Communications in Combinatorics and Optimization
Vol. 5 No. 1, 2020 pp.9-17
DOI: 10.22049/CCO.2019.26430.1108

CCO
Commun. Comb. Optim.

A study on some properties of leap graphs

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Received: 16 February 2019; Accepted: 12 June 2019
Published Online: 15 June 2019

Abstract: In a graph G, the first and second degrees of a vertex v are equal to the number of their first and second neighbors and are denoted by $d(v/G)$ and $d_2(v/G)$, respectively. The first, second and third leap Zagreb indices are the sum of squares of second degrees of vertices of G, the sum of products of second degrees of pairs of adjacent vertices in G and the sum of products of first and second degrees of vertices of G, respectively. In this paper, we initiate in studying a new class of graphs depending on the relationship between first and second degrees of vertices and is so-called a leap graph. Some properties of the leap graphs are presented. All leap trees and $\{C_3, C_4\}$-free leap graphs are characterized.

Keywords: Distance-degrees (of vertices), leap Zagreb indices, leap graphs

AMS Subject classification: 05C07, 05C12, 05C76

1. Introduction

In this paper, we are concerned with simple graphs, i.e., finite graphs having no loops, multiple and directed edges. Let $G = (V, E)$ be such a graph with vertex set $V(G)$ and edges set $E(G)$. As usual, we denote by $n = |V|$ and $m = |E|$ to the number of vertices and edges in a graph G, respectively. The distance $d_G(u, v)$ between any two vertices u and v of a graph G is equal to the length of (number of

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edges in) a shortest path connecting them. For a vertex $v \in V(G)$ and a positive integer k, the open k-neighborhood of v in a graph G is denoted by $N_k(v/G)$ and is defined as $N_k(v/G) = \{u \in V(G) : d_G(u, v) = k\}$. The k-distance degree of a vertex v in G is denoted by $d_k(v/G)$ (or simply $d_k(v)$, if no misunderstanding) and is defined as the number of k-neighbors of the vertex v in G, i.e., $d_k(v/G) = |N_k(v/G)|$. It is clear that $d_1(v/G) = d(v/G)$ for every $v \in V(G)$.

The complement $\overline{G}$ of a graph G is a graph with vertex set $V(G)$ and two vertices of $\overline{G}$ are adjacent if and only if they are not adjacent in G. If $G \cong \overline{G}$, then G is called a self-complementary graph (sc-graph, in short). A subdivision graph $S(G)$ of a graph G is a graph obtained from G by adding a new vertex on every edge of G. A crown graph S_n^0 is a graph obtained from a complete bipartite graph $K_{n,n}$ by removed the horizontal edges. For any two graphs G and H their cartesian product, $G \square H$, of them is the graph on the vertex set $V(G) \times V(H)$, and vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ of $V(G) \times V(H)$ are connected by an edge if and only if either $(u_1 = v_1 \textit{ and } u_2v_2 \in E(H))$ or $(u_2 = v_2 \textit{ and } u_1v_1 \in E(G))$.

If a graph G consists of disconnected components H_1 and H_2, then we write $G = H_1 \cup H_2$. If G consists of $p \geq 2$ disjoint copies of a graph H, then we write $G = pH$. For a vertex v of G, the eccentricity $e(v) = \max\{d_G(v, u) : u \in V(G)\}$, the diameter of G is $diam(G) = \max\{e(v) : v \in V(G)\}$, and the radius of G is $rad(G) = \min\{e(v) : v \in V(G)\}$. Let $H \subseteq V(G)$ be any subset of vertices of G. Then the induced subgraph $\langle H \rangle$ of G is the graph whose vertex set is H and whose edge set consists of all of the edges in $E(G)$ that have both endpoints in H. A graph G is called F-free graph if no induced subgraph of G is isomorphic to F. We follow [8], for unexplained graph theoretic terminologies and notations.

In the interdisciplinary area where chemistry, physics and mathematics meet, molecular graph based structure descriptors, usually referred to as topological indices, are of significant importance. A topological index of a graph is a graph invariant number calculated from a graph representing a molecule. Among the most important such structure descriptors are the classical first and second Zagreb indices, which introduced, more than fifty five years ago, by Gutman and Trinajestic [7], in (1972), and elaborated in [6]. They are defined as:

$$M_1(G) = \sum_{v \in V(G)} d_1^2(v/G) \qquad \textit{and} \qquad M_2(G) = \sum_{uv \in E(G)} d_1(u/G) d_1(v/G).$$

For properties of the two Zagreb indices see [4, 6, 12, 17], and for details of the theory of Zagreb indices see the survey [3] and the references cited therein. After most of the results on Zagreb indices were established, the inevitable occurred, Their various modifications have been proposed, thus opening the possibility to do analogous research and publish numerous additional papers. For these modifications see the recent survey [5].

