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Topological indices of the m^k-graph

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Abstract This paper is devoted to the study of a new graph, called m^k-graph and denoted by $m^k(G)$, that arises from a simple graph G by k successive iterations of a special kind of construction. We provide some of its topological indices such as Wiener index, Hyper-Wiener index, Wiener polarity, Zagreb indices, Schultz and modified Schultz indices and Wiener-type invariant. Some Formulas concerning classical graphs are settled to show the scope of this study.

1. Introduction

Throughout this paper, we consider a finite connected graph G that has no loops or multiple edges. We respectively denote by p and q the cardinality of its vertices set $V(G)$ and its edges set $E(G)$. Let $u, v \in V(G)$. As customary, we denote by $\delta_G(u)$ the degree of u and by $d_G(u,v)$ the distance between u and v (or $\delta_G(u)$ for short). The distance $d_G(u)$ of u is the sum, taken over all $v \in V(G)$, of the distances $d_G(u,v)$. The diameter $d(G)$ of G is the greatest distance between any two vertices u, v of G. Finally, for a non-negative integer $k = 0, 1, \ldots, d(G)$, we define $d(G,k)$ to be the number of unordered pairs of vertices in G that are at exactly distance k.

Note that $p = d(G,0), q = d(G,1) = 0$ for every $k > d(G)$. Let us recall some basic definitions and facts:

A *topological index* is a real number related to a graph, that must be a structural invariant. Several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules (Rajesh et al., 2016). The Wiener index is the first topological index to be used in chemistry (Behmaram et al., 2011). More precisely, in 1947, Harold Wiener introduced and developed this interesting index to determine physical properties of types of alkanes known as paraffin.

In a graph theoretic language, the *Wiener index* $W(G)$ of G is equal to the sum of all distances between vertices; that is

$$W(G) = \sum_{u,v \in V(G)} d(u,v) = \sum_{k=1}^{d(G)} k d(G,k).$$

In 1988, Hosoya introduced a related generating function $W(G;x)$ so that its derivative is a x-analog of $W(G)$ (Behmaram et al., 2011). Such a function is called the *Wiener polynomial* of G and it is defined as follows:

$$W(G;x) = \sum_{u,v \in V(G)} x^{d(u,v)} = \sum_{k=1}^{d(G)} d(G,k) x^k.$$

Subsequently, several other topological indices were deeply studied. We consider here certain of then which figure rather prominently.

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- The *Hyper-Wiener index* of acyclic graphs was introduced by Milan Randic in 1993 (Khalifeh et al., 2008). Then Klein et al., generalized Randic's definition for all connected graphs, as a generalization of the Wiener index (Cash, 2002; Fath-Tabar and Ashrafi, 2011). It is defined as

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{2}\sum_{\{u,v\} \subseteq V(G)} d(u,v)^2$$
$$= \frac{1}{2}\sum_{k=1}^{d(G)} k(k+1)d(G,k).$$

- The *Wiener polarity* of an organic molecule with molecular graph G is defined as $W_p(G) = d(G;3)$. In 1998, using this topological index, Lukovits and Linert demonstrated quantitative structure property relationships in a series of acyclic and cycle-containing hydrocarbons (Faghani et al., 2012).
- Suppose now that $\{d_G(u) : u \in V(G)\}$ consists of n elements. Then n is called the *Wiener dimension of* G, denoted by $dim_W(G)$ (Alizadeh et al., 2014). In other words, the Wiener dimension of G is the number of different distances of its vertices.
- Let λ be a given real number. In order to generalize the classical Wiener index, Zadeh and his co-authors (Hamzeh et al., 2013; Zadeh et al., 2009) introduced a new topological index termed the *Wiener-type invariant* of G associated to λ and defined as:

$$W_\lambda(G) = \sum_{k=1}^{d(G)} d(G,k)k^\lambda$$

It is evidently obtained that $W_1(G) = W(G)$.
- The *graph invariants* $M_1(G)$ and $M_2(G)$ were firstly considered by Gutman and Trinajstic (Dasa and Gutman, 2003; Horoldagva and Das, 2015) in 1972. They are defined as:

$$M_1(G) = \sum_{u\in v(G)} \delta^2(u) = \sum_{uv\in E(G)} \delta(u) + \delta(v)$$

and

$$M_2(G) = \sum_{uv\in E(G)} \delta(u)\delta(v)$$

These expressions, which now are called *the first and second Zagreb indices* respectively, were deduced within the study of the dependence of total π-electron energy on molecular structures (Mansour et al., 2016) and are measures of branching of the molecular carbon-atom skeleton (Gutman et al., 2015).
- The *Schultz* (Behmaram et al., 2011) and *Gutman* (Hamzeh et al., 2013) indices are defined as:

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

and

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

In Behmaram et al. (2011), Gutman introduced a polynomial version of the Schultz and the modified Schultz indices of a graph G as follows:

$$W_+(G;x) = \sum_{\{u,v\} \subseteq V(G)} (\delta(u) + \delta(v))x^{d(u,v)}$$

and

$$W_*(G;x) = \sum_{\{u,v\} \subseteq V(G)} \delta(u)\delta(v)\, x^{d(u,v)}.$$

It is a simple matter to verify that the derivative of $W_+(G;x)$ (resp., $W_*(G;x)$) evaluated at $x = 1$ provides $W_+(G)$ (resp., $W_*(G)$). For more information on this topic, we encourage the reader to consult (and, 2008) for historical background, mathematical properties and applications of the above recorded topological indices.

In this paper, we deal with a new graph called m^k-graph. For an integer $m \geqslant 2$, define $mG$to be the graph that consists of $m$copies $G_1, G_2, \ldots, G_m$ of G such that each vertex u of a copy G_i is adjacent to the corresponding vertex $v$in another copy G_j. (cf. Fig. 1). For instance, if G consists of one vertex, then $mG$is the complete graph K_m.

In order to take these ideas a stage further, we can make successive repetitions of this construction in the following fashion: for a non-negative integer k, we define

$$m^0G = G, m^1G = mG, m^2G = m(mG), \ldots, m^{k+1}G = m(m^kG).$$

For example, if Gconsists of one vertex, then we have $2G, 2^2G$ and 2^3G as Fig. 2. In fact, 2^kG is the cube graph Q_k of dimension k.

Our goal is to compute the previous topological indices for the m^k-graph. Consequently, we would be able to provide numerous significant applications which illustrate the importance of the graph under consideration.

For convenience, we will introduce the following parameter $t = 1 + (m-1)x$ which will be helpful in the proofs and convenient in the presentation of our formulas. Any unexplained terminology is standard, typically as in and (2008).

2. Preliminary results

In this section, we study some properties of the m^k-graph. It is a simple matter to verify the following statements.

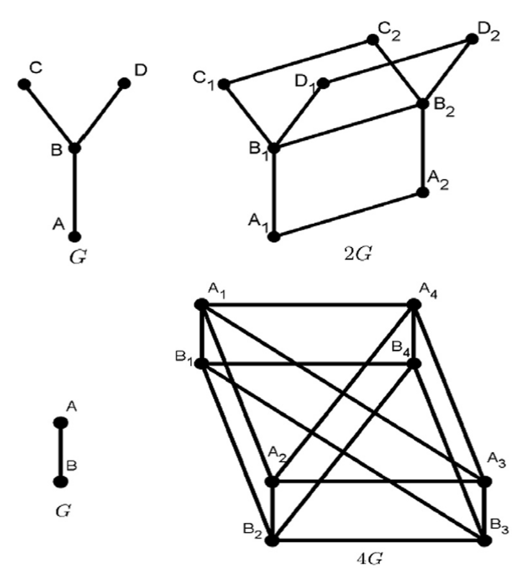

Fig. 1 2G, 4G.

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