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The Szeged index and the Wiener index of partial cubes with applications to chemical graphs

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ABSTRACT

In this paper, we study the Szeged index of partial cubes and hence generalize the result proved by Chepoi and Klavžar, who calculated this index for benzenoid systems. It is proved that the problem of calculating the Szeged index of a partial cube can be reduced to the problem of calculating the Szeged indices of weighted quotient graphs with respect to a partition coarser than Θ-partition. Similar result for the Wiener index was recently proved by Klavžar and Nadjafi-Arani. Furthermore, we show that such quotient graphs of partial cubes are again partial cubes. Since the results can be used to efficiently calculate the Wiener index and the Szeged index for specific families of chemical graphs, we consider C_4C_8 systems and show that the two indices of these graphs can be computed in linear time.

1. Introduction

In the present paper the Szeged index and the Wiener index of partial cubes are investigated. Our main result extends a parallel result about the Szeged index of benzenoid systems [6] to all partial cubes. In [6] the corresponding indices were expressed as the sum of indices of three weighted quotient trees, while in the general case these trees are quotient graphs of a partial cube with respect to a partition coarser than Θ-partition.

Partial cubes constitute a large class of graphs with a lot of applications and includes, for example, many families of chemical graphs (benzenoid systems, trees, C_4C_8 systems, phenylenes, cyclic phenylenes, polyphenylenes). Therefore, our results can be used to calculate the indices of a particular family of chemical graphs in linear time.

The Wiener index and the Szeged index are some of the most commonly studied topological indices. Their history goes back to 1947, when Wiener used the distances in the molecular graphs of alkanes to calculate their boiling points [29]. This research has led to the Wiener index, which is defined as

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

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In that paper it was also noticed that for every tree T it holds

$$W(T) = \sum_{e=uv\in E(T)} n_u(e)n_v(e),$$

where $n_u(e)$ denotes the number of vertices of T whose distance to u is smaller than the distance to v and $n_v(e)$ denotes the number of vertices of T whose distance to v is smaller than the distance to u. Therefore, a proper generalization to any graph was defined in [11] as

$$Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e).$$

This topological index was later named as the Szeged index. For some recent results on the Wiener index and the Szeged index see [1,10,21,22,24,27]. Moreover, some other variants of the Wiener index were introduced, for example Wiener polarity index (see [9,23,25]).

The Wiener index, due to its correlation with a large number of physico-chemical properties of organic molecules and its interesting mathematical properties, has been extensively studied in both theoretical and chemical literature. Later, the Szeged index was introduced and it was shown that it also has many applications, for example in drug modeling [16] and in networks [20,26].

The paper reads as follows. In the next section we give some basic definitions needed later. In Section 3 we prove that the problem of calculating the Szeged index of a partial cube can be reduced to the problem of calculating the Szeged indices of weighted quotient graphs with respect to a partition coarser than Θ-partition. It turns out that such quotient graphs are again partial cubes. We also consider a similar result for the Wiener index, which was proved in [19] under the name partition distance. In Section 4 we show that the mentioned results generalize already known results for benzenoid systems (see [4,6]) and apply them to C_4C_8 systems. Furthermore, we demonstrate with an example that the method can also be used to calculate the corresponding indices by hand.

2. Preliminaries

The *distance* $d_G(x, y)$ between vertices x and y of a graph G is the length of a shortest path between vertices x and y in G. We also write $d(x, y)$ for $d_G(x, y)$.

Two edges $e_1 = u_1v_1$ and $e_2 = u_2v_2$ of graph G are in relation Θ, $e_1\Theta e_2$, if

$$d_G(u_1, u_2) + d_G(v_1, v_2) \neq d_G(u_1, v_2) + d_G(u_1, v_2).$$

Note that this relation is also known as Djoković–Winkler relation (see [8,30]). The relation Θ is reflexive and symmetric, but not necessarily transitive. We denote its transitive closure (i.e. the smallest transitive relation containing Θ) by Θ^*. Let $\mathcal{E} = \{E_1, \ldots, E_r\}$ be the Θ^*-partition of the set $E(G)$. Then we say that a partition $\{F_1, \ldots, F_k\}$ of $E(G)$ is *coarser* than $\mathcal{E}$ if each set F_i is the union of one or more Θ^*-classes of G (see [19]).

The *hypercube* Q_n of dimension n is defined in the following way: all vertices of Q_n are presented as n-tuples $(x_1, x_2, \ldots, x_n)$ where $x_i \in \{0, 1\}$ for each $1 \leq i \leq n$ and two vertices of Q_n are adjacent if the corresponding n-tuples differ in precisely one coordinate. Therefore, the *Hamming distance* between two tuples x and y is the number of positions in x and y in which they differ.

Let G be a graph and $e = uv$ an edge of G. Throughout the paper we will use the following notation:

$$N_1(e|G) = \{x \in V(G) \mid d_G(x, u) < d_G(x, v)\},$$

$$N_2(e|G) = \{x \in V(G) \mid d_G(x, v) < d_G(x, u)\}.$$

Also, for $s \in \{1, 2\}$, let

$$n_s(e|G) = |N_s(e|G)|.$$

A subgraph H of G is called an *isometric subgraph* if for each $u, v \in V(H)$ it holds $d_H(u, v) = d_G(u, v)$. Any isometric subgraph of a hypercube is called a *partial cube*. We write $\langle S\rangle$ for the subgraph of G induced by $S \subseteq V(G)$. The following theorem puts forth two fundamental characterizations of partial cubes, cf. [13]:

Theorem 2.1. *For a connected graph G, the following statements are equivalent:*

(i) *G is a partial cube.*
(ii) *G is bipartite, and $\langle N_1(e|G)\rangle$ and $\langle N_2(e|G)\rangle$ are convex subgraphs of G for all $e \in E(G)$.*
(iii) *G is bipartite and $\Theta = \Theta^*$.*

Note that the characterization (ii) is due to Djoković [8], and (iii) to Winkler [30]. Is it also known that if G is a partial cube and E is a Θ-class of G, then $G - E$ has exactly two connected components, namely $\langle N_1(e|G)\rangle$ and $\langle N_2(e|G)\rangle$, where $ab \in E$. For more information about partial cubes see [13].

Let H and G be arbitrary graphs. Then a mapping $\alpha\colon V(H) \to V(G)$ is an *isometric embedding*, if $d_H(u, v) = d_G(\alpha(u), \alpha(v))$ for each $u, v \in V(H)$.