On distance spectral radius of uniform hypergraphs with cycles

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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 radius, respectively, and show the possible structure of the k-uniform unicyclic hypergraph(s) of fixed size with maximum distance spectral radius.

AMS classification: 05C65, 05C12, 05C50, 05C90

Key words: distance spectral radius, uniform hypergraph, graft transformation, unicyclic hypergraph, cycle

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.

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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 $V(G) = \{v_1, \dots, v_n\}$. 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 $x(G)$.

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 ordinary graphs have been studied extensively, see [4, 5, 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, 10, 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 radius, respectively.

For a k-uniform unicyclic hypergraph G with $V(G) = \{v_1, \dots, v_n\}$, if $E(G) = \{e_1, \dots, e_m\}$, where $e_i = \{v_{(i-1)(k-1)+1}, \dots, v_{(i-1)(k-1)+k}\}$ for $i = 1, \dots, m$ 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 labelled 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 $H_1, \dots, H_{g(k-1)}$ with $v_i \in V(H_i)$ for $i = 1, \dots, g(k-1)$. In this case, we denote G by $C^k_{g(k-1)}(H_1, \dots, H_{g(k-1)})$.

In this paper, we propose two types of graft transformations for the uniform hypergraph $C^k_{g(k-1)}(H_1, \dots, H_{g(k-1)})$ 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 radius, 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 $V(G) = \{v_1, \dots, v_n\}$. A column vector $x = (x_{v_1}, \dots, x_{v_n})^\top \in \mathbb{R}^n$ 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 $i = 1, \dots, n$. 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 $E' \subseteq E(G)$, let $G - E'$ be the subhypergraph of G obtained by deleting all the edges of E'. 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 $e_1, \dots, e_r \in E(G)$ 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 $E(G') = (E(G) \setminus \{e_1, \dots, e_r\}) \cup \{e'_1, \dots, e'_r\}$. Then we say that G' is obtained from G by moving edges $e_1, \dots, e_r$ from u to v.

A path $P = (v_0, e_1, v_1, \dots, v_{p-1}, e_p, v_p)$ 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 $e = \{w_1, \dots, w_k\}$ 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 $G, H_1, \dots, H_{k-1}$ are vertex-disjoint. For $0 \le s \le k-1$, let $G_{e,s}(H_1, \dots, H_{k-1})$ be the hypergraph obtained by identifying w_i of G and v_i of H_i for $s+1 \le i \le k-1$ and identifying w_k of G and v_i of H_i for all i with $1 \le i \le s$.

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

If P is a pendant path of a hypergraph G at u, we say G is obtained from H by attaching a pendant path P at u with $H = G[V(G) \setminus (V(P) \setminus \{u\})]$.

Let G be a connected k-uniform hypergraph with $|E(G)| \ge 1$. For $u \in V(G)$, and positive integers p and q, let $G_u(p, q)$ be the k-uniform hypergraph obtained from G by attaching two pendant paths of lengths p and q at u, respectively, and $G_u(p, 0)$ be the k-uniform hypergraph obtained from G by attaching a pendant path of length p at u.

Lemma 2.3. *[12] Let G be a connected k-uniform hypergraph $|E(G)| \ge 1$ and $u \in V(G)$. For integers $p \ge q \ge 1$, $\rho(G_u(p, q)) < \rho(G_u(p+1, q-1))$.*

Let G be a connected k-uniform hypergraph with $u, v \in e \in E(G)$. For positive integers p and q, let $G_{u,v}(p, q)$ be the k-uniform hypergraph obtained from G by attaching a pendant path of length p at u and a pendant path of length q at v, and $G_{u,v}(p, 0)$ be the k-uniform hypergraph obtained from G by attaching a pendant path of length p at u. Let $G_{u,v}(0, q) = G_{v,u}(q, 0)$.

Lemma 2.4. *[12] Let G be a connected k-uniform hypergraph with $|E(G)| \ge 2$ and $u, v \in e \in E(G)$. Suppose that $G - \{e\}$ consists of k components and $d_G(u) = d_G(v) = 1$. For $p \ge q \ge 1$, $\rho(G_{u,v}(p, q)) < \rho(G_{u,v}(p+1, q-1))$.*

The diameter of a connected k-uniform hypergraph G is the maximum distance between all vertex pairs of G.

3 Graft transformations and changes of distance spectral radius

A k-uniform hypertree in which all edges contain a common vertex (u) is known as a k-uniform hyperstar (with center u), denoted by $S_{d(k-1)+1,k}$. Obviously, $S_{1,k}$ consists of a single vertex, which is its center.

First we give a type of graft transformation on $C^k_{g(k-1)}(H_1, \dots, H_{g(k-1)})$ that decreases the distance spectral radius.

Theorem 3.1. *For $k \ge 3$ and $g \ge 4$ with $g + \sum_{i=1}^{g(k-1)} |E(H_i)| \ge 5$, let $G = C^k_{g(k-1)}(H_1, \dots, H_{g(k-1)})$, and let G^* be the k-uniform hypergraph obtained from G by moving each edge of $E_G(v_{(g-1)(k-1)+1}) \setminus \{e_g\}$ from $v_{(g-1)(k-1)+1}$ to v_1 and moving each edge of $E_G(v_k) \setminus \{e_1\}$ from v_k to v_1. If H_1 is a k-uniform hyperstar with center v_1, $|V(H_1)| = \max_{1 \le i \le g(k-1)} |V(H_i)|$, and $|V(H_i)| = 1$ for $2 \le i \le k-1$ and $(g-1)(k-1)+2 \le i \le g(k-1)$, then $\rho(G^*) < \rho(G)$.*

Proof. For $1 \le i \le g(k-1)$, let $V_i = V(H_i)$ and $t_i = |E(H_i)|$. Let $x = x(G^*)$. From the eigenequations of G^* at v_1 and v_k, we have

$$\begin{aligned}\rho(G^*)x_{v_1} &= x_{v_k} + \sum_{w\in V(G)\setminus\{v_1,v_k\}} d_{G^*}(v_1,w)x_w,\\ \rho(G^*)x_{v_k} &= x_{v_1} + \sum_{w\in V(G)\setminus\{v_1,v_k\}} d_{G^*}(v_k,w)x_w.\end{aligned}$$

Note that for $w \in V(G)\setminus\{v_1,v_k\}$, $2d_{G^*}(v_1,w) - d_{G^*}(v_k,w) \ge 0$. Then

$$\begin{aligned}(\rho(G^*)+1)(2x_{v_1} - x_{v_k}) &= x_{v_1} + x_{v_k} + \sum_{w\in V(G)\setminus\{v_1,v_k\}} (2d_{G^*}(v_1,w) - d_{G^*}(v_k,w))x_w\\ &> 0,\end{aligned}$$

and thus $2x_{v_1} - x_{v_k} > 0$, i.e., $2x_{v_1} > x_{v_k}$. By Lemma 2.1, the entry of x corresponding to each vertex of $(V_1\setminus\{v_1\})\cup(e_1\setminus\{v_1\})\cup(e_g\setminus\{v_1\})$ is the same, which we denote by a. Then $x_{v_1} > \frac{a}{2}$.

Case 1. $g = 2s$ with $s \ge 2$.

As we pass from G to G^*, the distance between v_k and a vertex of $U_1 = \left(\bigcup_{i=k}^{s(k-1)+1} V_i\right)\setminus\{v_k\}$ is increased by 1, the distance between v_k and a vertex of $U_2 = \left(\bigcup_{i=(s+1)(k-1)+1}^{(2s-1)(k-1)+1} V_i\right)\setminus\{v_{(2s-1)(k-1)+1}\}$ is decreased by 1, the distance between $v_{(2s-1)(k-1)+1}$ and a vertex of $U_3 = \left(\bigcup_{i=s(k-1)+1}^{(2s-1)(k-1)+1} V_i\right)\setminus\{v_{(2s-1)(k-1)+1}\}$ is increased by 1, the distance between $v_{(2s-1)(k-1)+1}$ and a vertex of $U_4 = \left(\bigcup_{i=k}^{(s-1)(k-1)+1} V_i\right)\setminus\{v_k\}$ is decreased by 1, the distance between a vertex of V_1 and a vertex of $U_5 = \left(\bigcup_{i=k}^{(2s-1)(k-1)+1} V_i\right)\setminus\{v_k, v_{(2s-1)(k-1)+1}\}$ is decreased by 1, the distance between a vertex of $e_1\setminus\{v_1,v_k\}$ and a vertex of $U_6 = \left(\bigcup_{i=s(k-1)+2}^{(2s-1)(k-1)+1} V_i\right)\setminus\{v_{(2s-1)(k-1)+1}\}$ is decreased by 1, the distance between a vertex of $e_{2s}\setminus\{v_1, v_{(2s-1)(k-1)+1}\}$ and a vertex of $U_7 = \left(\bigcup_{i=k}^{s(k-1)} V_i\right)\setminus\{v_k\}$ is decreased by 1, and the distance between any other vertex pair is decreased or remains unchanged. Then

$$\begin{aligned}&\frac{1}{2}(\rho(G)-\rho(G^*))\\ \ge\ & \frac{1}{2}x^\top(D(G)-D(G^*))x\\ \ge\ & x_{v_k}(-\sigma_{G^*}(U_1)+\sigma_{G^*}(U_2)) + x_{v_{(2s-1)(k-1)+1}}(-\sigma_{G^*}(U_3)+\sigma_{G^*}(U_4))\\ & +\sigma_{G^*}(V_1)\sigma_{G^*}(U_5) + \sigma_{G^*}(e_1\setminus\{v_1,v_k\})\sigma_{G^*}(U_6)\\ & +\sigma_{G^*}(e_{2s}\setminus\{v_1,v_{(2s-1)(k-1)+1}\})\sigma_{G^*}(U_7)\\ =\ & a(-\sigma_{G^*}(U_1)+\sigma_{G^*}(U_4)) + a(\sigma_{G^*}(U_2)-\sigma_{G^*}(U_3))\\ & +(t_1(k-1)a + x_{v_1})\sigma_{G^*}(U_5) + (k-2)a\sigma_{G^*}(U_6) + (k-2)a\sigma_{G^*}(U_7).\end{aligned}$$

Note that

$$-\sigma_{G^*}(U_1)+\sigma_{G^*}(U_4) = -\sigma_{G^*}\left(\bigcup_{i=(s-1)(k-1)+2}^{s(k-1)+1} V_i\right),$$

$$\sigma_{G^*}(U_2)-\sigma_{G^*}(U_3) = -\sigma_{G^*}\left(\bigcup_{i=s(k-1)+1}^{(s+1)(k-1)} V_i\right),$$

and $k\geq 3$. Thus

$$\begin{aligned}
&\frac{1}{2}(\rho(G)-\rho(G^*))\\
\geq\ & -a\left(\sigma_{G^*}\left(\bigcup_{i=(s-1)(k-1)+2}^{s(k-1)+1} V_i\right)+\sigma_{G^*}\left(\bigcup_{i=s(k-1)+1}^{(s+1)(k-1)} V_i\right)\right) \qquad (3.1)\\
&+(2t_1a+x_{v_1})\sigma_{G^*}(U_5)+a(\sigma_{G^*}(U_6)+\sigma_{G^*}(U_7)).
\end{aligned}$$

If $t_1\geq 1$, then since $\bigcup_{i=(s-1)(k-1)+2}^{(s+1)(k-1)} V_i\subseteq U_5$, from (3.1), we have

$$\begin{aligned}
\frac{1}{2}(\rho(G)-\rho(G^*)) \geq\ & -a\left(\sigma_{G^*}\left(\bigcup_{i=(s-1)(k-1)+2}^{s(k-1)+1} V_i\right)+\sigma_{G^*}\left(\bigcup_{i=s(k-1)+1}^{(s+1)(k-1)} V_i\right)\right)\\
&+2a\sigma_{G^*}\left(\bigcup_{i=(s-1)(k-1)+2}^{(s+1)(k-1)} V_i\right)\\
=\ & a\sigma_{G^*}\left(\bigcup_{i=s(k-1)+2}^{(s+1)(k-1)} V_i\right)+a\sigma_{G^*}\left(\bigcup_{i=(s-1)(k-1)+2}^{s(k-1)} V_i\right)\\
>\ & 0,
\end{aligned}$$

and thus $\rho(G^*)<\rho(G)$.

Suppose that $t_1=0$. Then $t_i=0$ and $V_i=\{v_i\}$ for $1\leq i\leq g(k-1)$, i.e., $G=C_{g(k-1),k}$. Since $g+\sum_{i=1}^{g(k-1)}|E(H_i)|\geq 5$, we have $2s=g\geq 6$, and thus $s\geq 3$.

