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Some edge-grafting transformations on the eccentricity resistance-distance sum and their applications☆

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ABSTRACT

The eccentricity resistance-distance sum of a connected graph G is defined as $\xi^R(G) = \sum_{\{u,v\}\subseteq V_G}(\varepsilon_G(u)+\varepsilon_G(v))R^G_{uv}$, where $\varepsilon_G(\cdot)$ is the eccentricity of the corresponding vertex and R^G_{uv} is the resistance distance between u and v in graph G. In this paper some edge-grafting transformations on the eccentricity resistance-distance sum of a connected graph are studied, which is mainly focused on the monotonicity on each of these edge-grafting transformations for ξ^R. As applications, on the one hand, we determined the graph with the minimum ξ^R-value among the set of all n-vertex cacti each of which contains just t cycles, and on the other hand, sharp lower bound on ξ^R of graphs among the n-vertex cacti is determined. The corresponding extremal graphs are identified.

1. Introduction

In this paper, we consider simple and finite graphs only and assume that all graphs are connected, and refer to Bondy and Murty [2] for notation and terminologies used but not defined here.

Let $G = (V_G, E_G)$ be a graph with vertex set V_G and edge set E_G. Then $G - v$, $G - uv$ denote the graph obtained from G by deleting vertex $v \in V_G$, or edge $uv \in E_G$, respectively (this notation is naturally extended if more than one vertex or edge is deleted). Similarly, $G + uv$ is obtained from G by adding an edge $uv \notin E_G$. The *distance*, $d_G(u, v)$, between two vertices u, v of G is the length of a shortest u-v path in G. The *eccentricity* $\varepsilon_G(v)$ of a vertex v is the distance between v and a furthest vertex from v. For a vertex subset S of V_G, denote by $G[S]$ the subgraph induced by S. Denote by P_n and C_n the path, and cycle on n vertices, respectively. A connected graph G is a *cactus* if any two of its cycles have at most one common vertex. For convenience, let $\mathcal{C}_{n,t}$ be the set of all n-vertex cacti each of which contains just t cycles.

A single number that can be used to characterize some properties of the graph of a molecule is called a *topological index*, or *graph invariant*. Topological index is a graph theoretic property that is preserved by isomorphism. The chemical information derived through topological index has been found useful in chemical documentation, isomer discrimination, structure–property correlations, etc. [1]. For quite some time there has been rising interest in the field of computational chemistry in topological indices. The interest in topological indices is mainly related to their use in nonempirical quantitative structure–property relationships and quantitative structure–activity relationships. The study of distances between vertices

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of a tree probably started from the classic *Wiener index* [29], which is one of the most well used chemical indices that correlate a chemical compounds structure (the "molecular graph") with the compounds physical–chemical properties. The Wiener index, introduced in 1947, is defined as the sum of distances between all pairs of vertices, namely that

$$W(G) = \sum_{\{u,v\}\subseteq V_G} d_G(u, v).$$

For more results on Wiener index one may be referred to those in [3,4,14,16,27] and the references therein.

The *degree distance index DD*(G) was introduced by Dobrynin and Kochetova [7] and Gutman [19] as a graph-theoretical descriptor for characterizing alkanes; it can be considered as a weighted version of the Wiener index

$$DD(G) = \sum_{\{u,v\}\subseteq V_G} (d_G(u) + d_G(v))d(u, v),$$

where the summation goes over all pairs of vertices in G. For further results on degree distance index, one may consult [20] and the references therein.

Recently, a novel graph invariant for predicting biological and physical properties-*eccentric distance sum* (EDS) was introduced by Gupta, Singh and Madan [12], which was defined as

$$\xi^d(G) = \sum_{\{u,v\}\subseteq V_G} (\varepsilon(v) + \varepsilon(u))d(u, v).$$

This topological index has vast potential in structure –activity/property relationships; it also displays high discriminating power with respect to both biological activity and physical properties; see [12]. For more research development on the eccentric distance sum of graphs, one may be referred to [10,21,23,25] and the references therein.

On the basis of electrical network theory, Klein and Randić [18] proposed a novel distance function, namely the *resistance distance*, on a graph. The term resistance distance was used because of the physical interpretation: place unit resistors on each edge of a graph G and take the resistance distance, R^G_{uv}, between vertices u and v of G to be the effective resistance between them. This novel parameter is in fact intrinsic to the graph and has some nice interpretations and applications in chemistry (see [16,17] for details). As an analogue to the Wiener index, define $K(G) = \sum_{\{u,v\}\subseteq V_G} R^G_{uv}$, known as the *Kirchhoff index* (a structure-descriptor) of G [18]. In particular, let $K_v(G) = \sum_{u\in V_G} R^G_{uv}$. Klein and Randić [18] showed that $K(G) \leqslant W(G)$ with equality if and only if G is a tree.

Comparing with the degree distance index of a graph, Gutman, Feng and Yu [13] first proposed the *degree resistance distance* as

$$D_R(G) = \sum_{\{u,v\}\subseteq V_G} (d_G(u) + d_G(v))R^G_{uv}$$

for graph G. Palacios [26] called this graph invariant as the *additive degree-Kirchhoff index*. It was systematically studied by Du, Su, Tu and Gutman in [8].

Attempting to compare analogues properties of above graph invariants, it is natural and interesting to define a new graph invariant, the *eccentricity resistance-distance sum* of graph G as

$$\xi^R(G) = \sum_{\{u,v\}\subseteq V_G} (\varepsilon_G(u) + \varepsilon_G(v))R^G_{uv}, \tag{1.1}$$

which can be defined, alternatively, as

$$\xi^R(G) = \sum_{v\in V_G} \varepsilon_G(v) \sum_{u\in V_G} R^G_{uv}.$$

Motivated from [8,9,15,22,24,28], we study some mathematical properties of $\xi^R(G)$; some extremal problems on $\xi^R(G)$ are considered. In this paper, we introduced several edge-grafting transformations to study the mathematical properties of $\xi^R(G)$. Using these nice mathematical properties, we characterize the extremal graph with the minimum eccentricity resistance-distance sum among graphs in $\mathcal{C}_{n,t}$ and the sharp lower bound on ξ^R of graphs among n-vertex cacti is also determined.

Further on we need the following lemmas.

Lemma 1.1 ([18]). *Let x be a cut vertex of G and u, v be vertices belonging to different components of $G-x$. Then $R^G_{uv} = R^G_{ux} + R^G_{xv}$.*

Lemma 1.2 ([13]). *Let C_k be a cycle with length k and $v \in C_k$. Then $K(C_k) = \frac{k^3-k}{12}$, $K_v(C_k) = \frac{k^2-1}{6}$.*