let G and H be graphs, $H < G$, $u \in V(H)$ and $v \in V(G) - V(H)$. Then every path connecting u and v contains a vertex of $\partial_G(H)$.*

Suppose $P = ua_1a_2 \cdots a_qv$ is an arbitrary path connecting u and v. Define $P_G(u, v)$ to be the following subgraph:

$$V(P_G(u, v)) = \{u, a_1, a_2, \ldots, a_q, v\},$$
$$E(P_G(u, v)) = \{ua_1, a_1v_2, \ldots, a_q, v\}.$$

If w is another vertex and $vb_1b_2 \cdots b_rw$ is path connecting v and w then $P_G(u, v)+P_G(v, w)$ denotes the following sequence:

$$ua_1a_2 \cdots a_qvb_1b_2 \cdots b_rw.$$

Suppose $\{a_i\}_{i=1}^q \cap \{b_i\}_{i=1}^r = \emptyset$. Then, $P_G(u, v) + P_G(v, w)$ is a path connecting u and w, when $u \neq w$ and a cycle, otherwise. Also, the length of $P_G(u, v)$ is denoted by $|P_G(u, v)|$.

Suppose G is a graph, H, K are subgraphs of G. The union and intersection of H and K are denoted by $H \cup K$ and $H \cap K$, respectively. These are defined as:

$$E(H \cup K) = E(H) \cup E(K); \qquad V(H \cup K) = V(H) \cup V(K)$$
$$E(H \cap K) = E(H) \cap E(K); \qquad V(H \cap K) = V(H) \cap V(K).$$

The union and intersection of a collection $\{H_i\}_{i=1}^r$ of subgraphs are denoted by $\bigcup_{i=1}^r H_i$ and $\bigcap_{i=1}^r H_i$, respectively.

A subgraph H of G is called *convex* if any shortest path of G between vertices of H is already in H. In other words, $u, v \in V(H)$ with $|P_G(u, v)| = d_G(u, v)$ implies that $P_G(u, v) \leq H$. It is clear that convexity is a transitive relation and every convex subgraph is isometric, but its converse is not generally correct.

It is easy to see that for each non-trivial simple graph G and its convex subgraph H containing an edge $e = uv$, $H - e$ is not isometric, since $d_{H-e}(u, v) \neq d_G(u, v) = 1$. So, H is not convex. On the other hand, it is not so difficult to construct a graph G having isometric subgraphs G_1 and G_2 such that $G_1 \cup G_2$ is not isometric. The same is true for the intersection of G_1 and G_2. On the other hand, one can construct a graph G having convex subgraphs G_1 and G_2 such that $G_1 \cup G_2$ is not convex, but the intersection of convex subgraphs have convex component(s). In general, we have the following lemma:

Lemma 2. *Suppose $\{H_i\}_{i=1}^k$ is a sequence of convex subgraphs of a connected graph G. Then each component of $\bigcap_{i=1}^k H_i$ is a convex subgraph of G.*

The previous lemma is not correct if we interchange the "convex subgraph" into "isometric subgraph". In the following two lemmas, two criteria for convexity and isometry of subgraphs are proved.

Lemma 3. *Suppose $H < G$. If $\langle V(H) \rangle_G = H$ and there exists an isometric subgraph I of G such that $\partial_G(H) \subseteq V(I) \subseteq V(H)$ then $H \ll G$.*

Proof. If it is not, take $u, v \in V(H)$ such that $d_G(u, v) < d_H(u, v)$. Suppose $P_G(u, v) = ua_1a_2 \cdots a_nv$ is a shortest path in G. Since $\langle V(H) \rangle_G = H$, there exists i, $1 \leq i \leq n$, such that $a_i \notin V(H)$. Consider $P_G(u, a_i) + P_G(a_i, v) = P_G(u, v)$ and apply Lemma 1, to obtain vertices a_r, a_s such that $\{a_r, a_s\} \subseteq \partial_G(H)$. Since there is $I \ll G$ such that $\{a_r, a_s\} \subseteq V(I)$, $d_G(a_r, a_s) = d_H(a_r, a_s)$. Therefore, $d_H(a_r, a_s) \leq d_G(a_r, a_i) + d_G(a_i, a_s)$, which is impossible. □

Lemma 4. *Suppose G is a graph and $H < G$. If $\langle V(H) \rangle_G = H$ and there exists a convex subgraph I of G such that $\partial_G(H) \subseteq V(I) \subseteq V(H)$ then H is convex.*

Proof. It is enough to prove that if $u, v \in V(H)$ and $P_G(u, v)$ is a path of length $d_G(u, v)$ then $P_G(u, v) \leq H$. If not, since $\langle V(H) \rangle_G = H$ there exists $w \in V(G) - V(H)$ such that $P_G(u, w) + P_G(w, v)$ is a shortest path between u and v. By Lemma 1, there are vertices $a_m, a_n \in \partial_G(H)$ such that $a_m \in V(P_G(u, w))$ and $a_n \in V(P_G(v, w))$. Now there are paths $P_G(a_m, w)$ and $P_G(a_n, w)$ such that $P_G(a_m, w) \leq P_G(u, w)$, $P_G(a_n, w) \leq P_G(v, w)$ and $P_G(a_m, w) + P_G(a_n, w)$ is a shortest path connecting a_m and a_n. Moreover, there is a convex subgraph I,$V(I) \subseteq V(H)$ such that $\partial_G(H) \subseteq V(I)$ and by definition $P_G(a_m, w) + P_G(a_n, w) \leq I$ and so $w \in V(H)$ which is a contradiction. □