Let $u_i=v_{(i-1)(k-1)+1}$ for $1\leq i\leq g$. Note that

$$e_s\setminus\{u_s\}=\bigcup_{i=(s-1)(k-1)+2}^{s(k-1)+1} V_i,\ e_{s+1}\setminus\{u_{s+2}\}=\bigcup_{i=s(k-1)+1}^{(s+1)(k-1)} V_i,$$

$$e_s\cup e_{s+1}=\bigcup_{i=(s-1)(k-1)+1}^{(s+1)(k-1)+1} V_i\subseteq U_5,\ e_{s+1}\setminus\{u_{s+1}\}=\bigcup_{i=s(k-1)+2}^{(s+1)(k-1)+1} V_i\subseteq U_6,$$

$$e_s\setminus\{u_{s+1}\}=\bigcup_{i=(s-1)(k-1)+1}^{s(k-1)} V_i\subseteq U_7,$$

and $x_{u_1}=x_{v_1}>\frac{a}{2}$. By (3.1), we have

$$\begin{aligned}
&\frac{1}{2}(\rho(G)-\rho(G^*))\\
\geq\ & -a\left[\sigma_{G^*}(e_s\setminus\{u_s\})+\sigma_{G^*}(e_{s+1}\setminus\{u_{s+2}\})\right]
\end{aligned}$$

$$\begin{aligned}
&\quad +\frac{a}{2}\cdot\sigma_{G^*}(e_s\cup e_{s+1})+a\left(\sigma_{G^*}(e_{s+1}\setminus\{u_{s+1}\})+\sigma_{G^*}(e_s\setminus\{u_{s+1}\})\right)\\
&= -a\left[\sigma_{G^*}(e_s\setminus\{u_s,u_{s+1}\})+\sigma_{G^*}(e_{s+1}\setminus\{u_{s+1},u_{s+2}\})+2x_{u_{s+1}}\right]\\
&\quad +a\left[\sigma_{G^*}(e_s\setminus\{u_s,u_{s+1}\})+\sigma_{G^*}(e_{s+1}\setminus\{u_{s+1},u_{s+2}\})+x_{u_s}+x_{u_{s+2}}\right]\\
&\quad +\frac{a}{2}\cdot\sigma_{G^*}(e_s\cup e_{s+1})\\
&= a\left(x_{u_s}+x_{u_{s+2}}-2x_{u_{s+1}}\right)+\frac{a}{2}\cdot\sigma_{G^*}(e_s\cup e_{s+1})\\
&= \frac{a}{2}\left(2x_{u_s}+2x_{u_{s+2}}-4x_{u_{s+1}}+\sigma_{G^*}(e_s\cup e_{s+1})\right).
\end{aligned}$$

Since $\{u_s,u_{s+1},u_{s+2}\}\subset e_s\cup e_{s+1}$, we have

$$\begin{aligned}
\frac{1}{2}(\rho(G)-\rho(G^*)) &> \frac{a}{2}\left(2x_{u_s}+2x_{u_{s+2}}-4x_{u_{s+1}}+x_{u_s}+x_{u_{s+1}}+x_{u_{s+2}}\right)\\
&= \frac{3a}{2}\left(x_{u_s}+x_{u_{s+2}}-x_{u_{s+1}}\right).
\end{aligned}$$

Let $W=V(G)\setminus\{u_s,u_{s+1},u_{s+2}\}$. From the eigenequations of G^* at u_s, u_{s+1} and u_{s+2}, we have

$$\begin{aligned}
\rho(G^*)x_{u_s} &= x_{u_{s+1}}+2x_{u_{s+2}}+\sum_{w\in W}d_{G^*}(u_s,w)x_w,\\
\rho(G^*)x_{u_{s+1}} &= x_{u_s}+x_{u_{s+2}}+\sum_{w\in W}d_{G^*}(u_{s+1},w)x_w,\\
\rho(G^*)x_{u_{s+2}} &= 2x_{u_s}+x_{u_{s+1}}+\sum_{w\in W}d_{G^*}(u_{s+2},w)x_w.
\end{aligned}$$

Note that for $w\in W$, $d_{G^*}(u_s,w)+d_{G^*}(u_{s+2},w)-d_{G^*}(u_{s+1},w)\geq 0$. Then

$$\rho(G^*)\left(x_{u_s}+x_{u_{s+2}}-x_{u_{s+1}}\right)\geq x_{u_s}+2x_{u_{s+1}}+x_{u_{s+2}}>0,$$

and thus $x_{u_s}+x_{u_{s+2}}-x_{u_{s+1}}>0$. Therefore $\rho(G)-\rho(G^*)>0$, i.e., $\rho(G^*)<\rho(G)$.

Case 2. $g=2s+1$ with $s\geq 2$.

As we pass from G to G^*, the distance between v_k and a vertex of $U_1=\left(\bigcup_{i=k}^{(s+1)(k-1)}V_i\right)\setminus\{v_k\}$ is increased by 1, the distance between v_k and a vertex of $U_2=\left(\bigcup_{i=(s+1)(k-1)+2}^{2s(k-1)+1}V_i\right)\setminus\{v_{2s(k-1)+1}\}$ is decreased by 1, the distance between $v_{2s(k-1)+1}$ and a vertex of $U_3=\left(\bigcup_{i=s(k-1)+2}^{2s(k-1)+1}V_i\right)\setminus\{v_{2s(k-1)+1}\}$ is increased by 1, the distance between $v_{2s(k-1)+1}$ and a vertex of $U_4=\left(\bigcup_{i=k}^{s(k-1)}V_i\right)\setminus\{v_k\}$ is decreased by 1, the distance between a vertex of V_1 and a vertex of $U_5=\left(\bigcup_{i=k}^{2s(k-1)+1}V_i\right)\setminus\{v_k,v_{2s(k-1)+1}\}$ is decreased by 1, the distance between a vertex of $e_1\setminus\{v_1,v_k\}$ and a vertex of $U_6=\left(\bigcup_{i=(s+1)(k-1)+1}^{2s(k-1)+1}V_i\right)\setminus\{v_{2s(k-1)+1}\}$ is decreased by 1, the distance between a vertex of $e_{2s+1}\setminus\{v_1,v_{2s(k-1)+1}\}$ and a vertex of $U_7=\left(\bigcup_{i=k}^{s(k-1)+1}V_i\right)\setminus\{v_k\}$

is decreased by 1, and the distance between any other vertex pair is decreased or remains unchanged. Then

$$\begin{aligned}\frac{1}{2}(\rho(G)-\rho(G^*)) &\geq \frac{1}{2}x^\top(D(G)-D(G^*))x\\ &\geq x_{v_k}(-\sigma_{G^*}(U_1)+\sigma_{G^*}(U_2))+x_{v_{2s(k-1)+1}}(-\sigma_{G^*}(U_3)+\sigma_{G^*}(U_4))\\ &\quad+\sigma_{G^*}(V_1)\sigma_{G^*}(U_5)+\sigma_{G^*}(e_1\setminus\{v_1,v_k\})\sigma_{G^*}(U_6)\\ &\quad+\sigma_{G^*}(e_{2s+1}\setminus\{v_1,v_{2s(k-1)+1}\})\sigma_{G^*}(U_7)\\ &\geq a(-\sigma_{G^*}(U_1)+\sigma_{G^*}(U_4))+a(\sigma_{G^*}(U_2)-\sigma_{G^*}(U_3))\\ &\quad+(t_1(k-1)a+x_{v_1})\sigma_{G^*}(U_5)+(k-2)a(\sigma_{G^*}(U_6)+\sigma_{G^*}(U_7)).\end{aligned}$$

Note that

$$\begin{aligned}-\sigma_{G^*}(U_1)+\sigma_{G^*}(U_4) &= -\sigma_{G^*}\left(\bigcup_{i=s(k-1)+1}^{(s+1)(k-1)} V_i\right),\\ \sigma_{G^*}(U_2)-\sigma_{G^*}(U_3) &= -\sigma_{G^*}\left(\bigcup_{i=s(k-1)+2}^{(s+1)(k-1)+1} V_i\right),\end{aligned}$$

and $k\geq 3$. Thus

$$\begin{aligned}&\frac{1}{2}(\rho(G)-\rho(G^*))\\ \geq\ & -a\left(\sigma_{G^*}\left(\bigcup_{i=s(k-1)+1}^{(s+1)(k-1)} V_i\right)+\sigma_{G^*}\left(\bigcup_{i=s(k-1)+2}^{(s+1)(k-1)+1} V_i\right)\right)\\ &+(2t_1a+x_{v_1})\sigma_{G^*}(U_5)+a(\sigma_{G^*}(U_6)+\sigma_{G^*}(U_7)).\end{aligned}\tag{3.2}$$

If $t_1\geq 1$, then since $\bigcup_{i=s(k-1)+1}^{(s+1)(k-1)+1} V_i\subseteq U_5$, we have

$$\begin{aligned}\frac{1}{2}(\rho(G)-\rho(G^*)) &\geq -a\left(\sigma_{G^*}\left(\bigcup_{i=s(k-1)+1}^{(s+1)(k-1)} V_i\right)+\sigma_{G^*}\left(\bigcup_{i=s(k-1)+2}^{(s+1)(k-1)+1} V_i\right)\right)\\ &\quad+2a\sigma_{G^*}\left(\bigcup_{i=s(k-1)+1}^{(s+1)(k-1)+1} V_i\right)\\ &= a\sigma_{G^*}(V_{(s+1)(k-1)+1})+a\sigma_{G^*}(V_{s(k-1)+1})\\ &> 0,\end{aligned}$$

and thus $\rho(G)-\rho(G^*)>0$. Therefore $\rho(G^*)<\rho(G)$.

Suppose that $t_1=0$. Then $t_i=0$ and $V_i=\{v_i\}$ for $1\leq i\leq g(k-1)$, i.e., $G=C_{g(k-1),k}$.

Let $u_i=v_{(i-1)(k-1)+1}$ for $1\leq i\leq g$. Note that

$$e_{s+1}\setminus\{u_{s+1}\}=\bigcup_{i=s(k-1)+2}^{(s+1)(k-1)+1} V_i,\ e_{s+1}\setminus\{u_{s+2}\}=\bigcup_{i=s(k-1)+1}^{(s+1)(k-1)} V_i,$$

$$(e_s \setminus \{u_s\}) \cup e_{s+1} \cup (e_{s+2} \setminus \{u_{s+3}\}) = \bigcup_{i=(s-1)(k-1)+2}^{(s+2)(k-1)} V_i \subseteq U_5,$$

$$e_{s+2} \setminus \{u_{s+3}\} = \bigcup_{i=(s+1)(k-1)+1}^{(s+2)(k-1)} V_i \subseteq U_6,\ e_s \setminus \{u_s\} = \bigcup_{i=(s-1)(k-1)+2}^{s(k-1)+1} V_i \subseteq U_7.$$

By (3.2), we have

$$\begin{aligned}
\frac{1}{2}(\rho(G) - \rho(G^*)) &\geq -a\left[\sigma_{G^*}(e_{s+1} \setminus \{u_{s+2}\}) + \sigma_{G^*}(e_{s+1} \setminus \{u_{s+1}\})\right] \\
&\quad + \frac{a}{2} \cdot \sigma_{G^*}((e_s \setminus \{u_s\}) \cup e_{s+1} \cup (e_{s+2} \setminus \{u_{s+3}\})) \\
&\quad + a\left[\sigma_{G^*}(e_s \setminus \{u_s\}) + \sigma_{G^*}(e_{s+2} \setminus \{u_{s+3}\})\right] \\
&= -a\left[2\sigma_{G^*}(e_{s+1} \setminus \{u_{s+1}, u_{s+2}\}) + x_{u_{s+1}} + x_{u_{s+2}}\right] \\
&\quad + \frac{a}{2}\left[\sigma_{G^*}(e_s \setminus \{u_s, u_{s+1}\}) + \sigma_{G^*}(e_{s+1} \setminus \{u_{s+1}, u_{s+2}\})\right. \\
&\quad \left. + \sigma_{G^*}(e_{s+2} \setminus \{u_{s+2}, u_{s+3}\}) + x_{u_{s+1}} + x_{u_{s+2}}\right] \\
&\quad + a\left[\sigma_{G^*}(e_s \setminus \{u_s, u_{s+1}\}) + \sigma_{G^*}(e_{s+2} \setminus \{u_{s+2}, u_{s+3}\})\right. \\
&\quad \left. + x_{u_{s+1}} + x_{u_{s+2}}\right] \\
&= \frac{3a}{2}\left[\sigma_{G^*}(e_s \setminus \{u_s, u_{s+1}\}) + \sigma_{G^*}(e_{s+2} \setminus \{u_{s+2}, u_{s+3}\})\right. \\
&\quad \left. - \sigma_{G^*}(e_{s+1} \setminus \{u_{s+1}, u_{s+2}\})\right] + \frac{a}{2}\left(x_{u_{s+1}} + x_{u_{s+2}}\right).
\end{aligned}$$

Let $w_i \in e_i \setminus \{u_i, u_{i+1}\}$ for $s \leq i \leq s+2$, and $W = V(G) \setminus \{w_s, w_{s+1}, w_{s+2}\}$. From the eigenequations of G^* at w_s, w_{s+1}, and w_{s+2}, we have

$$\begin{aligned}
\rho(G^*)x_{w_s} &= 2x_{w_{s+1}} + 3x_{w_{s+2}} + \sum_{w \in W} d_{G^*}(w_s, w)x_w, \\
\rho(G^*)x_{w_{s+1}} &= 2x_{w_s} + 2x_{w_{s+2}} + \sum_{w \in W} d_{G^*}(w_{s+1}, w)x_w, \\
\rho(G^*)x_{w_{s+2}} &= 3x_{w_s} + 2x_{w_{s+1}} + \sum_{w \in W} d_{G^*}(w_{s+2}, w)x_w.
\end{aligned}$$

Note that for $w \in W$, $d_{G^*}(w_s, w) + d_{G^*}(w_{s+2}, w) - d_{G^*}(w_{s+1}, w) \geq 0$. We have

$$\rho(G^*)\left(x_{w_s} + x_{w_{s+2}} - x_{w_{s+1}}\right) \geq x_{w_s} + x_{w_{s+2}} + 4x_{w_{s+1}} > 0,$$

and then $x_{w_s} + x_{w_{s+2}} - x_{w_{s+1}} > 0$. By Lemma 2.1, the entry of x corresponding to each vertex of $e_i \setminus \{u_i, u_{i+1}\}$ for $s \leq i \leq s+2$ is the same. Thus

$$\begin{aligned}
&\quad \sigma_{G^*}(e_s \setminus \{u_s, u_{s+1}\}) + \sigma_{G^*}(e_{s+2} \setminus \{u_{s+2}, u_{s+3}\}) - \sigma_{G^*}(e_{s+1} \setminus \{u_{s+1}, u_{s+2}\}) \\
&= (k-2)(x_{w_s} + x_{w_{s+2}} - x_{w_{s+1}}) \\
&> 0.
\end{aligned}$$

Therefore $\rho(G) - \rho(G^*) > 0$, i.e., $\rho(G^*) < \rho(G)$. □

Let $C_g^k(t_1, \ldots, t_g) = C_{g(k-1)}^k(H_1, \ldots, H_{g(k-1)})$, where $H_j = S_{t_i(k-1)+1,k}$ with center v_j, and $t_i \geq 0$ for $j = (i-1)(k-1)+1$ with $i = 1, \ldots, g$, and $H_j = S_{1,k}$ otherwise.