In 2017, Naji et al. [11] have introduced a new distance-degree-based topological indices conceived depending on the second degrees of vertices, and are so-called leap Zagreb indices of a graph G and are defined as:

$$LM_1(G) = \sum_{v \in V(G)} d_2^2(v/G)$$

$$LM_2(G) = \sum_{uv \in E(G)} d_2(u/G)d_2(v/G)$$

$$LM_3(G) = \sum_{v \in V(G)} d(v/G)d_2(v/G).$$

The leap Zagreb indices have several chemical applications. Surprisingly, the first leap Zagreb index has very good correlation with physical properties of chemical compounds like boiling point, entropy, DHVAP, HVAP and accentric factor [2].

In a later work [10], the first leap Zagreb index of graph operations was studied. In [1], the expressions for these three leap Zagreb indices of generalized xyz point line transformation graphs $T^{xyz}(G)$, when $z = 1$ are obtained. The authors in [13], generalized the results of [11], pertaining to trees and unicyclic graphs. They determined upper and lower bounds on leap Zagreb indices and characterized the extremal graphs. Leap Zagreb indices are considered in a recent survey [5]. For more study on leap Zagreb indices see [9, 14, 15].
In this paper, we initiate studying of a new class of graphs depending on relationship between first and second degrees of vertices and so-called a leap graph. Some properties of leap graphs are presented. All leap trees and (C_3, C_4)-free leap graphs are characterized.

The following fundamental results which will be required for many of our arguments in this paper.

Lemma 1. [16, 18] *Let G be a connected graph with n vertices and m edges. Then*

$$d_2(v/G) \leq \Big(\sum_{u \in N_1(v/G)} d_1(u/G) \Big) - d_1(v/G).$$

Equality holds if and only if G is $\{C_3, C_4\}$-free graph.

Observation 1. [11] Let G be a connected graph with n vertices. Then for any vertex $v \in V(G)$,

$$d_2(v/G) \leq d_1(v/\overline{G}) = n - 1 - d_1(v/G).$$

Equality holds if and only if G having diameter at most two.

Corollary 1. [11] *Let G be a $\{C_3, C_4\}$-free k-regular graph with n vertices. Then*

$$d_2(v/G) = k(k-1).$$

Theorem 2. [11] *Let G be a connected graph with n vertices and m edges. Then*

$$LM_3(G) \leq \sqrt{M_1(G)LM_1(G)}.$$

Equality holds if one of the following conditions is satisfied:
(a) G is regular graph with diameter $diam(G) \leq 2$.
(b) G is regular and $\{C_3, C_4\}$-free.

2. Leap graphs

Definition 1. Let G be a graph with n vertices. Then G is called a leap graph if and only if for every vertex $v \in V(G)$

$$d(v/G) = d_2(v/G).$$

It is clear, from this definition, that if G is a leap graph, then

$$LM_1(G) = LM_3(G) = M_1(G) \quad \textit{and} \quad LM_2(G) = M_2(G).$$

Example 1. We herewith present some examples of leap graphs.

1. A totally disconnected graph $\overline{K_n}$, for $n \geq 1$, is a leap graph.
2. Every cycle C_n with $n \geq 5$ vertices is a leap graph.
3. A subdivision graph $S(K_{1,3})$ of a star $K_{1,3}$ is a leap graph, see Figure 1 (a).
4. A crown graph S_n^0 for $n \geq 3$ is a leap graph, see Figure 1 (b).
5. $K_2 \square C_4$, $K_3 \square K_3$ and $K_3 \square P_3$, each one is a leap graph.
6. Some other examples of leap graphs shown in figure 1.

From Observation 1, the following result follows.

Proposition 1. *Let G be a connected nontrivial leap graph with n vertices and m edges. Then*

(a) $n \geq 5$,

(b) $m \leq \frac{n(n-1)}{4}$,

(c) $\Delta(G) \leq \lfloor \frac{n-1}{2} \rfloor$,

(d) $diam(G) \geq 2$.

