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Discrete Applied Mathematics ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Discrete Applied Mathematics

journal homepage: www.elsevier.com/locate/dam

On distance spectral radius of uniform hypergraphs with cycles

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ARTICLE INFO

Article history:
Received 27 September 2016
Received in revised form 5 December 2017
Accepted 7 December 2017
Available online xxxx

Keywords:
Distance spectral radius
Uniform hypergraph
Graft transformation
Unicyclic hypergraph
Cycle

ABSTRACT

We study the effect of two types of graft transformations on the distance spectral radius of connected uniform hypergraphs containing at least one cycle, determine the unique k-uniform unicyclic hypergraphs of fixed size with minimum and second minimum distance spectral radii, respectively, and show the possible structure of the k-uniform unicyclic hypergraph(s) of fixed size with maximum distance spectral radius.

1. Introduction

A hypergraph G is a pair (V, E), where $V = V(G)$ is a nonempty finite set called the vertex set of G and $E = E(G)$ is a family of subsets of $V(G)$ called the edge set of G, see [3]. The size of G is the cardinality of $E(G)$. For an integer $k \geq 2$, a hypergraph is k-uniform if all its edges have cardinality k. A (simple) graph is a 2-uniform hypergraph. For $v \in V(G)$, let $E_G(v)$ be the set of edges of G containing v. The degree of a vertex v in G is the number of edges containing it, denoted by $d_G(v)$, i.e., $d_G(v) = |E_G(v)|$.

For $u, v \in V(G)$, a walk from u to v in G is defined to be a sequence of vertices and edges $(v_0, e_1, v_1, \ldots, v_{p-1}, e_p, v_p)$ with $v_0 = u$ and $v_p = v$ such that edge e_i contains vertices v_{i-1} and v_i, and $v_{i-1} \neq v_i$ for $i = 1, \ldots, p$. The value p is the length of this walk. A path is a walk with all v_i distinct and all e_i distinct. A cycle is a walk containing at least two edges, all e_i are distinct and all v_i are distinct except $v_0 = v_p$. A vertex $u \in V(G)$ is viewed as a path (from u to u) of length 0. If there is a path from u to v for any $u, v \in V(G)$, then we say that G is connected. A component of a hypergraph G is a maximal connected subhypergraph of G. A hypertree is a connected hypergraph with no cycles. A unicyclic hypergraph is a connected hypergraph with exactly one cycle. Note that a k-uniform unicyclic hypergraph with m edges always has order $(k-1)m$.

Let G be a connected k-uniform hypergraph with $V(G) = \{v_1, \ldots, v_n\}$. For $u, v \in V(G)$, the distance between u and v is the length of a shortest path from u to v in G, denoted by $d_G(u, v)$. In particular, $d_G(u, u) = 0$. The distance matrix of G is the $n \times n$ matrix $D(G) = (d_G(u, v))_{u,v \in V(G)}$. The eigenvalues of $D(G)$ are called the distance eigenvalues of G. Since $D(G)$ is real and symmetric, the distance eigenvalues of G are real. The distance spectral radius of G, denoted by $\rho(G)$, is the largest absolute value of the distance eigenvalues of G. Since $D(G)$ is an irreducible nonnegative matrix, the Perron–Frobenius theorem implies that $\rho(G)$ is the largest distance eigenvalue, and there is a unique positive unit eigenvector corresponding to $\rho(G)$, which is called the distance Perron vector of G, denoted by $x(G)$.

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https://doi.org/10.1016/j.dam.2017.12.011
0166-218X/

Please cite this article in press as: H. Lin, B. Zhou, On distance spectral radius of uniform hypergraphs with cycles, Discrete Applied Mathematics (2018), https://doi.org/10.1016/j.dam.2017.12.011.

Balaban et al. [2] proposed the use of the distance spectral radius of ordinary graphs (2-uniform hypergraphs) as a molecular descriptor, and it was successfully used to make inferences about the extent of branching and boiling points of alkanes, see [2,8]. Now the distance spectral radius of an ordinary graph has been studied extensively, see [4–6] for classical results, and see survey [1] (and references therein, e.g., [14,16]) for recent results. Particularly, Yu et al. [16] determined the unique unicyclic graphs with minimum (maximum, respectively) distance spectral radius. They showed that the graph obtained by adding an edge to a star is the unique unicyclic graph with minimum distance spectral radius, while the graph obtained from a path by adding an edge between a terminal vertex and the vertex of distance two from it is the unique unicyclic graph with maximum distance spectral radius.

As graph representation of molecular structures is widely used in computational chemistry and theoretical chemical researches, hypergraph theory also found applications in chemistry [7,9–11]. As noted in [10], the hypergraph model gave a higher accuracy of molecular structure description: the higher the accuracy of the model, the greater the diversity of the behavior of its invariants. For 'general' k-uniform hypergraphs, Sivasubramanian [15] gave a formula for the inverse of a few q-analogs of the distance matrix of a 3-uniform hypertree, and we studied the distance spectral radius of k-uniform hypergraphs in [12] and determined the k-uniform hypertrees with maximum, second maximum, minimum, and second minimum distance spectral radii, respectively.

For a hypergraph G with $E' \subseteq E(G)$, let $G - E'$ be the subhypergraph of G obtained by deleting all the edges of E'.