By Theorem 3.1, we have the following corollary.

Corollary 3.1. *For $k \geq 3$, $g \geq 4$, and $t_i \geq 0$ with $1 \leq i \leq g$ and $g + \sum_{i=1}^{g} t_i \geq 5$, if $t_1 = \max_{1 \leq i \leq g} t_i$, then*

$$\rho(C_{g-2}^k(t_1 + t_2 + t_g + 2, t_3, \ldots, t_{g-1})) < \rho(C_g^k(t_1, \ldots, t_g)).$$

Next we give a type of graft transformation on $C_{g(k-1)}^k(H_1, \ldots, H_{g(k-1)})$ that increases the distance spectral radius.

Theorem 3.2. *For $k \geq 3$ and $g \geq 3$, let $G = C_{g(k-1)}^k(H_1, \ldots, H_{g(k-1)})$, and let G_1^* be the k-uniform hypergraph obtained from G by moving e_1 from v_k to $v_{(g-1)(k-1)+1}$, and G_2^* be the k-uniform hypergraph obtained from G by moving e_g from $v_{(g-1)(k-1)+1}$ to v_k. Then $\rho(G_1^*) > \rho(G)$ or $\rho(G_2^*) > \rho(G)$.*

Proof. For $1 \leq i \leq g(k-1)$, let $V_i = V(H_i)$. Let $A_1 = \bigcup_{i=k}^{\frac{g(k-1)}{2}} V_i$ and $A_2 = \bigcup_{i=\frac{g(k-1)}{2}+2}^{(g-1)(k-1)+1} V_i$ if g is even, and $A_1 = \bigcup_{i=k}^{\frac{(g-1)(k-1)}{2}+1} V_i$ and $A_2 = \bigcup_{i=\frac{(g+1)(k-1)}{2}+1}^{(g-1)(k-1)+1} V_i$ if g is odd. Let $x = x(G)$. Suppose that $\sigma_G(A_1) \geq \sigma_G(A_2)$. As we pass from G to G_1^*, the distance between a vertex of $\bigcup_{i=2}^{k-1} V_i$ and a vertex of A_1 is increased by at least 1, the distance between a vertex of $\bigcup_{i=2}^{k-1} V_i$ and a vertex of A_2 is decreased by 1, and the distance between any other vertex pair is increased or remains unchanged. Then

$$\begin{aligned}
\frac{1}{2}(\rho(G_1^*) - \rho(G)) &\geq \frac{1}{2} x^\top (D(G_1^*) - D(G))x \\
&\geq \sigma_G\left(\bigcup_{i=2}^{k-1} V_i\right)(\sigma_G(A_1) - \sigma_G(A_2)) \\
&\geq 0.
\end{aligned}$$

Thus $\rho(G_1^*) \geq \rho(G)$. If $\rho(G) = \rho(G_1^*)$, then $\rho(G_1^*) = x^\top D(G_1^*)x$, and thus x is also the distance Perron vector of G_1^*, implying that

$$\begin{aligned}
\rho(G_1^*)x_{v_1} - \rho(G)x_{v_1} &= (D(G_1^*)x)_{v_1} - (D(G)x)_{v_1} \\
&= \sum_{v \in V(G)} (d_{G_1^*}(v_1, v) - d_G(v_1, v))x_v \\
&\geq \sum_{v \in V_k} x_v \\
&> 0,
\end{aligned}$$

a contradiction. Thus $\rho(G_1^*) > \rho(G)$.

Suppose that $\sigma_G(A_1) < \sigma_G(A_2)$. As we pass from G to G_2^*, the distance between a vertex of $\bigcup_{i=(g-1)(k-1)+2}^{g(k-1)} V_i$ and a vertex of A_2 is increased by at least 1, the distance between a vertex of $\bigcup_{i=(g-1)(k-1)+2}^{g(k-1)} V_i$ and a vertex of A_1 is decreased by 1, and the distance between any other vertex pair is increased or remains unchanged. Then

$$\begin{aligned}\frac{1}{2}(\rho(G_2^*)-\rho(G)) &\geq \frac{1}{2}x^\top(D(G_2^*)-D(G))x\\ &\geq \sigma_G\left(\bigcup_{i=(g-1)(k-1)+2}^{g(k-1)} V_i\right)(\sigma_G(A_2)-\sigma_G(A_1))\\ &> 0.\end{aligned}$$

Thus $\rho(G_2^*) > \rho(G)$. □

The results in this section will be used to study the distance spectral radius of uniform unicyclic hypergraphs in the next sections.

4 Minimum distance spectral radius of uniform unicyclic hypergraphs

In this section, we determine the unique hypergraphs with minimum and second minimum distance spectral radius respectively in the set of k-uniform unicyclic hypergraphs of fixed size.

Lemma 4.1. *For $k \geq 3$ and $t \geq 0$, $\rho(C_2^k(t,0))$ is the largest root of $f(\rho)=0$, where*

$$\begin{aligned}f(\rho) &= \rho^4+\rho^3(-2tk-2k+2t+7)+\rho^2(-3k^2-2tk^2-tk+3k+3t+7)\\ &\quad +\rho(-4k^2-tk^2-4tk+6k+5t+1)-k^2+k-2tk+2t.\end{aligned}$$

Proof. Let $G=C_2^k(t,0)$. Let (u,e_1,v,e_2,u) be the unique cycle of G, where $d_G(v)=2+t$. Let $x=x(G)$. By Lemma 2.1, the entry of x corresponding to each vertex of $(e_1\cup e_2)\setminus\{u,v\}$ is the same, which we denote by x_1, and the entry of x corresponding to each vertex of $V(G)\setminus(e_1\cup e_2)$ is the same, which we denote by x_2. Let $w_1\in(e_1\cup e_2)\setminus\{u,v\}$ and $w_2\in V(G)\setminus(e_1\cup e_2)$. By the eigenequations of G at u, v, w_1, and w_2, we have

$$\begin{aligned}\rho(G)x_u &= x_v+(2k-4)x_1+(2k-2)tx_2,\\ \rho(G)x_v &= x_u+(2k-4)x_1+(k-1)tx_2,\\ \rho(G)x_1 &= x_u+x_v+(3k-7)x_1+(2k-2)tx_2,\\ \rho(G)x_2 &= 2x_u+x_v+(4k-8)x_1+((2k-2)(t-1)+k-2)x_2.\end{aligned}$$

We view these equations as a homogeneous linear system in the four variables x_u, x_v, x_1 and x_2. Since it has a nontrivial solution, we have

$$\det\begin{pmatrix}-\rho & 1 & 2k-4 & (2k-2)t\\ 1 & -\rho & 2k-4 & (k-1)t\\ 1 & 1 & 3k-7-\rho & (2k-2)t\\ 2 & 1 & 4k-8 & (2k-2)(t-1)+k-2-\rho\end{pmatrix}=0,$$

where $\rho = \rho(G)$. By direct calculation, this determinant is equal to $f(\rho(G))$. Now the result follows easily. $\square$

Lemma 4.2. *For $k \geq 3$, we have*

$$\rho(C_{4k-4,k}) > \rho(C_2^k(2,0)).$$

Proof. Let $G = C_{4k-4,k}$ with edges $e_i = \{v_{(i-1)(k-1)+1}, \dots, v_{(i-1)(k-1)+k}\}$ for $1 \leq i \leq 4$, where $v_{4k-3} = v_1$. Let $\rho^* = \rho(G)$ and $x = x(G)$. By Lemma 2.1, the entry of x corresponding to each vertex of $\{v_1, v_k, v_{2k-1}, v_{3k-2}\}$ is the same, which we denote by α, and the entry of x corresponding to each vertex of $V(G)\setminus\{v_1, v_k, v_{2k-1}, v_{3k-2}\}$ is the same, which we denote by β. Then from the eigenequations of G at v_1 and v_2, we have

$$\rho(G)\alpha = 4\alpha + 6(k-2)\beta,$$
$$\rho(G)\beta = 6\alpha + (8k-17)\beta.$$

Thus ρ^* is the largest root of $\rho^2 - 8k\rho + 13\rho - 4k + 4 = 0$, i.e., $\rho^* = \frac{8k-13+\sqrt{64k^2-192k+153}}{2}$.

Let $G' = C_2^k(2,0)$. By Lemma 4.1, $\rho(G')$ is the largest root of $f(\rho) = 0$, where

$$f(\rho) = \rho^4 + \rho^3(11-6k) + \rho^2(13+k-7k^2) + \rho(11-2k-6k^2) + 4 - 3k - k^2.$$

Let $\rho_1 \geq \rho_2 \geq \rho_3 \geq \rho_4$ be the roots of $f(\rho) = 0$, where $\rho_1 = \rho(G')$. Then $\rho_1 + \rho_2 + \rho_3 + \rho_4 = 6k - 11$. Note that

$$\begin{aligned} f(-2k+2) &= (k-1)(k-2)(36k^2 - 116k + 91) > 0, \\ f(0) &= -(k+4)(k-1) < 0, \\ f(\rho^*) &= \rho^*(72k^3 - 411k^2 + 743k - 436) + 36k^3 - 185k^2 + 285k - 136 > 0. \end{aligned}$$

Then $\rho^* > \rho_1$, or $\rho^* < \rho_2$. Suppose that $\rho^* < \rho_2$. Then

$$\begin{aligned} \rho_1 + \rho_2 + \rho_3 + \rho_4 &\geq 2\rho^* + 0 + (-2k+2) \\ &= 6k - 11 + \sqrt{64k^2 - 192k + 153} \\ &> 6k - 11, \end{aligned}$$

a contradiction. Thus $\rho(G) = \rho^* > \rho_1 = \rho(G')$, as desired. $\square$

Lemma 4.3. *For $k \geq 3$ and $t_1 \geq t_2 \geq t_3 \geq 0$, we have*
(i) if $t_2 \geq 1$, then $\rho(C_3^k(t_1, t_2, t_3)) > \rho(C_3^k(t_1 + t_2 + t_3, 0, 0))$;
(ii) if $t_1 \geq 1$, then $\rho(C_3^k(t_1, 0, 0)) > \rho(C_2^k(t_1 + 1, 0))$.

Proof. Let $G = C_3^k(t_1, t_2, t_3)$. Let C be the unique cycle of G with edges $e_i = \{v_{(i-1)(k-1)+1}, \dots, v_{(i-1)(k-1)+k}\}$ for $i = 1, 2, 3$ and $v_{3k-2} = v_1$. Let $T_i = V(S_{t_i(k-1)+1,k}) \setminus \{v_{(i-1)(k-1)+1}\}$ for $1 \leq i \leq 3$.

First we prove (i). Let G' be the k-uniform hypergraph obtained from G by moving each edge of $E_G(v_k) \setminus \{e_1, e_2\}$ from v_k to v_1, and moving each edge of $E_G(v_{2k-1}) \setminus \{e_2, e_3\}$ from v_{2k-1} to v_1. It is easily seen that $G' \cong C_3^k(t_1 + t_2 + t_3, 0, 0)$. Let $x = x(G')$. By Lemma 2.1, the entry of x corresponding to each vertex of

$(e_1 \setminus \{v_1, v_k\}) \cup (e_3 \setminus \{v_1, v_{2k-1}\})$ is the same, which we denote by α, the entry of x corresponding to each vertex of $e_2 \setminus \{v_k, v_{2k-1}\}$ is the same, which we denote by β, the entry of x corresponding to each vertex of $T_1 \cup T_2 \cup T_3$ is the same, which we denote by γ, and $x_{v_k} = x_{v_{2k-1}}$.

As we pass from G to G', the distance between a vertex of T_2 and a vertex of $T_1 \cup (e_3 \setminus \{v_{2k-1}\})$ is decreased by 1, the distance between a vertex of T_2 and a vertex of $e_2 \setminus \{v_{2k-1}\}$ is increased by 1, the distance between a vertex of T_3 and a vertex of $T_1 \cup (e_1 \setminus \{v_k\})$ is decreased by 1, the distance between a vertex of T_3 and a vertex of $e_2 \setminus \{v_k\}$ is increased by 1, and the distance between any other vertex pair is decreased or remains unchanged. Then

$$\begin{aligned}
& \frac{1}{2}(\rho(G) - \rho(G')) \\
\geq\ & \frac{1}{2}x^\top(D(G) - D(G'))x \\
\geq\ & \sigma_{G'}(T_2)[\sigma_{G'}(T_1) + x_{v_1} + \sigma_{G'}(e_3 \setminus \{v_1, v_{2k-1}\}) - \sigma_{G'}(e_2 \setminus \{v_{2k-1}\})] \\
& +\sigma_{G'}(T_3)[\sigma_{G'}(T_1) + x_{v_1} + \sigma_{G'}(e_1 \setminus \{v_1, v_k\}) - \sigma_{G'}(e_2 \setminus \{v_k\})] \\
=\ & \sigma_{G'}(T_2)[\sigma_{G'}(T_1) + x_{v_1} + \sigma_{G'}(e_3 \setminus \{v_1, v_{2k-1}\}) - \sigma_{G'}(e_2 \setminus \{v_k, v_{2k-1}\}) - x_{v_k}] \\
& +\sigma_{G'}(T_3)[\sigma_{G'}(T_1) + x_{v_1} + \sigma_{G'}(e_1 \setminus \{v_1, v_k\}) - \sigma_{G'}(e_2 \setminus \{v_k, v_{2k-1}\}) - x_{v_{2k-1}}] \\
=\ & t_2(k-1)\gamma[t_1(k-1)\gamma + x_{v_1} + (k-2)\alpha - (k-2)\beta - x_{v_k}] \\
& +t_3(k-1)\gamma[t_1(k-1)\gamma + x_{v_1} + (k-2)\alpha - (k-2)\beta - x_{v_k}] \\
=\ & (t_2 + t_3)(k-1)\gamma[t_1(k-1)\gamma + x_{v_1} + (k-2)\alpha - (k-2)\beta - x_{v_k}] \\
\geq\ & (t_2 + t_3)(k-1)\gamma[(k-1)\gamma + x_{v_1} + (k-2)\alpha - (k-2)\beta - x_{v_k}],
\end{aligned}$$

and thus

$$\frac{1}{2}(\rho(G) - \rho(G')) \geq (t_2 + t_3)(k-1)\gamma[(k-1)\gamma + x_{v_1} + (k-2)\alpha - (k-2)\beta - x_{v_k}]. \quad (4.1)$$