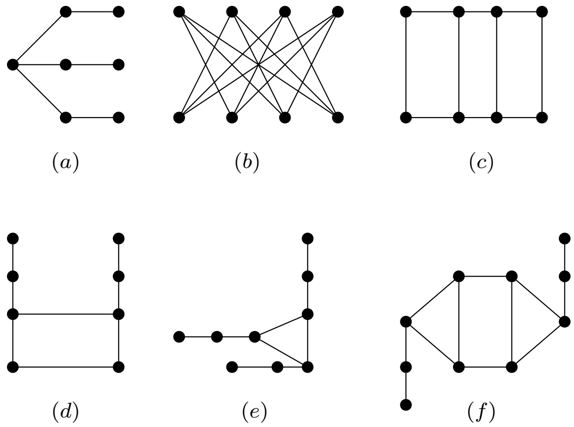

Figure 1. **Some examples of leap graphs**

Corollary 2. *If G is a leap graph with $diam(G) = 2$, then G is a sc-graph.*

The converse of Corollary 2, in general case, is not true. For instance, the graph G in Figure 2, is a sc-graph with $diam(G) = 2$ but is not a leap graph.

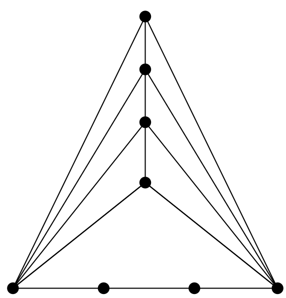

Figure 2. **A sc-graph with $diam = 2$ but not a leap graph.**

Corollary 3. *The join $G + H$ of any two graphs G and H is not a leap graph.*

Theorem 3. *Let G be a connected leap graph with n vertices. Then $\overline{G}$ is a leap graph if and only if the following conditions are satisfied:*

1. *G is regular sc-graph.*
2. *$n \equiv 1 \pmod 4$.*
3. *$diam(G) = 2$.*

Proof. Let G and $\overline{G}$ be leap graphs. Then from the definition of leap graph and using Observation 1, we get for every vertex $v \in V(G)$,

$$d_1(v/G) = d_2(v/G) \leq d_1(v/\overline{G}) = d_2(v/\overline{G}) \leq d_1(v/G).$$

Thus, $d_1(v/G) = d_1(v/\overline{G}) = n - 1 - d_1(v/G)$ and hence $d_1(v/G) = d_1(v/\overline{G}) = \frac{n-1}{2}$. Therefore, G is $\frac{n-1}{2}$-regular sc-graph. Since $d_1(v/G)$ is an integer number, it follows that n is an odd and since G is a $\frac{n-1}{2}$-regular then $\frac{n-1}{2}$ must be an even. Therefore, $n \equiv 1 \pmod 4$. Since for every vertex $v \in V(G)$, $d_2(v/G) = d_1(v/\overline{G})$, it follows from Observation 1, that $diam(G) \leq 2$. But for every graph G with $diam(G) \leq 1$, if G is leap graph, then $\overline{G}$ is not leap graph. Therefore, $diam(G) = 2$.
Conversely, if G is a leap graph and all above conditions are satisfied, then it is immediate to check that $\overline{G}$ is also a leap graph. ∎

Theorem 4. *Let G be a k-regular $\{C_3, C_4\}$-free graph with $n \geq 5$ vertices. Then G is a leap graph if and only if $G \cong C_n$.*

Proof. Let G be a k-regular $\{C_3, C_4\}$-free graph with $n \geq 5$ vertices. Then by Corollary 1, $d_2(v/G) = k(k-1)$ for every $v \in V(G)$ and if G is a leap graph, then $d_2(v/G) = d(v/G)$ this implies that $d(v/G) = 2$ for every $v \in V(G)$. Therefore $G \cong C_n$. The converse is trivial. ∎

Theorem 5. *Let T be a tree with n vertices. Then T is a leap graph if and only if $T \cong S(K_{1,3})$.*

Proof. Let T be a tree such that T is a leap graph. Since every tree has at least two pendent vertices (vertices with degree one). Firstly, let v_1 be a pendent vertex of T and let $\{v_2\} = N_1(v/T)$. Then By Lemma 1, $d_2(v_1/T) = d_1(v_2/T) - d_1(v_1/T)$ this led to $d_1(v_2/T) = 2$. Now, let $v_3 \in N_1(v_2/T) = N_2(v_1/T)$. Then by Lemma 1, and bring in mind that T is a leap graph, we obtain $d_1(v_3/T) = 3$. Let $N_1(v_3/T) = \{v_2, v_4, v_5\}$, again by Lemma 1, we obtain that $d_2(v_3/T) = d_1(v_2/T) + d_1(v_4/T) + d_1(v_5/T) - d_1(v_3/T)$ which gives $d_1(v_4/T) + d_1(v_5/T) = 4$. Since T is a connected leap graph, it follows that $d_1(v_4/T) = d_1(v_5/T) = 2$. Otherwise, suppose, without lost of generality, that $d_1(v_4/T) = 1$ and $d_1(v_5/T) = 3$ and hence $d_2(v_4/T) = 2 \neq d_1(v_4/T)$, a contradiction. Finally, let $N_1(v_4/T) = \{v_3, v_6\}$. Then $d_2(v_4/T) = d_1(v_3/T) + d_1(v_6/T) - d_1(v_4/T)$ which give $d_1(v_6/T) = 1$. Similarly for v_5. Therefore, $T \cong S(K_{1,3})$. ∎