For a k-uniform unicyclic hypergraph G with $V(G) = \{v_1, \ldots, v_n\}$, if $E(G) = \{e_1, \ldots, e_m\}$, where $e_i = \{v_{(i-1)(k-1)+1}, \ldots, v_{(i-1)(k-1)+k}\}$ for $i = 1, \ldots, m$ and $v_{(m-1)(k-1)+k} = v_1$, then we call G a k-uniform loose cycle, denoted by $C_{n,k}$.

Let G be a connected k-uniform hypergraph with an induced subhypergraph $C_{g(k-1),k}$, where $k \geq 3$ and $g \geq 2$. Let the vertices of $C_{g(k-1),k}$ be labeled as above with $v_{(g-1)(k-1)+k} = v_1$. Suppose that $G - E(C_{g(k-1),k})$ consists of $g(k-1)$ components, denoted by $H_1, \ldots, H_{g(k-1)}$ with $v_i \in V(H_i)$ for $i = 1, \ldots, g(k-1)$. In this case, we denote G by $C^k_{g(k-1)}(H_1, \ldots, H_{g(k-1)})$.

In this paper, we propose two types of graft transformations for the uniform hypergraph $C^k_{g(k-1)}(H_1, \ldots, H_{g(k-1)})$ that decrease or increase the distance spectral radius, determine the unique k-uniform unicyclic hypergraphs of size $m \geq 2$ with minimum and second minimum distance spectral radii, respectively, and discuss the possible structure of the k-uniform unicyclic hypergraph(s) of fixed size with maximum distance spectral radius.

2. Preliminaries

Let G be a k-uniform hypergraph with $V(G) = \{v_1, \ldots, v_n\}$. A column vector $x = (x_{v_1}, \ldots, x_{v_n})^\top \in \mathbb{R}^n$ can be considered as a function defined on $V(G)$ which maps vertex v_i to x_{v_i}, i.e., $x(v_i) = x_{v_i}$ for $i = 1, \ldots, n$. Then

$$x^\top D(G)x = \sum_{\{u,v\}\subseteq V(G)} 2d_G(u, v)x_u x_v,$$

and ρ is a distance eigenvalue with corresponding eigenvector x if and only if $x \neq 0$ and for each $u \in V(G)$,

$$\rho x_u = \sum_{v\in V(G)} d_G(u, v)x_v.$$

The above equation is called the eigenequation of G (at u). For a unit column vector $x \in \mathbb{R}^n$ with at least one nonnegative entry, by Rayleigh's principle, we have

$$\rho(G) \geq x^\top D(G)x$$

with equality if and only if $x = x(G)$.

Lemma 2.1 ([12]). *Let G be a connected k-uniform hypergraph with η being an automorphism of G, and x the distance Perron vector of G. Then $\eta(v_i) = v_j$ implies that $x_{v_i} = x_{v_j}$.*

For $X \subseteq V(G)$ with $X \neq \emptyset$, let $G[X]$ be the subhypergraph of G induced by X, i.e., $G[X]$ has vertex set X and edge set $\{e \subseteq X : e \in E(G)\}$, and let $\sigma_G(X)$ be the sum of the entries of the distance Perron vector of G corresponding to the vertices in X. For $u \in V(G)$, let $G - u$ be the subhypergraph of G obtained by deleting u and all edges containing u.

Let G be a k-uniform hypergraph with $u, v \in V(G)$ and $e_1, \ldots, e_r \in E(G)$ such that $u \in e_i, v \notin e_i$ and $e'_i \notin E(G)$ for $1 \leq i \leq r$, where $e'_i = (e_i \setminus \{u\}) \cup \{v\}$. Let G' be the hypergraph with $V(G') = V(G)$ and $E(G') = (E(G) \setminus \{e_1, \ldots, e_r\}) \cup \{e'_1, \ldots, e'_r\}$. Then we say that G' is obtained from G by moving edges $e_1, \ldots, e_r$ from u to v.

A path $P = (v_0, e_1, v_1, \ldots, v_{p-1}, e_p, v_p)$ with $p \geq 1$ in a k-uniform hypergraph G is called a pendant path of length p at v_0, if $d_G(v_0) \geq 2$, $d_G(v_i) = 2$ for $1 \leq i \leq p - 1$, $d_G(v) = 1$ for $v \in e_i \setminus \{v_{i-1}, v_i\}$ with $1 \leq i \leq p$, and $d_G(v_p) = 1$. If $p = 1$, then we call P or e_1 a pendant edge at v_0.

Let G be a connected k-uniform hypergraph with $|E(G)| \geq 2$, and let $e = \{w_1, \ldots, w_k\}$ be a pendant edge of G at w_k. For $1 \leq i \leq k - 1$, let H_i be a connected k-uniform hypergraph with $v_i \in V(H_i)$. Suppose that $G, H_1, \ldots, H_{k-1}$ are vertex-disjoint. For $0 \leq s \leq k - 1$, let $G_{e,s}(H_1, \ldots, H_{k-1})$ be the hypergraph obtained by identifying w_i of G and v_i of H_i for $s + 1 \leq i \leq k - 1$ and identifying w_k of G and v_i of H_i for all i with $1 \leq i \leq s$.

Lemma 2.2 ([12]). *Suppose that $|E(H_j)| \geq 1$ for some j with $1 \leq j \leq k - 1$. Then $\rho(G_{e,0}(H_1, \ldots, H_{k-1})) > \rho(G_{e,s}(H_1, \ldots, H_{k-1}))$ for $j \leq s \leq k - 1$.*

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