Let $u \in (e_1 \setminus \{v_1, v_k\}) \cup (e_3 \setminus \{v_1, v_{2k-1}\})$, $v \in e_2 \setminus \{v_k, v_{2k-1}\}$ and $w \in T_1 \cup T_2 \cup T_3$. From the eigenequations of G' at v_1, v_k, u, v and w, we have

$$\begin{aligned}
\rho(G')x_{v_1} &= 2x_{v_k} + 2(k-2)\alpha + 2(k-2)\beta + (t_1 + t_2 + t_3)(k-1)\gamma, \\
\rho(G')x_{v_k} &= x_{v_1} + x_{v_k} + 3(k-2)\alpha + (k-2)\beta + 2(t_1 + t_2 + t_3)(k-1)\gamma, \\
\rho(G')\alpha &= x_{v_1} + 3x_{v_k} + (3k-7)\alpha + 2(k-2)\beta + 2(t_1 + t_2 + t_3)(k-1)\gamma, \\
\rho(G')\beta &= 2x_{v_1} + 2x_{v_k} + 4(k-2)\alpha + (k-3)\beta + 3(t_1 + t_2 + t_3)(k-1)\gamma, \\
\rho(G')\gamma &= x_{v_1} + 4x_{v_k} + 4(k-2)\alpha + 3(k-2)\beta \\
&\quad +(2(t_1 + t_2 + t_3 - 1)(k-1) + (k-2))\gamma.
\end{aligned}$$

Then

$$\begin{aligned}
& \rho(G')(\gamma(k-1) + x_{v_1} + \alpha(k-2) - \beta(k-2) - x_{v_k}) \\
=\ & 5x_{v_k}(k-1) + \alpha(k-2)(3k-4) + \beta(k-2)(4k-3) \\
& +\gamma(k-1)((t_1 + t_2 + t_3)(k-1) - k)
\end{aligned}$$

$$\begin{aligned} &\geq 5x_{v_k}(k-1)+\alpha(k-2)(3k-4)+\beta(k-2)(4k-3)+\gamma(k-1)(k-2) \\ &> 0, \end{aligned}$$

and thus $(k-1)\gamma + x_{v_1} + (k-2)\alpha - (k-2)\beta - x_{v_k} > 0$. Therefore by (4.1), $\rho(G) > \rho(G')$.

Now we prove (ii). Let G'' be the k-uniform hypergraph obtained from G by moving e_2 from v_k to v_1. It is easily seen that $G'' \cong C_2^k(t_1+1, 0)$. Let $x = x(G'')$. By Lemma 2.1, the entry of x corresponding to each vertex of $T_1 \cup (e_1 \setminus \{v_1\})$ is the same, which we denote by α, the entry of x corresponding to each vertex of $(e_2 \cup e_3) \setminus \{v_1, v_k, v_{2k-1}\}$ is the same, which we denote by β.

As we pass from G to G'', the distance between v_k and a vertex of $e_2 \setminus \{v_k\}$ is increased by 1, the distance between a vertex of T_1 and a vertex of $e_2 \setminus \{v_k, v_{2k-1}\}$ is decreased by 1, and the distance between any other vertex pair remains unchanged. Note that $t_1 \geq 3$ and $k \geq 3$. Then

$$\begin{aligned} \frac{1}{2}(\rho(G) - \rho(G'')) &\geq \frac{1}{2}x^\top(D(G) - D(G''))x \\ &= -x_{v_k}\sigma_{G''}(e_2 \setminus \{v_k\}) + \sigma_{G''}(T_1)\sigma_{G''}(e_2 \setminus \{v_k, v_{2k-1}\}) \\ &= -\alpha(x_{v_{2k-1}} + (k-2)\beta) + t_1(k-1)\alpha(k-2)\beta \qquad (4.2) \\ &= -\alpha x_{v_{2k-1}} + (k-2)(t_1(k-1)-1)\alpha\beta \\ &\geq \alpha(\beta - x_{v_{2k-1}}). \end{aligned}$$

Let $u \in (e_2 \cup e_3) \setminus \{v_1, v_k, v_{2k-1}\}$. From the eigenequations of G'' at v_{2k-1} and u, we have

$$\begin{aligned} \rho(G'')x_{v_{2k-1}} &= 2(k-2)\beta + x_{v_1} + 2(t_1+1)(k-1)\alpha, \\ \rho(G'')\beta &= x_{v_{2k-1}} + (3k-7)\beta + x_{v_1} + 2(t_1+1)(k-1)\alpha, \end{aligned}$$

and thus $\rho(G'')(\beta - x_{v_{2k-1}}) = x_{v_{2k-1}} + (k-3)\beta > 0$, implying that $\beta - x_{v_{2k-1}} > 0$. Therefore by (4.2), $\rho(G) > \rho(G'')$. □

Lemma 4.4. *For $k \geq 3$, $1 \leq b \leq \left\lfloor \frac{n-2k+2}{2(k-1)} \right\rfloor$ and $a = \frac{n-2k+2}{k-1} - b$, we have*

$$\rho(C_2^k(a, b)) > \rho(C_2^k(a+1, b-1)).$$

Proof. Let $G = C_2^k(a, b)$. Let C be the unique cycle of G with edges $e_i = \{v_{(i-1)(k-1)+1}, \ldots, v_{(i-1)(k-1)+k}\}$, where $1 \leq i \leq 2$ and $v_{2k-1} = v_1$. Let $x = x(G)$. By Lemma 2.1, the entry of x corresponding to each vertex of $\cup_{e \in E_G(v_1)} e \setminus (e_1 \cup e_2)$ is the same, which we denote by α, the entry of x corresponding to each vertex of $\cup_{e \in E_G(v_k)} e \setminus (e_1 \cup e_2)$ is the same, which we denote by β, and the entry of x corresponding to each vertex of $(e_1 \cup e_2) \setminus \{v_1, v_k\}$ is the same, which we denote by γ. Let $u_1 \in \cup_{e \in E_G(v_1)} e \setminus (e_1 \cup e_2)$ and $u_2 \in \cup_{e \in E_G(v_k)} e \setminus (e_1 \cup e_2)$. From the eigenequations of G at u_1, u_2, v_2, v_1 and v_k, we have

$$\begin{aligned} \rho(G)\alpha &= (2(k-1)a - k)\alpha + 3(k-1)b\beta + 4(k-2)\gamma + x_{v_1} + 2x_{v_k}, \\ \rho(G)\beta &= 3(k-1)a\alpha + (2(k-1)b - k)\beta + 4(k-2)\gamma + 2x_{v_1} + x_{v_k}, \end{aligned}$$

$$\begin{aligned}
\rho(G)\gamma &= 2(k-1)a\alpha + 2(k-1)b\beta + (3k-7)\gamma + x_{v_1} + x_{v_k},\\
\rho(G)x_{v_1} &= (k-1)a\alpha + 2(k-1)b\beta + 2(k-2)\gamma + x_{v_k},\\
\rho(G)x_{v_k} &= 2(k-1)a\alpha + (k-1)b\beta + 2(k-2)\gamma + x_{v_1}.
\end{aligned}$$

Thus $\rho(G)$ is the largest root of the equation $g_b(t) = 0$, where

$$\begin{aligned}
g_b(t) &= t^5 - t^4(2ak + 2bk + k - 2a - 2b - 7)\\
&\quad -t^3(5k^2 + 5abk^2 + 4ak^2 + 4bk^2 - 10k\\
&\quad -10abk - ak - bk - 7 + 5ab - 3b - 3a)\\
&\quad -t^2(3k^3 + abk^3 + 2ak^3 + 2bk^3 + k^2 + 5abk^2 + 2ak^2 + 2bk^2\\
&\quad -13k - 13abk + ak + bk - 1 + 7ab - 5b - 5a)\\
&\quad -t(4k^3 + ak^3 + bk^3 - 5k^2 + 4abk^2 + 4ak^2 + 4bk^2\\
&\quad -2k - 8abk - 3ak - 3bk + 4ab - 2b - 2a)\\
&\quad -k(k-1)(k + 2b + 2a).
\end{aligned}$$

For $1 \le b \le \left\lfloor \frac{n-2k+2}{2(k-1)} \right\rfloor$, it is easily seen that

$$g_b(t) - g_{b-1}(t) = -(a + 1 - b)(k-1)^2 t[t^2 + (k+7)t + 4].$$

Let $\rho_b = \rho(C_2^k(a, b))$. Then

$$\begin{aligned}
g_b(\rho_{b-1}) &= g_b(\rho_{b-1}) - g_{b-1}(\rho_{b-1})\\
&= -(a + 1 - b)(k-1)^2 \rho_{b-1}[\rho_{b-1}^2 + (k+7)\rho_{b-1} + 4]\\
&< 0,
\end{aligned}$$

from which, together with the fact that $g_b(t) > 0$ for $t > \rho_b$, we have $\rho_b > \rho_{b-1}$. $\square$

Theorem 4.1. *For $k \ge 3$, let G be a k-uniform unicyclic hypergraph of size $m \ge 2$ with minimum distance spectral radius. Then $G \cong C_{3k-3,k}$ if $m = 3$, and $G \cong C_2^k(m-2, 0)$ otherwise.*

Proof. It is trivial if $m = 2$. Suppose that $m \ge 3$. Let g be the length of the unique cycle of G. Let C be the unique cycle of G with edges $e_i = \{v_{(i-1)(k-1)+1}, \dots, v_{(i-1)(k-1)+k}\}$, where $i = 1, \dots, g$ and $v_{g(k-1)+1} = v_1$. For $1 \le i \le g(k-1)$, let H_i be the component of $G - E(C)$ containing v_i.

Claim 1. For each i and j with $1 \le i \le g$ and $2 \le j \le k-1$,

$$V(H_{(i-1)(k-1)+j}) = \{v_{(i-1)(k-1)+j}\}.$$

Suppose that there exist some i and some j with $1 \le i \le g$ and $2 \le j \le k-1$ such that $V(H_{(i-1)(k-1)+j}) \ne \{v_{(i-1)(k-1)+j}\}$, i.e., $V(H_{(i-1)(k-1)+j}) \setminus \{v_{(i-1)(k-1)+j}\} \ne \emptyset$. Then $H_{(i-1)(k-1)+j}$ is a k-uniform hypertree with at least one edge.

Let G' be the k-uniform hypergraph obtained from G by moving each edge of $E_G(v_{(i-1)(k-1)+j}) \setminus \{e_i\}$ from $v_{(i-1)(k-1)+j}$ to $v_{(i-1)(k-1)+k}$. Obviously, G' is a k-uniform unicyclic hypergraph of size m.

As we pass from G to G', the distance between a vertex of $V(H_{(i-1)(k-1)+j}) \setminus \{v_{(i-1)(k-1)+j}\}$ and $v_{(i-1)(k-1)+j}$ is increased by 1, the distance between a vertex of $V(H_{(i-1)(k-1)+j}) \setminus \{v_{(i-1)(k-1)+j}\}$ and a vertex of $e_{i+1} \setminus \{v_{i(k-1)+k}\}$ is decreased by 1, and the distance between any other vertex pair is decreased or remains unchanged. Let $x = x(G')$ and $U = V(H_{(i-1)(k-1)+j}) \setminus \{v_{(i-1)(k-1)+j}\}$. Then

$$\begin{aligned}\frac{1}{2}(\rho(G) - \rho(G')) &\geq \frac{1}{2}x^\top(D(G) - D(G'))x \\ &\geq \sigma_{G'}(U)\left[-x_{v_{(i-1)(k-1)+j}} + \sigma_{G'}\left(e_{i+1} \setminus \{v_{i(k-1)+k}\}\right)\right] \quad (4.3) \\ &\geq \sigma_{G'}(U)\left(-x_{v_{(i-1)(k-1)+j}} + x_{v_{i(k-1)+1}} + x_{v_{i(k-1)+2}}\right).\end{aligned}$$

Let $W = V(G) \setminus \{v_{(i-1)(k-1)+j}, v_{i(k-1)+1}, v_{i(k-1)+2}\}$. From the eigenequations of G' at $v_{(i-1)(k-1)+j}$, $v_{i(k-1)+1}$ and $v_{i(k-1)+2}$, we have

$$\begin{aligned}\rho(G')x_{v_{(i-1)(k-1)+j}} &= x_{v_{i(k-1)+1}} + 2x_{v_{i(k-1)+2}} + \sum_{w \in W} d_{G'}(v_{(i-1)(k-1)+j}, w)x_w, \\ \rho(G')x_{v_{i(k-1)+1}} &= x_{v_{(i-1)(k-1)+j}} + x_{v_{i(k-1)+2}} + \sum_{w \in W} d_{G'}(v_{i(k-1)+1}, w)x_w, \\ \rho(G')x_{v_{i(k-1)+2}} &= x_{v_{i(k-1)+1}} + 2x_{v_{(i-1)(k-1)+j}} + \sum_{w \in W} d_{G'}(v_{i(k-1)+2}, w)x_w.\end{aligned}$$

Note that for $w \in W$,

$$d_{G'}\left(v_{i(k-1)+1}, w\right) + d_{G'}\left(v_{i(k-1)+2}, w\right) - d_{G'}\left(v_{(i-1)(k-1)+j}, w\right) \geq 0.$$

Then

$$(\rho(G') + 1)\left(-x_{v_{(i-1)(k-1)+j}} + x_{v_{i(k-1)+1}} + x_{v_{i(k-1)+2}}\right) \geq 2x_{v_{(i-1)(k-1)+j}} + x_{v_{i(k-1)+1}} > 0,$$

implying that $-x_{v_{(i-1)(k-1)+j}} + x_{v_{i(k-1)+1}} + x_{v_{i(k-1)+2}} > 0$. Thus by (4.3), $\rho(G) > \rho(G')$, a contradiction. Therefore Claim 1 follows.