Theorem 6. *If G is a connected $\{C_3, C_4\}$-free leap graph, then*

$$LM_1(G) = LM_2(G) = LM_3(G) = M_1(G) = M_2(G) = 4m.$$

Proof. Let G be a connected leap $\{C_3, C_4\}$-free graph. Then, from the definition of leap graph,

$$LM_1(G) = LM_3(G) = M_1(G) \ \ and \ \ LM_2(G) = M_2(G). \tag{1}$$

From Theorem 2, and since G is $\{C_3, C_4\}$-free graph it follows that

$$LM_3(G) = 2M_2(G) - M_1(G). \tag{2}$$

Combine equations 1 and 2, we obtain $LM_1(G) = LM_2(G)$. Therefore,

$$LM_1(G) = LM_2(G) = LM_3(G) = M_1(G) = M_2(G). \tag{3}$$

Now, by Lemma 1, and since G is a $\{C_3, C_4\}$-free leap graph then, for every $v \in V(G)$

$$2d_1(v/G) = \sum_{u \in N_1(v/G)} d_1(u/G).$$

Hence,

$$2 \sum_{v \in V(G)} d_1(v/G) = \sum_{v \in V(G)} \sum_{u \in N_1(v/G)} d_1(u/G),$$

which led to $4m = M_1(G)$. This complete the proof. ∎

Corollary 4. *Let G be a connected $\{C_3, C_4\}$-free graph with n vertices and m edges. If G is a leap graph, then $G = S(K_{1,3})$ or G is a unicyclic graph.*

Proof. Let G be a connected $\{C_3, C_4\}$-free leap graph. Then from Theorem 6, for every $i = 1, 2, 3$, $LM_i(G) = 4m$ and by using the well-known result $M_1(G) \geq \frac{4m^2}{n}$, we obtain $m \leq n$. Hence we have the following cases:

Case1: $m < n$, then G is a tree and by Theorem 5, $G \cong S(K_{1,3})$.

Case2: $m = n$, then G is a unicyclic graph.

∎

We denote by UC_n and LUC_n, for $n \geq 3$, to unicyclic and leap unicyclic graphs, respectively.
By check various unicyclic graphs and by trying to construct a leap unicyclic graph, we found that LUC_3 and LUC_4, shown in Figure 1.d and 1.e, are the leap unicyclic graphs only. But we can not write a logical proof for that. Hence, we leave this result in the following conjecture.

Conjecture: Let G be a unicyclic graph. Then G is a leap graph if and only if $G \cong LUC_3$ or LUC_4.

Theorem 7. *For every positive integers $n \geq 5$ and $2 \leq k \leq \lfloor \frac{n-1}{2} \rfloor$, such that k is even, there is a k-regular leap graph with n vertices.*

Proof. If $n \in \{5, 6, 7, 8\}$, then $k = 2$, and $G = C_n$ have the desired property. Hence we assume that $n \geq 9$ and let k be an even number such that $2 \leq k \leq \lfloor \frac{n-1}{2} \rfloor$. Let G be a graph obtained from a cycle C_n with vertex set $v_1, v_2, ..., v_n$, by joining every vertex v_i into every vertex v_j in C_n if and only if $d_{C_n}(v_i, v_j) \leq \frac{k}{2}$, where the indices being taken modulo n. By easy check, for every $v_i \in V(G)$, $i = 1, 2, ..., n$, we obtain that

$$N_1(v_i/G) = \{v_{i-\frac{k}{2}}, ..., v_{i-2}, v_{i-1}, v_{i+1}, v_{i+2}, ..., v_{i+\frac{k}{2}}\}$$
$$N_2(v_i/G) = \{v_{i-k}, ..., v_{i-2-\frac{k}{2}}, v_{i-1-\frac{k}{2}}, v_{i+1+\frac{k}{2}}, v_{i+2+\frac{k}{2}}, ..., v_{i+k}\}.$$

Hence, $d_1(v_i/G) = d_2(v_i/G) = k$. Therefore, G is a k-regular leap graph. ∎

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