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On the monotonicity of topological indices and the connectivity of a graph

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ABSTRACT

Let $I(G)$ be a topological index of a graph. If $I(G+e) < I(G)$ (or $I(G+e) > I(G)$, respectively) for each edge $e \notin G$, then $I(G)$ decreases (or increases, respectively) with addition of edges. In this paper, we determine the extremal values of some monotonic topological indices in terms of the number of cut vertices, or the number of cut edges, or the vertex connectivity, or the edge connectivity of a graph, and characterize the corresponding extremal graphs among all graphs of order n.

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1. Introduction

The structural invariants of a (molecular) graph are numerical parameters of a (molecular) graph which characterize its topology and are usually called topological indices in chemical graph theory. They are the final results of a logical and mathematical procedure which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the results of some standardized experiment, and have been shown to be useful in modeling many physicochemical properties in numerous QSAR and QSPR studies [4,19,27]. Some of the most famous topological indices are based on the graph-distances (the Wiener index, the Harary index, the Kirchhoff index, the detour index, etc.), the edge contributions (the Randić index, the Zagreb index, the Szeged index, the PI-index, etc.) and a variety of quantities to describe the structure of graphs (the energy, the matching energy, the Estrada index, the Hosoya index, the Merrifield–Simmons index, etc.), respectively.

On the other hand, many important topological indices have the monotonicity, i.e., decrease (or increase, respectively) with addition of edges, including the Wiener index, the Kirchhoff index, the Hosoya index, the matching energy, the Zagreb index, etc. In [31], Zhou and Trinajstić obtained the minimum Kirchhoff index and Wiener index of connected graphs in terms of the number of vertices and matching number. In [2], we determined the extremal values of some monotonic topological indices in all bipartite graphs with a given matching number. In [23], Li and Fan provided an upper bound of the Harary index in terms of the vertex or edge connectivity of a graph and characterized the unique graph with the maximum Harary index among all graphs with a given number of cut vertices or vertex connectivity or edge connectivity.

Motivated from [1,2,9,14,21–23,28,29], we continue to study the mathematical properties of the monotonic topological indices and concentrate on the extremal values of some monotonic topological indices and the connectivity of a graph.

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2. Basic properties

Throughout this paper we consider only simple and connected graphs. First, we consider the effect of edge addition (or deletion) on topological indices.

Let $I(G)$ be a topological index of a graph G. If $I(G+e) < I(G)$ (or $I(G+e) > I(G)$, respectively) for each edge $e \notin G$, then $I(G)$ decreases (or increases, respectively) with addition of edges.

For example, the Wiener index and the Merrifield–Simmons index decrease with addition of edges, the spectral radius, the Zagreb index, the Hosoya index and the matching energy increase with addition of edges.

In this section, we discuss the property of graphs with the minimum or maximum topological indices decrease or increase with addition of edges among all graphs with a given number of cut vertices, given vertex connectivity or given edge connectivity.

Let $G = (V, E)$ be a graph with vertex set $V = V(G)$ and edge set $E = E(G)$. For a vertex $v \in V(G)$, denote by $N_G(v)$ the neighborhood of v in G and by $d_G(v) = |N_G(v)|$ the degree of v in G. A vertex of G is called pendent if it has degree 1, and the edge incident with a pendent vertex is a pendent edge. A pendent path at v in a graph G is a path in which no vertex other than v is incident with any edge of G outside the path, where the degree of v is at least three. A cut vertex of a graph is a vertex whose removal increases the number of components of the graph. A block of a connected graph is defined to be a maximum connected subgraph without cut vertices. The vertex connectivity (respectively, edge connectivity) of a graph is the minimum number of vertices (respectively, minimum number of edges) whose deletion yields the resulting graph disconnected or a singleton.

We may associate with any graph G a bipartite graph $B(G)$ with bipartition $(\mathcal{B}, S)$, where $\mathcal{B}$ is the set of blocks of G and S the set of cut vertices of G, a block B and a cut vertex v being adjacent in $B(G)$ if and only if B contains v. Then the graph $B(G)$ is a tree, called the block tree of G.

The distance $d_G(u, v)$ between vertices u and v in G is the length of any shortest path in G connecting u and v. When the graph is clear from the context, we will omit the subscript G from the notation.

The vertex-disjoint union of the graphs G and H is denoted by $G \cup H$. Let $G \vee H$ be the graph obtained from $G \cup H$ by adding all possible edges from vertices of G to vertices of H, i.e., $G \vee H = \overline{\overline{G} \cup \overline{H}}$. Let K_n be the complete graph with n vertices. $\overline{K_n}$ consists of n isolated vertices. For $X \subset V(G)$, let $G - X$ be the graph formed from G by deleting the vertices in X and the edges incident with them.

Many literatures have been involved in the research of the extremal values for some topological indices in terms of the number of cut vertices, cut edges and the connectivity. Gutman and Zhang [14] determined the graph with the minimum Wiener index among all n-vertex graphs with (vertex or edge) connectivity k. This result was extended to the Zagreb and the hyper-Wiener indices by Behtoei et al. [1], to the zeroth-order general Randić index, the general sum-connectivity index and the general Randić connectivity index by Tomescu et al. [28], to the first and second Zagreb indices when connectivity is at most k by Li and Zhou [22] and Xu et al. [29], and to the matching energy by Li and Yan [21]. Feng et al. [9], Chen and Liu [3] and Zhao and Li [30] obtained the extremal values of Zagreb indices over all connected graphs with n vertices and k cut edges or cut vertices, respectively. Fang and Shu [8] characterized the extremal graphs with the largest spectral radius in the set of connected graphs with n vertices, k cut edges and t cut vertices. Li and Fan [23] characterized the graph with the maximum Harary index among all graphs with a given number of cut vertices or vertex connectivity or edge connectivity. Du and Zhou [5] and Du et al. [6] determined the graph with maximum Estrada index among graphs with given number of cut vertices, cut edges, connectivity, and edge connectivity, respectively.

In fact, all topological indices in these literatures above are monotonic, and the extremal graphs for these indices have some common structural characteristics over all graphs of order n with a given number of cut vertices or cut edges, or vertex connectivity, or edge connectivity. In the following, we will give a unified approach to this kind of problems in extremal graph theory.

Proposition 1. *Let G be a graph with (i) the minimal I-value for the topological index I which decreases with addition of edges, or (ii) the maximal I-value for the topological index I which increases with addition of edges, among all graphs with n vertices and k cut vertices. Then each block of G is complete, and each cut vertex of G is contained in exactly two blocks.*

Proof. Without loss of generality, we assume I is a topological index I which decreases with addition of edges. Let G be a graph with the minimal I-value among all the graphs with n vertices and k cut vertices. If G has a block B which is not complete, then adding an edge e between a pair of non-adjacent vertices in B, we will get a new graph $G+e$, which possesses the same numbers of vertices and cut vertices as G. However, $I(G) > I(G+e)$, a contradiction. If G has a cut vertex v contained in at least three blocks, let B_1 and B_2 be two blocks containing the cut vertex v, then adding edges between the vertices of B_1 and the vertices of B_2, we will get a new graph G', which possesses the same numbers of vertices and cut vertices as G. But $I(G) > I(G')$, a contradiction again. □

Similarly, we have

Proposition 2. *Let G be a graph with (i) the minimal I-value for the topological index I which decreases with addition of edges, or (ii) the maximal I-value for the topological index I which increases with addition of edges, among all graphs with n vertices and k cut edges $e_1, e_2, \dots, e_k$. Then each component of $G - \{e_1, e_2, \dots, e_k\}$ is complete.*

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