If $m = 3$, then by Claim 1, $G \cong C_{3k-3,k}$ or $C_2^k(1,0)$, and by Theorem 3.2, we have $\rho(C_{3k-3,k}) < \rho(C_2^k(1,0))$, implying that $G \cong C_{3k-3,k}$.

Suppose that $m \geq 4$.

Claim 2. For each i with $1 \leq i \leq g$, $H_{(i-1)(k-1)+1}$ is a k-uniform hyperstar with center $v_{(i-1)(k-1)+1}$.

Suppose that some $H_{(i-1)(k-1)+1}$, say H_1 is not a k-uniform hyperstar with center v_1. Then $|E(H_1)| \geq 2$. We choose an edge $e \in E_G(v_1) \setminus \{e_1, e_g\}$ such that $e \setminus \{v_1\}$ contains at least one vertex of degree at least 2 in G. Let $e = \{w_1, w_2, \ldots, w_k\}$, where $v_1 = w_k$. For $1 \leq j \leq k-1$, let W_j be the component of $G - e$ containing w_j. Then $G = H_{e,0}(W_1, \ldots, W_{k-1})$, where $H = G[V(G) \setminus \cup_{j=1}^{k-1}(V(W_j) \setminus \{w_j\})]$. Note that there is some j with $1 \leq j \leq k-1$ such that $|E(W_j)| \geq 1$. Let $G' = H_{e,k-1}(W_1, \ldots, W_{k-1})$. It is easily seen that G' is a k-uniform unicyclic hypergraph of size m. By Lemma 2.2, we have $\rho(G) > \rho(G')$, a contradiction. This proves Claim 2.

If $m=4$, then by Claims 1 and 2, we have $G\cong C_{4k-4,k}$, $C_3^k(1,0,0)$, $C_2^k(1,1)$ or $C_2^k(2,0)$, and then by Lemmas 4.2, 4.3 (ii), and 4.4, we have

$$\min\{\rho(C_{4k-4,k}),\rho(C_3^k(1,0,0)),\rho(C_2^k(1,1))\}>\rho(C_2^k(2,0)),$$

implying that $G\cong C_2^k(2,0)$.

Suppose that $m\geq 5$. For $1\leq i\leq g$, let $t_i=|E(H_{(i-1)(k-1)+1})|$. By Claims 1 and 2, $G\cong C_g^k(t_1,\dots,t_g)$, where $\sum_{i=1}^g t_i=m-g$. Suppose without loss of generality that $t_1=\max_{1\leq i\leq g}t_i$.

Suppose that g is odd. Suppose that $g\geq 5$. Let $G'=C_{g-2}^k(t_1+t_2+t_g+2,t_3,\dots,t_{g-1})$. Obviously, G'' is a k-uniform unicyclic hypergraph of size m. By Corollary 3.1, we have $\rho(G)>\rho(G'')$, a contradiction. Thus $g=3$. Therefore we have $G\cong C_3^k(t_1,t_2,t_3)$ with $t_1+t_2+t_3=m-3$. We may assume that $t_1\geq t_2\geq t_3$. By Lemma 4.3 (i), we have $t_1=m-3$ and $t_2=t_3=0$, i.e., $G\cong C_3^k(m-3,0,0)$. Obviously, $C_2^k(m-2,0)$ is a k-uniform unicyclic hypergraph of size m. By Lemma 4.3 (ii), $\rho(G)>\rho(C_2^k(m-2,0))$, a contradiction. Thus g is even.

Suppose that $g\geq 4$. Let $G^*=C_{g-2}^k(t_1+t_2+t_g+2,t_3,\dots,t_{g-1})$. Obviously, G^* is a k-uniform unicyclic hypergraph of size m. By Corollary 3.1, we have $\rho(G)>\rho(G^*)$, a contradiction. Then $g=2$, and thus $G\cong C_2^k(t_1,t_2)$ with $t_1\geq t_2$ and $t_1+t_2=m-2$. By Lemma 4.4, $t_1=m-2$ and $t_2=0$, i.e., $G=C_2^k(m-2,0)$. $\square$

Lemma 4.5. *For $k\geq 3$ and $t_1=\max_{1\leq i\leq 4}t_i\geq 0$, we have $\rho(C_4^k(t_1,t_2,t_3,t_4))<\rho(C_3^k(t_1+t_2+1,t_3,t_4))$ if $t_1=0$ and $k=3$, and $\rho(C_4^k(t_1,t_2,t_3,t_4))>\rho(C_3^k(t_1+t_2+1,t_3,t_4))$ otherwise.*

Proof. Let $G=C_4^k(t_1,t_2,t_3,t_4)$. Let C be the unique cycle of G with edges $e_i=\{v_{(i-1)(k-1)+1},\dots,v_{(i-1)(k-1)+k}\}$, where $i=1,\dots,4$, and $v_{4k-3}=v_1$. For $1\leq i\leq 4k-4$, let H_i be the component of $G-E(C)$ containing v_i. Let G' be the hypergraph obtained from G by moving each edge of $E_G(v_k)\setminus\{e_1\}$ from v_k to v_1. Then $G'\cong C_3^k(t_1+t_2+1,t_3,t_4)$. Let $x=x(G')$. By Lemma 2.1, the entry of x corresponding to each vertex of $(e_1\cup V(H_1))\setminus\{v_1\}$ is the same, which we denote by α_1, the entry of x corresponding to each vertex of $e_i\setminus\{v_{(i-1)(k-1)+1},v_{(i-1)(k-1)+k}\}$ for $i=2,3,4$ is the same, which we denote by α_i.

Suppose that $t_1=0$. Then $G\cong C_{4k-4,k}$. By the proof of Lemma 4.2, we have $\rho*=\rho(G)=\frac{8k-13+\sqrt{64k^2-192k+153}}{2}$. By Lemma 2.1, $\alpha_2=\alpha_4$ and $x_{v_{2k-1}}=x_{v_{3k-2}}$. Then from the eigenequations of G' at v_2, v_{k+1}, v_{2k}, v_1 and v_{2k-1}, we have

$$\begin{aligned}
\rho(G')\alpha_1 &= (k-2)\alpha_1+(4k-8)\alpha_2+(3k-6)\alpha_3+x_{v_1}+4x_{v_{2k-1}},\\
\rho(G')\alpha_2 &= (2k-2)\alpha_1+(3k-7)\alpha_2+(2k-4)\alpha_3+x_{v_1}+3x_{v_{2k-1}},\\
\rho(G')\alpha_3 &= (3k-3)\alpha_1+(4k-8)\alpha_2+(k-3)\alpha_3+2x_{v_1}+2x_{v_{2k-1}},\\
\rho(G')x_{v_1} &= (k-1)\alpha_1+(2k-4)\alpha_2+(2k-4)\alpha_3+2x_{v_{2k-1}},\\
\rho(G')x_{v_{2k-1}} &= (2k-2)\alpha_1+(3k-6)\alpha_2+(k-2)\alpha_3+x_{v_1}+x_{v_{2k-1}}.
\end{aligned}$$

Thus $\rho(G')$ is the largest root of $f(\rho)=0$, where

$$f(\rho) \;=\; \rho^5-\rho^4(5k-11)-\rho^3(18k^2-28k-4)-\rho^2(8k^3+10k^2-39k+4)$$

$$-\rho(9k^3-4k^2-14k-3)-9k^2+16k-3.$$

If $k=3$, then $f(\rho^*)=-1539-125\sqrt{153}<0$, which together with the fact that $f(\rho)>0$ for $\rho>\rho(G')$, implying that $\rho^*<\rho(G')$.

Suppose that $k\geq 4$. Let $\rho_1\geq\rho_2\geq\rho_3\geq\rho_4\geq\rho_5$ be the roots of $f(\rho)=0$, where $\rho_1=\rho(G')$. Note that

$$\begin{aligned}
f(-k) &= (4k^3-10k^2+7k-3)(k-1)^2>0,\\
f(0) &= -(9k^2-16k+3)<0,\\
f(\rho^*) &= \rho^*(320k^4-2585k^3+7476k^2-9300k+4241)\\
&\quad +160k^4-1200k^3+3135k^2-3424k+1333>0.
\end{aligned}$$

Then $\rho^*>\rho_1$ or $\rho^*<\rho_2$. Suppose that $\rho^*<\rho_2$. Note that $0<\rho_3<\rho^*$, $-k<\rho_4<0$ and $5k-11=\rho_1+\rho_2+\rho_3+\rho_4+\rho_5$. Then

$$\rho_5<5k-11-2\rho^*-0-(-k)=-2k+2-\sqrt{64k^2-192k+153}<-(8k-10),$$

However, since the maximum row sum of $D(G')$ is $8k-10$ and $\rho(G')$ is bounded above by the maximum row sum of $D(G')$ (see [13, p. 24, Theorem 1.1]), we have $|\rho_5|\leq\rho(G')\leq 8k-10$, a contradiction. Thus $\rho^*>\rho_1=\rho(G')$, as desired.

Now suppose that $t_1\geq 1$. As we pass from G to G', the distance between v_k and a vertex of $(V(H_k)\setminus\{v_k\})\cup V(H_{2k-1})\cup(e_3\setminus\{v_{2k-1},v_{3k-2}\})$ is increased by 1, the distance between a vertex of $V(H_1)$ and a vertex of $(V(H_k)\setminus\{v_k\})\cup V(H_{2k-1})\cup(e_2\setminus\{v_k,v_{2k-1}\})$ is decreased by 1, and the distance between any other vertex pair is decreased or remains unchanged. Note that $|V(H_1)|\geq k\geq 3$. Thus

$$\begin{aligned}
&\frac{1}{2}(\rho(G)-\rho(G'))\\
\geq\ &\frac{1}{2}x^\top(D(G)-D(G'))x\\
\geq\ &-x_{v_k}[\sigma_{G'}(V(H_k)\setminus\{v_k\})+\sigma_{G'}(V(H_{2k-1}))+\sigma_{G'}(e_3\setminus\{v_{2k-1},v_{3k-2}\})]\\
&+\sigma_{G'}(V(H_1))[\sigma_{G'}(V(H_k)\setminus\{v_k\})+\sigma_{G'}(V(H_{2k-1})+\sigma_{G'}(e_2\setminus\{v_k,v_{2k-1}\})]\\
\geq\ &-\alpha_1[\sigma_{G'}(V(H_k)\setminus\{v_k\})+\sigma_{G'}(V(H_{2k-1}))+(k-2)\alpha_3]\\
&+(2\alpha_1+x_{v_1})[\sigma_{G'}(V(H_k)\setminus\{v_k\})+\sigma_{G'}(V(H_{2k-1}))+(k-2)\alpha_2]\\
>\ &(k-2)\alpha_1(2\alpha_2-\alpha_3).
\end{aligned}$$

Let $W=V(G)\setminus\{v_{k+1},v_{2k}\}$. From the eigenequations of G' at v_{k+1} and v_{2k}, we have

$$\begin{aligned}
\rho(G')\alpha_2 &= 2\alpha_3+\sum_{w\in W}d_{G'}(v_{k+1},w)x_w,\\
\rho(G')\alpha_3 &= 2\alpha_2+\sum_{w\in W}d_{G'}(v_{2k},w)x_w.
\end{aligned}$$

Note that for $w\in W$, $2d_{G'}(v_{k+1},w)-d_{G'}(v_{2k},w)\geq 0$. Then $(\rho(G')+1)(2\alpha_2-\alpha_3)\geq 3\alpha_3>0$, implying that $2\alpha_2-\alpha_3>0$. Thus $\rho(G)>\rho(G')$. □

For $k \geq 3$, let $F_2^k(t) = C_{2k-2}^k(H_1, \ldots, H_{2k-2})$ when $|V(H_1)| = |V(H_i)| = 1$ for $3 \leq i \leq 2k-2$ and H_2 is a hyperstar $S_{t(k-1)+1,k}$ with center v_2. In particular, $F_2^k(0) = C_{2k-2,k}$.

For $k \geq 3$, let $H_2^k = C_{2k-2}^k(H_1, \ldots, H_{2k-2})$ when $|V(H_i)| = 1$ for $2 \leq i \leq 2k-2$ and H_1 is a k-uniform pendant path of length 2 at v_1.

Lemma 4.6. *For $k \geq 3$ and $t \geq 1$, we have*
(i) if $t \geq 1$, then $\rho(C_3^k(t,0,0)) < \rho(F_2^k(t+1))$,
(ii) if $t = 1$, then $\rho(C_3^k(t,0,0)) < \min\{\rho(C_2^k(1,1)), \rho(H_2^k)\}$.

Proof. Let $G = C_3^k(t,0,0)$. Let C be the unique cycle of G with edges $e_i = \{v_{(i-1)(k-1)+1}, \ldots, v_{(i-1)(k-1)+k}\}$, where $i = 1,2,3$, and $v_{3k-2} = v_1$. Let H_1 be the component of $G - E(C)$ containing v_1. Let $x = x(G)$. By Lemma 2.1, the entry of x corresponding to each vertex of $(e_1 \cup e_3) \setminus \{v_1, v_k, v_{2k-1}\}$ is the same, which we denote by α, the entry of x corresponding to each vertex of $e_2 \setminus \{v_k, v_{2k-1}\}$ is the same, which we denote by β, and $x_{v_k} = x_{v_{2k-1}}$.

