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On the extremal graphs of diameter 2 with respect to the eccentric resistance-distance sum ☆

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ABSTRACT

Given a connected graph G, the eccentric resistance-distance sum of G is defined as $\xi^R(G) = \sum_{\{u,v\}\subseteq V_G}(\varepsilon_G(u)+\varepsilon_G(v))R_{uv}$, where $\varepsilon_G(\cdot)$ is the eccentricity of the corresponding vertex and R_{uv} is the resistance-distance between u and v in G. In this paper, the graphs of diameter 2 with the largest, second largest, third largest, smallest, second smallest and third smallest eccentric resistance-distance sums are identified, respectively. The main tools are standard results of electrical networks.

1. Introduction

In this paper, we consider simple and finite graphs only and assume that all graphs are connected. For all the notations and terminologies not defined here we refer the reader to Bondy and Murty [3].

Let $G = (V_G, E_G)$ be a graph with vertex set $V_G = \{v_1, v_2, \dots, v_n\}$ and edge set E_G. Then $G - uv$ denotes the graph obtained from G by deleting edge $uv \in E_G$, (this notation is naturally extended if more than one 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. The *diameter* of G is defined as the maximum of the eccentricities of vertices of G. The symbol $\sim$ denotes that two vertices in question are adjacent. The degree $d(v)$ of a vertex v is equal to the number of all adjacent vertices. The number $\Delta(G) := \max\{d(v)|v \in V_G\}$ is the maximum degree of G. Denote by S_n and K_n the star, and complete graph on n vertices, respectively. For a vertex subset $S \subseteq V_G$, let $G[S]$ denote the subgraph induced by S.

The *join* $G \vee H$ of two vertex disjoint graphs G and H is the graph consisting of the union $G \cup H$, together with all edges of the type xy, where $x \in V_G$ and $y \in V_H$. Let $A(G) = (a_{ij})_{n\times n}$ be the *adjacency matrix* of G whose $a_{ij} = 1$ if vertices v_i and v_j are adjacent and 0 otherwise. Let $D(G) = \mathrm{diag}(d(v_1), d(v_2), \dots, d(v_n))$ be the diagonal matrix of degrees. The (*combinatorial*) *Laplacian matrix* of G is defined as $L(G) = D(G) - A(G)$.

A single number that can be used to characterize some properties of the molecular graph is called a *topological index*, or *graph invariant*. The 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. [2]. For quite some time there has been rising interest in the field of computational chemistry in topological indices.

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The study of distances between vertices of a tree probably started from the classic *Wiener index* [33], 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 equivalently as the sum of distances between all pairs of vertices, i.e.,

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

For more results on Wiener index one may be referred to those in [5,10,21] and the references therein.

The *degree distance index* $DD(G)$ was defined as

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

which can be considered as a weighted version of the Wiener index. It was introduced, independently, by Dobrynin and Kochetova [6], and Gutman [13] as a graph-theoretical descriptor for characterizing alkanes. For further results on degree distance index, one may consult [4,22] and the references therein.

In 2002, Gupta, Singh and Madan [12] introduced a novel graph invariant for predicting biological and physical properties–*eccentric distance sum* (EDS), 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 [11,16,17,24–26,29,30] and the references therein.

On the basis of electrical network theory, Klein and Randić [20] 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_{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 [18,19] for details). In electrical network G, one usually lets $U_u(G)$ (or U_u) denote the voltage of the vertex u and $U_{uv}(G)$ (or U_{uv}) be the electrical potential difference between two vertices u and v.

We get to know from [32] that the monotonicity law (see also in [7], p. 67) states that if in a given network the resistance of an individual resistor is decreased, then the effective resistance between any two vertices of the network can only decrease. Therefore, if we add an edge to a graph, as the resistance between the vertices where the edge is added decreases from infinity to 1, the effective resistance between any two vertices of the new graph is bounded above by the effective resistance between those same vertices in the original graph. The monotonicity law will be repeatedly used in our paper.

As an analogue to the Wiener index, define $Kf(G)=\sum_{\{u,v\}\subseteq V_G}R_{uv}$, known as the *Kirchhoff index* (a structure-descriptor) of G [27]. Klein and Randić [20] showed that $Kf(G)\leqslant W(G)$ with equality if and only if G is a tree. Given an n-vertex graph G, it is shown, independently, by Gutman and Mohar [15], and Zhu et al. [34] that

$$Kf(G)=\sum_{i<j}R_{ij}=n\sum_{i=2}^{n}\frac{1}{\mu_i}, \tag{1.1}$$

where $0=\mu_1<\mu_2\leqslant\cdots\leqslant\mu_n\,(n\geqslant 2)$ are the eigenvalues of $L(G)$.

Gutman, Feng and Yu [14] first proposed the *degree resistance distance* of a graph G as

$$D_R(G)=\sum_{\{u,v\}\subseteq V_G}(d_G(u)+d_G(v))R_{uv}.$$

It is an analogue of the degree distance index of a graph. Palacios [31] called $D_R(G)$ 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 *eccentric resistance-distance sum* of graph G as

$$\xi^R(G)=\sum_{\{u,v\}\subseteq V_G}(\varepsilon_G(u)+\varepsilon_G(v))R_{uv}. \tag{1.2}$$

This graph invariant was recently proposed and studied by Li and Wei [23].

This paper is motivated directly from [32] in which Palacios used the standard results on electric networks to identify the graphs of diameter 2 with the extremal Kirchhoff indices. In this paper, we determine the graph of diameter 2 with the largest, second largest, third largest, smallest, second smallest, third smallest eccentric resistance-distance sums. The tools used are well known facts of electric networks. It is a surprise to see that the extremal graphs obtained in our paper are not consistent with those obtained by Palacios in [32].