First we prove (i). Let G' be the k-uniform hypergraph obtained from G by moving e_2 from v_k to v_{3k-3}. It is easily seen that $G' \cong F_2^k(t+1)$. As we pass from G to G', the distance between v_{3k-3} and a vertex of $e_2 \setminus \{v_k, v_{2k-1}\}$ is decreased by 1, the distance between a vertex of $e_2 \setminus \{v_k, v_{2k-1}\}$ and a vertex of $e_1 \setminus \{v_1, v_k\}$ is increased by 1, the distance between v_k and v_{2k-1} is increased by 1, and the distance between any other vertex pair is increased or remains unchanged. Then

$$\begin{aligned}
\frac{1}{2}(\rho(G') - \rho(G)) &\geq \frac{1}{2}x^\top(D(G') - D(G))x \\
&\geq -x_{v_{3k-3}}\sigma_G(e_2 \setminus \{v_k, v_{2k-1}\}) \\
&\quad +\sigma_G(e_2 \setminus \{v_k, v_{2k-1}\})\sigma_G(e_1 \setminus \{v_1, v_k\}) + x_{v_k}x_{v_{2k-1}} \\
&= -(k-2)\alpha\beta + (k-2)^2\alpha\beta + x_{v_k}x_{v_{2k-1}} \\
&= (k-2)(k-3)\alpha\beta + x_{v_k}x_{v_{2k-1}} \\
&> 0.
\end{aligned}$$

Thus $\rho(G') > \rho(G)$.

Now we prove (ii). Let $E(H_1) = \{e_4\}$, where $e_1 \cap e_4 = \{v_1\}$. Let G^* be the hypergraph obtained from G by moving e_1 from v_k to v_{2k-1}. It is easily seen that $G^* \cong C_2^k(1,1)$. As we pass from G to G^*, the distance between v_{2k-1} and a vertex of $e_1 \setminus \{v_1, v_k\}$ is decreased by 1, the distance between v_k and a vertex of $e_4 \cup (e_1 \setminus \{v_1, v_k\})$ is increased by 1, and the distance between any other vertex pair remains unchanged. Then

$$\begin{aligned}
\frac{1}{2}(\rho(G^*) - \rho(G)) &\geq \frac{1}{2}x^\top(D(G^*) - D(G))x \\
&= -x_{v_{2k-1}}\sigma_G(e_1 \setminus \{v_1, v_k\}) + x_{v_k}(\sigma_G(e_4) + \sigma_G(e_1 \setminus \{v_1, v_k\})) \\
&= x_{v_k}\sigma_G(e_1 \setminus \{v_1, v_k\}) \\
&> 0.
\end{aligned}$$

Thus $\rho(G^*) > \rho(G)$.

Let G^{**} be the hypergraph obtained from G by moving e_1 from v_1 to v_{2k-1}. Obviously, $G^{**} \cong H_2^k$. As we pass from G to G^{**}, the distance between a vertex of e_4 and a vertex of $e_1 \setminus \{v_1\}$ is increased by 1, the distance between v_{2k-1} and a vertex of $e_1 \setminus \{v_1, v_k\}$ is decreased by 1, and the distance between any other vertex pair remains unchanged. Then

$$\begin{aligned}\frac{1}{2}(\rho(G^{**}) - \rho(G)) &\geq \frac{1}{2}x^\top (D(G^{**}) - D(G))x \\ &= \sigma_G(e_4)\sigma_G(e_1 \setminus \{v_1\}) - x_{v_{2k-1}}\sigma_G(e_1 \setminus \{v_1, v_k\})) \\ &> (\sigma_G(e_4) - x_{v_{2k-1}})\sigma_G(e_1 \setminus \{v_1, v_k\})).\end{aligned}$$

Let $u \in e_4 \setminus \{v_1\}$. Note that for $w \in V(G)\setminus\{v_1, v_{2k-1}, u\}$, $d_G(v_1, w) + d_G(v_{2k-1}, w) - d_G(u, w) \geq 0$. From the eigenequations of G at v_1, v_{2k-1} and u, we have $\rho(G)(x_{v_1} + x_u - x_{v_{2k-1}}) \geq -x_u + 3x_{v_{2k-1}}$, and then $(\rho(G)+1)(x_{v_1} + x_u - x_{v_{2k-1}}) \geq x_{v_1} + 2x_{v_{2k-1}} > 0$, implying that $x_{v_1} + x_u - x_{v_{2k-1}} > 0$. Thus $\sigma_G(e_4) - x_{v_{2k-1}} > x_{v_1} + x_u - x_{v_{2k-1}} > 0$. Therefore $\rho(G^{**}) > \rho(G)$. □

Theorem 4.2. *For $k \geq 3$, let G be a k-uniform unicyclic hypergraph of size $m \geq 3$ not isomorphic to $C_{3k-3,k}$ for $m = 3$ and $C_2^k(m-2, 0)$ otherwise with minimum distance spectral radius. Then $G \cong C_2^k(1, 0)$ if $m = 3$, $G \cong C_{4k-4,k}$ if $k = 3$ and $m = 4$, and $G \cong C_3^k(m-3, 0, 0)$ otherwise.*

Proof. Let g be the length of the unique cycle of G. Let C be the unique cycle of G with edges $e_i = \{v_{(i-1)(k-1)+1}, \dots, v_{(i-1)(k-1)+k}\}$, where $i = 1, \dots, g$, and $v_{g(k-1)+1} = v_1$. For $1 \leq i \leq g(k-1)$, let H_i be the component of $G - E(C)$ containing v_i.

If $m = 3$, then since $G \ncong C_{3k-3,k}$, we have $G \cong C_2^k(1, 0)$ or $F_2^k(1)$, and by similar argument as in Claim 1 in the proof of Theorem 4.1, we have $\rho(C_2^k(1, 0)) < \rho(F_2^k(1))$, implying that $G \cong C_2^k(1, 0)$.

Suppose that $m \geq 4$. Note that $G \ncong C_2^k(m-2, 0)$. As in the proof of Theorem 4.1, we have the following Claims 1 and 2.

Claim 1. For $g \geq 3$, each $1 \leq i \leq g$ and each $2 \leq j \leq k-1$,

$$V(H_{(i-1)(k-1)+j}) = \{v_{(i-1)(k-1)+j}\}.$$

Claim 2. If $m \geq 4$ and $g \geq 3$, then for each $1 \leq i \leq g$, $H_{(i-1)(k-1)+1}$ is a k-uniform hyperstar with center $v_{(i-1)(k-1)+1}$.

Suppose that $m = 4$. If $g = 2$, then since $G \ncong C_2^k(m-2, 0)$ and by similar argument as in Claim 1 in the proof of Theorem 4.1, we have $G \cong C_2^k(1, 1)$, $F_2^k(2)$ or H_2^k, and if $g = 3, 4$, then by Claim 1, we have $G \cong C_3^k(1, 0, 0)$ or $C_{4k-4,k}$. By Lemmas 4.5 and 4.6, we have $\rho(C_{4k-4,k}) < \min\{\rho(C_2^k(1, 1)), \rho(F_2^k(2)), \rho(H_2^k), \rho(C_3^k(1, 0, 0))\}$ if $k = 3$ and $\rho(C_3^k(1, 0, 0)) < \min\{\rho(C_2^k(1, 1)), \rho(F_2^k(2)), \rho(H_2^k), \rho(C_{4k-4,k})\}$ otherwise. Therefore $G \cong C_{4k-4,k}$ if $k = 3$, and $G \cong C_3^k(m-3, 0, 0)$ otherwise, as desired.

Suppose that $m \geq 5$.

Claim 3. g is odd.

Suppose that g is even. Suppose that $g \geq 6$. Then $m \geq 6$. For $1 \leq i \leq g$, let $t_i = |E(H_{(i-1)(k-1)+1})|$. By Claims 1 and 2, $G \cong C_g^k(t_1, \dots, t_g)$, where $\sum_{i=1}^{g} t_i = m - g$. Suppose without loss of generality that $t_1 = \max_{1 \leq i \leq g} t_i$. Let

$G' = C^k_{g-2}(t_1+t_2+t_g+2, t_3, \dots, t_{g-1})$. Obviously, G' is a k-uniform unicyclic hypergraph of size m and $G' \ncong C^k_2(m-2,0)$. By Corollary 3.1, we have $\rho(G) > \rho(G')$, a contradiction. Thus $g = 2$ or 4.

Suppose that $g = 4$. Obviously, by Claims 1 and 2, $G \cong C^k_4(t_1,t_2,t_3,t_4)$ with $t_1 = \max_{1\le i\le 4} t_i \ge 1$. Obviously, $C^k_3(t_1+t_2+1, t_3, t_4)$ is a k-uniform unicyclic hypergraph of size m and it is not isomorphic to $C^k_2(m-2,0)$. By Lemma 4.5, we have $\rho(G) \ge \rho\left(C^k_3(t_1+t_2+1,t_3,t_4)\right)$, a contradiction. Thus $g = 2$ and $G \cong C^k_{2k-2}(H_1,\dots,H_{2k-2})$.

Let $m_i = |E(H_i)|$, where $1 \le i \le 2k-2$ and $\sum_{i=1}^{2k-2} m_i + 2 = m$. Suppose without loss of generality that $m_1 \ge m_k \ge 0$ and $m_2 = \max\{m_j : 2 \le j \le 2k-2,\ j \ne k\}$.

We will show that $m_2 = 0$. Suppose that $m_2 \ge 1$. Then $G \ncong C^k_2(m-2,0)$. By similar argument as in Claim 2 in the proof of Theorem 4.1, each H_i is a k-uniform hyperstar with center v_i for $1 \le i \le 2k-2$.

Suppose that $m_1 \ge 1$. Let G' be the hypergraph obtained from G by moving each edge of $E_G(v_2)\setminus e_1$ from v_2 to v_k. Obviously, G' is a unicyclic hypergraph of size m and $G' \ncong C^k_2(m-2,0)$. Let $x = x(G')$. From the eigenequations of G' at v_2, v_k and v_{k+1}, we have $\rho(G')\left(x_{v_k}+x_{v_{k+1}}-x_{v_2}\right) \ge -x_{v_{k+1}} + 3x_{v_2}$. Then $(\rho(G')+1)\left(x_{v_k}+x_{v_{k+1}}-x_{v_2}\right) \ge x_{v_k}+2x_{v_2} > 0$. Thus $x_{v_k}+x_{v_{k+1}}-x_{v_2} > 0$. As we pass from G to G', the distance between a vertex of $V(H_2)\setminus\{v_2\}$ and v_2 is increased by 1, the distance between a vertex of $V(H_2)\setminus\{v_2\}$ and a vertex of $\{v_k, v_{k+1}\}$ is decreased by 1, and the distance between any other vertex pair is decreased or remains unchanged. Then

$$\begin{aligned}\frac{1}{2}(\rho(G)-\rho(G')) &\ge \frac{1}{2}x^\top(D(G)-D(G'))x\\ &\ge \sigma_{G'}(V(H_2)\setminus\{v_2\})\left(x_{v_k}+x_{v_{k+1}}-x_{v_2}\right)\\ &> 0.\end{aligned}$$

Thus $\rho(G) > \rho(G')$, a contradiction. Thus $m_1 = m_k = 0$.

Suppose that there exists some $i \in \{j : 3 \le j \le 2k-2 \text{ and } j \ne k\}$ such that $m_i \ge 1$. Let G' be the hypergraph obtained from G by moving each edge of $E_G(v_i)\setminus e_1$ from v_i to v_k if $3 \le i \le k-1$, and the hypergraph obtained from G by moving each edge of $E_G(v_i)\setminus e_2$ from v_i to v_k if $k+1 \le i \le 2k-2$. Obviously, G' is a unicyclic hypergraph of size m and $G' \ncong C^k_2(m-2,0)$. By similar argument as above, we have $\rho(G) > \rho(G')$, a contradiction. Thus $m_i = 0$ for $i \in \{j : 3 \le j \le 2k-2 \text{ and } j \ne k\}$.

Since $m_i = 0$ for $1 \le i \le 2k-2$ with $i \ne 2$, we have $G \cong F^k_2(m-2)$. Obviously, $C^k_3(m-3,0,0)$ is a unicyclic hypergraph of size m and it is not isomorphic to $C^k_2(m-2,0)$. By Lemma 4.6 (i), $\rho(G) > \rho(C^k_3(m-3,0,0))$, a contradiction. Now we have $m_2 = 0$.

Suppose that $m_k \ge 1$. Note that $m_1 \ge m_k$ and $m_1 + m_k = m-2$. By similar argument as in Claim 2 in the proof of Theorem 4.1, both H_1 and H_k are k-uniform hyperstars with centers v_1 and v_k, respectively. Then $G \cong C^k_2(m_1, m_k)$. By Lemma 4.4, we have $G \cong C^k_2(m-3,1)$. Now by Theorem 3.2, $\rho(G) > \rho(C^k_3(m-3,0,0))$, a contradiction. It follows that $m_k = 0$.

Let u_0 be the vertex in $V(H_1)$ such that $d_G(u_0, v_1)$ is as large as possible. Let $p = d_G(u_0, v_1)$. Since $m_2 = m_k = 0$ and $G \not\cong C_2^k(m-2, 0)$, we have $p \geq 2$. Let $(u_0, e_1', u_1, \dots, e_p', u_p)$ be the unique path connecting u_0 and v_1 in H_1, where $u_p = v_1$. Note that e_1' is a pendant edge at u_1. Let $e_p' = \{w_1, \dots, w_k\}$, where $w_{k-1} = u_{p-1}$ and $w_k = u_p$. Let W_j be the component of $G - e_p'$ containing w_j for $1 \leq j \leq k-1$. Then $G = H_{e_p',0}(W_1, \dots, W_{k-1})$, where $H = G[V(G) \setminus \cup_{j=1}^{k-1}(V(W_j) \setminus \{w_j\})]$. Note that $|E(W_{k-1})| \geq 1$.

Suppose that $p \geq 3$. Let $G' = H_{e_p',k-1}(W_1, \dots, W_{k-1})$. Obviously, G' is a k-uniform unicyclic hypergraph of size m and $G' \not\cong C_2^k(m-2, 0)$. By Lemma 2.2, we have $\rho(G) > \rho(G')$, a contradiction. Thus $p = 2$, implying that W_i is a k-uniform hyperstar with center w_i for $2 \leq i \leq k-1$.

Let G'' be the hypergraph obtained from G by moving e_1 from v_k to $w_{k-1} (= u_1)$. Let $x = x(G'')$. By Lemma 2.1, the entry of x corresponding to each vertex of $e_1' \setminus \{w_{k-1}\}$ is the same. Let $z_0 \in e_1' \setminus \{w_{k-1}\}$. From the eigenequations of G'' at z_0, w_{k-1} and v_k, we have $\rho(G'')\left(2x_{z_0} + x_{w_{k-1}} - x_{v_k}\right) \geq -2x_{z_0} + 8x_{v_k}$. Then $(\rho(G'') + 1)\left(2x_{z_0} + x_{w_{k-1}} - x_{v_k}\right) \geq x_{w_{k-1}} + 7x_{v_k} > 0$. Thus $2x_{z_0} + x_{w_{k-1}} - x_{v_k} > 0$.

As we pass from G to G'', the distance between a vertex of $e_1 \setminus \{v_1, v_k\}$ and a vertex of $V(W_{k-1})$ is decreased by 1, the distance between a vertex of $e_1 \setminus \{v_1, v_k\}$ and v_k is increased by 1, and the distance between any other vertex pair remains unchanged. Then

$$
\begin{aligned}
\frac{1}{2}(\rho(G) - \rho(G'')) &\geq \frac{1}{2}x^\top (D(G) - D(G''))x \\
&= \sigma_{G''}(e_1 \setminus \{v_1, v_k\})\,(\sigma_{G''}(V(W_{k-1})) - x_{v_k}) \\
&\geq \sigma_{G''}(e_1 \setminus \{v_1, v_k\})\,(\sigma_{G''}(e_1') - x_{v_k}) \\
&\geq \sigma_{G''}(e_1 \setminus \{v_1, v_k\})\left((k-1)x_{z_0} + x_{w_{k-1}} - x_{v_k}\right) \\
&\geq \sigma_{G''}(e_1 \setminus \{v_1, v_k\})\left(2x_{z_0} + x_{w_{k-1}} - x_{v_k}\right) \\
&> 0.
\end{aligned}
$$

Thus $\rho(G) > \rho(G'')$, also a contradiction. Now Claim 3 follows.

By Claim 3, g is odd. By Claims 1 and 2, $G \cong C_g^k(t_1, \dots, t_g)$ with $t_1 = \max_{1 \leq i \leq g} t_i$ and $\sum_{i=1}^g t_i + g = m$. Suppose that $g \geq 5$. Let $G^* = C_{g-2}^k(t_1 + t_2 + t_g + 2, t_3, \dots, t_{g-1})$. Obviously, G^* is a k-uniform unicyclic hypergraph of size m and $G^* \not\cong C_2^k(m-2, 0)$. By Corollary 3.1, we have $\rho(G) > \rho(G^*)$, a contradiction. It follows that $g = 3$. Therefore we have $G \cong C_3^k(t_1, t_2, t_3)$ with $t_1 \geq t_2 \geq t_3 \geq 0$ and $t_1 + t_2 + t_3 = m - 3$. By Lemma 4.3 (i), we have $t_1 = m - 3$ and $t_2 = t_3 = 0$, i.e., $G \cong C_3^k(m-3, 0, 0)$. □

5 Maximum distance spectral radius of uniform unicyclic hypergraphs

In this section, we discuss the unique hypergraphs with maximum distance spectral radius in the set of k-uniform unicyclic hypergraphs of fixed size.

Lemma 5.1. *For $k \geq 4$, let G be a k-uniform unicyclic hypergraph with cycle length 2. Let e be an edge on the cycle of G containing two vertices u and v of degree 1. For $p \geq q \geq 1$, $\rho(G_{u,v}(p,q)) < \rho(G_{u,v}(p+1,q-1))$.*

Proof. Let $H = G_{u,v}(p,q)$. Let C be the cycle of G with edges $e = e_1 = \{v_1, \dots, v_k\}$ and $e_2 = \{v_k, \dots, v_{2k-1}\}$, where $v_{2k-1} = v_1$. Let H_i be the component of $H - E(C)$ containing v_i for $1 \leq i \leq 2k-2$. We may assume $u = v_2$ and $v = v_{k-1}$. Let $H_2 = (v_2, e_1', u_1, \dots, u_{p-1}, e_p', u_p)$ and $H_{k-1} = (v_{k-1}, e_1'', y_1, \dots, y_{q-1}, e_q'', y_q)$, where $e_1' = \{v_2, u_1, w_1, \dots, w_{k-2}\}$ and $e_1'' = \{v_{k-1}, y_1, w_1', \dots, w_{k-2}'\}$.

Let $x = x(H)$. Suppose that $\sigma_H(V(H_2)) \geq \sigma_H(V(H_{k-1}))$. Let $l_i = |E(H_i)|$ for $1 \leq i \leq 2k-2$. Let $I = \{i : l_i \geq 1, 3 \leq i \leq k-2\}$. Let H' be the k-uniform hypergraph obtained from H by moving each edge of $E_H(v_i) \setminus e_1$ from v_i to w_{i-2}' for all $i \in I$, moving each edge of $E_H(v_1) \setminus e_1$ from v_1 to w_{k-3}', and moving each edge of $E_H(v_k) \setminus e_1$ from v_k to w_{k-2}'. It is easily seen that $H' \cong G_{u,v}(p+1, q-1)$.

As we pass from H to H', for $i \in I$, the distance between a vertex of $V(H_i) \setminus \{v_i\}$ and a vertex of $V(H_2) \cup (e_1 \setminus \{v_2, v_i, v_{k-1}\})$ is increased by 1, the distance between a vertex of $V(H_i) \setminus \{v_i\}$ and v_i is increased by 2, the distance between a vertex of $V(H_i) \setminus \{v_i\}$ and a vertex of $V(H_{k-1}) \setminus \{v_{k-1}, w_{i-2}'\}$ is decreased by 1, and the distance between a vertex of $V(H_i) \setminus \{v_i\}$ and w_{i-2}' is decreased by 2, the distance between a vertex of $V(H_1) \setminus \{v_1\}$ and a vertex of $V(H_2) \cup (e_1 \setminus \{v_1, v_2, v_{k-1}\})$ is increased by 1, the distance between a vertex of $V(H_1) \setminus \{v_1\}$ and v_1 is increased by 2, the distance between a vertex of $V(H_1) \setminus \{v_1\}$ and a vertex of $V(H_{k-1}) \setminus \{v_{k-1}, w_{k-3}'\}$ is decreased by 1, the distance between a vertex of $V(H_1) \setminus \{v_1\}$ and w_{k-3}' is decreased by 2, the distance between a vertex of $V(H_k) \setminus \{v_k\}$ and a vertex of $V(H_2) \cup (e_1 \setminus \{v_2, v_{k-1}, v_k\})$ is increased by 1, the distance between a vertex of $V(H_k) \setminus \{v_k\}$ and v_k is increased by 2, the distance between a vertex of $V(H_k) \setminus \{v_k\}$ and a vertex of $V(H_{k-1}) \setminus \{v_{k-1}, w_{k-2}'\}$ is decreased by 1, the distance between a vertex of $V(H_k) \setminus \{v_k\}$ and w_{k-2}' is decreased by 2, the distance between a vertex of $\bigcup_{i=k+1}^{2k-2} V(H_i)$ and a vertex of $V(H_2) \cup (e_1 \setminus \{v_1, v_{k-1}, v_k\})$ is increased by 1, the distance between a vertex of $\bigcup_{i=k+1}^{2k-2} V(H_i)$ and a vertex of $\{v_1, v_k\}$ is increased by 2, the distance between a vertex of $\bigcup_{i=k+1}^{2k-2} V(H_i)$ and a vertex of $V(H_{k-1}) \setminus \{v_{k-1}, w_{k-3}', w_{k-2}'\}$ is decreased by 1, the distance between a vertex of $\bigcup_{i=k+1}^{2k-2} V(H_i)$ and a vertex of $\{w_{k-3}', w_{k-2}'\}$ is decreased by 2, and the distance between any other vertex pair remains unchanged. Note that $\sigma_H(e_1) \geq x_{v_1} + x_{v_2} + x_{v_{k-1}} + x_{v_k}$. Let $A = \bigcup_{i=k+1}^{2k-2} V(H_i)$. Then

$$
\begin{aligned}
& \frac{1}{2}(\rho(H') - \rho(H)) \\
\geq\ & \frac{1}{2} x^\top (D(H') - D(H)) x \\
=\ & \sum_{i \in I} \sigma_H(V(H_i) \setminus \{v_i\}) \Big[\sigma_H(V(H_2)) + \big(\sigma_H(e_1) - x_{v_2} - x_{v_i} - x_{v_{k-1}}\big) + 2x_{v_i} \\
& - \Big(\sigma_H(V(H_{k-1})) - x_{v_{k-1}} - x_{w_{i-2}'}\Big) - 2x_{w_{i-2}'} \Big] \\
& + \sigma_H(V(H_1) \setminus \{v_1\}) \Big[\sigma_H(V(H_2)) + \big(\sigma_H(e_1) - x_{v_1} - x_{v_2} - x_{v_{k-1}}\big) + 2x_{v_1}
\end{aligned}
$$

$$
\begin{aligned}
&-\Big(\sigma_H(V(H_{k-1}))-x_{v_{k-1}}-x_{w'_{k-3}}\Big)-2x_{w'_{k-3}}\Big]\\
&+\sigma_H(V(H_k)\setminus\{v_k\})\Big[\sigma_H(V(H_2))+\big(\sigma_H(e_1)-x_{v_2}-x_{v_{k-1}}-x_{v_k}\big)+2x_{v_k}\\
&-\Big(\sigma_H(V(H_{k-1}))-x_{v_{k-1}}-x_{w'_{k-2}}\Big)-2x_{w'_{k-2}}\Big]\\
&+\sigma_H(A)\Big[\sigma_H(V(H_2))+\big(\sigma_H(e_1)-x_{v_1}-x_{v_{k-1}}-x_{v_k}\big)+2x_{v_1}+2x_{v_k}\\
&-\Big(\sigma_H(V(H_{k-1}))-x_{v_{k-1}}-x_{w'_{k-3}}-x_{w'_{k-2}}\Big)-2x_{w'_{k-3}}-2x_{w'_{k-2}}\Big]\\
= &\sum_{i\in I}\sigma_H(V(H_i)\setminus\{v_i\})\Big(\sigma_H(V(H_2))-\sigma_H(V(H_{k-1}))+(\sigma_H(e_1)-x_{v_2})+x_{v_i}-x_{w'_{i-2}}\Big)\\
&+\sigma_H(V(H_1)\setminus\{v_1\})\Big(\sigma_H(V(H_2))-\sigma_H(V(H_{k-1}))+(\sigma_H(e_1)-x_{v_2})+x_{v_1}-x_{w'_{k-3}}\Big)\\
&+\sigma_H(V(H_k)\setminus\{v_k\})\Big(\sigma_H(V(H_2))-\sigma_H(V(H_{k-1}))+(\sigma_H(e_1)-x_{v_2})+x_{v_k}-x_{w'_{k-2}}\Big)\\
&+\sigma_H(A)\Big(\sigma_H(V(H_2))-\sigma_H(V(H_{k-1}))+\sigma_H(e_1)+x_{v_1}+x_{v_k}-x_{w'_{k-3}}-x_{w'_{k-2}}\Big)\\
> &\sum_{i\in I}\sigma_H(V(H_i)\setminus\{v_i\})\Big(\sigma_H(V(H_2))-\sigma_H(V(H_{k-1}))+x_{v_i}+x_{v_{k-1}}-x_{w'_{i-2}}\Big)\\
&+\sigma_H(V(H_1)\setminus\{v_1\})\Big(\sigma_H(V(H_2))-\sigma_H(V(H_{k-1}))+x_{v_1}+x_{v_{k-1}}-x_{w'_{k-3}}\Big)\\
&+\sigma_H(V(H_k)\setminus\{v_k\})\Big(\sigma_H(V(H_2))-\sigma_H(V(H_{k-1}))+x_{v_k}+x_{v_{k-1}}-x_{w'_{k-2}}\Big)\\
&+\sigma_H(A)\Big(\sigma_H(V(H_2))-\sigma_H(V(H_{k-1}))+x_{v_1}+x_{v_2}+x_{v_{k-1}}+x_{v_k}-x_{w'_{k-3}}-x_{w'_{k-2}}\Big),
\end{aligned}
$$

and thus

$$
\begin{aligned}
&\frac{1}{2}(\rho(H')-\rho(H))\\
\geq &\sum_{i\in I}\sigma_H(V(H_i)\setminus\{v_i\})\Big(x_{v_i}+x_{v_{k-1}}-x_{w'_{i-2}}\Big)\\
&+\sigma_H(V(H_1)\setminus\{v_1\})\Big(x_{v_1}+x_{v_{k-1}}-x_{w'_{k-3}}\Big) \qquad (5.1)\\
&+\sigma_H(V(H_k)\setminus\{v_k\})\Big(x_{v_k}+x_{v_{k-1}}-x_{w'_{k-2}}\Big)\\
&+\sigma_H(A)\Big(x_{v_1}+x_{v_2}+x_{v_{k-1}}+x_{v_k}-x_{w'_{k-3}}-x_{w'_{k-2}}\Big).
\end{aligned}
$$

For $w\in W=V(H)\setminus\{v_i,v_{k-1},w'_{i-2}\}$ with $3\leq i\leq k-2$, we have $d_H(v_i,w)+d_H(v_{k-1},w)-d_H(w'_{i-2},w)\geq 0$. From the eigenequations of H at v_i,v_{k-1} and w'_{i-2}, we have

$$
\begin{aligned}
&\rho(H)(x_{v_i}+x_{v_{k-1}}-x_{w'_{i-2}})\\
\geq\ &-x_{v_i}+3x_{w'_{i-2}}+\sum_{w\in W}(d_H(v_i,w)+d_H(v_{k-1},w)-d_H(w'_{i-2},w))x_w\\
\geq\ &-x_{v_i}+3x_{w'_{i-2}},
\end{aligned}
$$

implying that $(\rho(H)+1)(x_{v_i}+x_{v_{k-1}}-x_{w'_{i-2}}) \geq x_{v_{k-1}}+2x_{w'_{i-2}} > 0$, and thus $x_{v_i}+x_{v_{k-1}}-x_{w'_{i-2}} > 0$. Similarly, we have $x_{v_1}+x_{v_{k-1}}-x_{w'_{k-3}} > 0$, $x_{v_k}+x_{v_{k-1}}-x_{w'_{k-2}} > 0$ and $x_{v_1}+x_{v_2}+x_{v_{k-1}}+x_{v_k}-x_{w'_{k-3}}-x_{w'_{k-2}} > 0$. Thus by (5.1),

$$\frac{1}{2}(\rho(H')-\rho(H)) \geq \sigma_H(A)\left(x_{v_1}+x_{v_2}+x_{v_{k-1}}+x_{v_k}-x_{w'_{k-3}}-x_{w'_{k-2}}\right) > 0.$$

It follows that $\rho(H) < \rho(H')$.

Suppose that $\sigma_H(V(H_2)) < \sigma_H(V(H_{k-1}))$. Let H'' be the k-uniform hypergraph obtained from H by moving each edge of $E_H(v_i) \setminus e_1$ from v_i to w_{i-2} for all $3 \leq i \leq k-2$, moving each edge of $E_H(v_1) \setminus e_1$ from v_1 to w_{k-3}, and moving each edge of $E_H(v_k) \setminus e_1$ from v_k to w_{k-2}. It is easily seen that $H'' \cong G_{u,v}(p-1, q+1)$. By similar argument as above, we have $\rho(H) < \rho(H'')$.

Now we have proved that

$$\rho(G_{u,v}(p,q)) < \max\{\rho(G_{u,v}(p+1,q-1)), \rho(G_{u,v}(p-1,q+1))\}. \tag{5.2}$$

If $p = q$, then the result follows easily. Suppose that $p > q$. Suppose that $\rho(G_{u,v}(p,q)) < \rho(G_{u,v}(p-1,q+1))$. Note that $G_{u,v}(\lceil \frac{p+q+1}{2} \rceil, \lfloor \frac{p+q-1}{2} \rfloor) \cong G_{u,v}(\lfloor \frac{p+q-1}{2} \rfloor, \lceil \frac{p+q+1}{2} \rceil)$. Using (5.2) repeatedly, we have

$$\begin{aligned}\rho(G_{u,v}(p,q)) &\leq \rho\left(G_{u,v}\left(\left\lceil \frac{p+q+1}{2} \right\rceil, \left\lfloor \frac{p+q-1}{2} \right\rfloor\right)\right) \\ &< \rho\left(G_{u,v}\left(\left\lfloor \frac{p+q-1}{2} \right\rfloor, \left\lceil \frac{p+q+1}{2} \right\rceil\right)\right),\end{aligned}$$

which is impossible. Thus $\rho(G_{u,v}(p,q)) < \rho(G_{u,v}(p+1,q-1))$, as desired. □

For $k \geq 3$, let $\widetilde{C}_2^k(l_1, l_2) = G_{v_2,v_{k+1}}(l_1, l_2)$, where $G = C_{2k-2,k}$ and $l_1 \geq l_2 \geq 0$.

Theorem 5.1. *For $k \geq 3$, let G be a k-uniform unicyclic hypergraph of size $m \geq 2$ with maximum distance spectral radius. Then $G \cong \widetilde{C}_2^k(l_1, l_2)$, where $l_1 \geq l_2 \geq 0$ and $l_1 + l_2 + 2 = m$.*

Proof. It is trivial if $m = 2$. Suppose that $m \geq 3$. By Theorem 3.2, the cycle length of G is 2. Let C be the unique cycle with edges $e_1 = \{v_1, \dots, v_k\}$ and $e_2 = \{v_k, \dots, v_{2k-1}\}$, where $v_{2k-1} = v_1$. Let H_i be the component of $G - E(C)$ containing v_i, which is a k-uniform hypertree, where $1 \leq i \leq 2k-2$. Then $G \cong C_{2k-2}^k(H_1, \dots, H_{2k-2})$. Let $x = x(G)$.

Claim 1. $|V(H_1)| = |V(H_k)| = 1$.

Suppose that there is at least one edge in H_1. We may assume $\sigma_G\left(\bigcup_{i=2}^{k-1} V(H_i)\right) \geq \sigma_G\left(\bigcup_{i=k+1}^{2k-2} V(H_i)\right)$. Let G' be the k-uniform hypergraph obtained from G by moving each edge of $E_G(v_1) \setminus \{e_1, e_2\}$ from v_1 to v_{2k-2}. As we pass from G to G', the distance between a vertex of $V(H_1) \setminus \{v_1\}$ and a vertex of $\{v_1\} \cup \left(\bigcup_{i=2}^{k-1} V(H_i)\right)$ is increased by 1, the distance between a vertex of $V(H_1) \setminus \{v_1\}$ and a vertex of $V(H_{2k-2})$ is decreased by 1, and the distance between any other vertex pair remains unchanged. Then

$$\frac{1}{2}(\rho(G')-\rho(G)) \geq \frac{1}{2}x^\top(D(G')-D(G))x$$

$$
\begin{aligned}
&= \sigma_G(V(H_1)\setminus\{v_1\})\left(x_{v_1}+\sigma_G\left(\bigcup_{i=2}^{k-1}V(H_i)\right)-\sigma_G(V(H_{2k-2}))\right)\\
&> \sigma_G(V(H_1)\setminus\{v_1\})\left(\sigma_G\left(\bigcup_{i=2}^{k-1}V(H_i)\right)-\sigma_G\left(\bigcup_{i=k+1}^{2k-2}V(H_i)\right)\right)\\
&\geq 0,
\end{aligned}
$$

and thus $\rho(G')>\rho(G)$, a contradiction. Therefore $|V(H_1)|=1$. Similarly, we have $|V(H_k)|=1$. Claim 1 follows.

Claim 2. Each H_i with $|V(H_i)|>1$ is a pendant path at v_i, where $2\leq i\leq 2k-2$ and $i\neq k$.

Suppose that $d_{H_i}(v_i)\geq 2$. Let $U_1,\ldots,U_{d_{H_i}(v_i)}$ be the vertex-disjoint subhypergraphs of H_i-v_i with $\cup_{j=1}^{d_{H_i}(v_i)}V(U_j)=V(H_i)\setminus\{v_i\}$ such that $H_i[V(U_j)\cup\{v_i\}]$ is a k-uniform hypertree for $1\leq j\leq d_{H_i}(v_i)$. Note that $d_{H_i}(w)=d_G(w)$ for each $w\in V(U_j)$, where $1\leq j\leq d_{H_i}(v_i)$.

Suppose that there is one vertex of degree at least 3 in $V(U_j)$ for some j with $1\leq j\leq d_{H_i}(v_i)$. Choose a vertex u of degree at least 3 such that $d_G(v_i,u)$ is as large as possible. Let $N_1,\ldots,N_{d_G(u)}$ be the vertex-disjoint subhypergraphs of $G-u$ with $\cup_{l=1}^{d_G(u)}V(N_j)=V(G)\setminus\{u\}$ such that $G[V(N_1)\cup\{u\}]$ is a k-uniform unicyclic hypergraph and $G[V(N_l)\cup\{u\}]$ is a k-uniform hypertree for $2\leq l\leq d_G(u)$.

Suppose that $G[V(N_l)\cup\{u\}]$ is not a pendant path at u for some l with $2\leq l\leq d_G(u)$. Then there are at least three vertices of degree 2 in some edge of $E(G[V(N_l)\cup\{u\}])$. We choose such an edge $e=\{w_1,\ldots,w_k\}$ by requiring that $d_G(u,w_1)$ is as large as possible, where $d_G(u,w_1)=d_G(u,w_r)-1$ for $2\leq r\leq k$. Then there are two pendant paths, say P and Q with lengths p and Q at different vertices w_s and w_t of e respectively, where $2\leq s<t\leq k$. We may assume that $p\geq q$. Then $G\cong F_{w_s,w_t}(p,q)$, where $F=G[V(G)\setminus(V(P\cup Q)\setminus\{w_s,w_t\})]$. Obviously, $d_F(w_s)=d_F(w_t)=1$ and $G''=F_{w_s,w_t}(p+1,q-1)$ is a k-uniform unicyclic hypergraph of size m. By Lemma 2.4, we have $\rho(G)<\rho(G'')$, a contradiction. Thus for each l with $2\leq l\leq d_G(u)$, $G[V(N_l)\cup\{u\}]$ is a pendant path at u, the length of which is denoted by p_l. We may assume that $p_2\geq p_3$. Then $G\cong N_u(p_2,p_3)$, where $N=G[V(G)\setminus V(N_2\cup N_3)]$. Obviously, $G^*=N_u(p_2+1,p_3-1)$ is a k-uniform unicyclic hypergraph of size m. By Lemma 2.3, we have $\rho(G)<\rho(G^*)$, a contradiction. Thus for $1\leq j\leq d_{H_i}(v_i)$, each vertex of $V(U_j)$ is of degree at most 2.

By similar argument as above, there is no edge in $E(G[V(U_j)\cup\{v_i\}])$ with at least three vertices of degree 2, and thus $G[V(U_j)\cup\{v_i\}]$ is a pendant path at v_i for $1\leq j\leq d_{H_i}(v_i)$. Let q_j be the length of $G[V(U_j)\cup\{v_i\}]$, where $1\leq j\leq d_{H_i}(v_i)$. We may assume that $q_1\geq q_2$. Then $G\cong\widetilde{N}_{v_i}(q_1,q_2)$, where $\widetilde{N}=G[V(G)\setminus V(U_1\cup U_2)]$. Obviously, $G^{**}=\widetilde{N}_{v_i}(q_1+1,q_2-1)$ is a k-uniform unicyclic hypergraph of size m. By Lemma 2.3, we have $\rho(G)<\rho(G^{**})$, a contradiction. Therefore $d_{H_i}(v_i)=1$.

By similar argument as above, each vertex of $V(H_i)\setminus\{v_i\}$ is of degree at most 2, and there is at most two vertices of degree at least 2 in each edge of $E(H_i)$, Thus H_i is a pendant path at v_i in G. This proves Claim 2.

By Claims 1 and 2, $|V(H_1)|=|V(H_k)|=1$ and each H_i with $|V(H_i)|>1$ is a pendant path at v_i, where $2\leq i\leq 2k-2$ and $i\neq k$. Let $m_i=|E(H_i)|$ for

$1 \leq i \leq 2k-2$. Then $m_1 = m_k = 0$.

If $k = 3$, then $G \cong \widetilde{C}_2^k(m_2, m_4)$ with $m_2 + m_4 + 2 = m$, and thus the result follows.

Suppose that $k \geq 4$. Suppose that there exist at least two integers i and j with $2 \leq i < j \leq k-1$ such that $m_i \geq m_j \geq 1$. Then by Claims 2, we have $G \cong H_{v_i,v_j}(m_i, m_j)$, where $H = G[V(G) \setminus (V(H_i \cup H_j) \setminus \{v_i, v_j\})]$. Let $G' = H_{v_i,v_j}(m_i+1, m_j-1)$. By Lemma 5.1, $\rho(G) < \rho(G')$, a contradiction. Thus there exists at most one integer i with $2 \leq i \leq k-1$ such that $m_i \geq 1$. Similarly, there exists at most one integer j with $k+1 \leq j \leq 2k-2$ such that $m_j \geq 1$. Thus $G \cong \widetilde{C}_2^k(m_i, m_j)$ with $2 \leq i \leq k-1$, $k+1 \leq j \leq 2k-2$ and $m_i + m_j + 2 = m$, and the result follows. □

By direct calculation, we list $\rho\left(\widetilde{C}_2^k(l_1, l_2)\right)$ for $k = 3, 4$ and $l_1 + l_2 = 2, 3, 4$ in Table 1.

Table 1: $\rho\left(\widetilde{C}_2^k(l_1, l_2)\right)$ for $k = 3, 4$ and $l_1 + l_2 = 2, 3, 4$.

G	$\widetilde{C}_2^3(1,1)$	$\widetilde{C}_2^3(2,0)$	$\widetilde{C}_2^3(2,1)$	$\widetilde{C}_2^3(3,0)$	$\widetilde{C}_2^3(2,2)$	$\widetilde{C}_2^3(3,1)$	$\widetilde{C}_2^3(4,0)$
$\rho(G)$	14.7150	14.1580	22.3219	21.4508	31.5138	31.2036	30.1133
G	$\widetilde{C}_2^4(1,1)$	$\widetilde{C}_2^4(2,0)$	$\widetilde{C}_2^4(2,1)$	$\widetilde{C}_2^4(3,0)$	$\widetilde{C}_2^4(2,2)$	$\widetilde{C}_2^4(3,1)$	$\widetilde{C}_2^4(4,0)$
$\rho(G)$	23.2481	23.8118	35.5228	34.6496	49.5106	49.1982	48.1116

Based on Table 1, we conjecture that $\rho\left(\widetilde{C}_2^k\left(\lceil \frac{m}{2} \rceil - 1, \lfloor \frac{m}{2} \rfloor - 1\right)\right) > \rho\left(\widetilde{C}_2^k(l_1, l_2)\right)$ for l_1 and l_2 with $l_1 + l_1 + 2 = m$ and $(l_1, l_2) \neq \left(\lceil \frac{m}{2} \rceil - 1, \lfloor \frac{m}{2} \rfloor - 1\right)$. If this is proved, then by Theorem 5.1, $\widetilde{C}_2^k\left(\lceil \frac{m}{2} \rceil - 1, \lfloor \frac{m}{2} \rfloor - 1\right)$ is the unique k-uniform unicyclic hypergraph of size $m \geq 2$ with maximum distance spectral radius for $k \geq 3$.

Acknowledgement. This work was supported by the National Natural Science Foundation of China (No. 11671156), the Postdoctoral Science Foundation of China (No. 2017M621066) and the Scientific Research Fund of the Science and Technology Program of Guangzhou, China (No. 201510010265). We thank the references for helpful suggestions and comments.

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