Research Article

On the Maximum Estrada Index of 3-Uniform Linear Hypertrees

Faxu Li,^{1,2} Liang Wei,³ Jinde Cao,^{4,5} Feng Hu,^{1,2} and Haixing Zhao²

¹ School of Computer Science, Shaanxi Normal University, Xi'an 710062, China

² College of Computer, Qinghai Normal University, Xining 810008, China

³ Department of Mathematics, Qinghai Normal University, Xining 810008, China

⁴ Department of Mathematics, Southeast University, Nanjing 210096, China

⁵ Department of Mathematics, Faculty of Science, King Abdulaziz University, Jeddah 21589, Saudi Arabia

Correspondence should be addressed to Haixing Zhao; h.x.zhao@163.com

Received 3 July 2014; Accepted 12 August 2014; Published 28 August 2014

Academic Editor: Jianlong Qiu

Copyright © 2014 Faxu Li et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

For a simple hypergraph H on n vertices, its Estrada index is defined as $EE(H) = \sum_{i=1}^n e^{\lambda_i}$, where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of its adjacency matrix. In this paper, we determine the unique 3-uniform linear hypertree with the maximum Estrada index.

1. Introduction

Let $G = (V, E)$ be a simple graph, and let n and m be the number of vertices and the number of edges of G , respectively. The characteristic polynomial of a graph G is written as $P(G, \lambda) = \det(\lambda I - A(G))$, where $A(G)$ is the adjacency matrix of G . The eigenvalues of G are the eigenvalues of its adjacency matrix $A(G)$, which are denoted by $\lambda_1, \lambda_2, \dots, \lambda_n$. A graph-spectrum-based invariant, nowadays named Estrada index, proposed by Estrada in 2000, is defined as [1]

$$EE(G) = \sum_{i=1}^n e^{\lambda_i}. \quad (1)$$

Since then, the Estrada index has already found remarkable applications in biology, chemistry, and complex networks [2–5]. Some mathematical properties of the Estrada index, especially bounds for it have been established in [6–15]. For more results on the Estrada index, the readers are referred to recent papers [16–19].

Let $H = (V, \mathcal{E})$ be a simple and finite hypergraph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and hyperedge set $\mathcal{E}(G) = \{E_1, E_2, \dots, E_m\}$. The hypergraph H is called linear if two hyperedges intersect in one vertex at most and also h -uniform if $|E_i| = h$ for each E_i in $\mathcal{E}$, $i = 1, 2, \dots, m$. An h -uniform hypertree is a connected linear h -hypergraph without cycles. An h -uniform linear hypertree is called 3-uniform linear

hypertree if h is equal to 3. Denoted by $\mathcal{S}_m^h$ an h -uniform linear star with m hyperedges. More details on hypergraphs can be found in [20].

Let $A(H)$ denote a square symmetric matrix in which the diagonal elements a_{ii} are zero, and other elements a_{ij} represent the number of hyperedges containing both vertices v_i and v_j (for undirected hypergraphs, $a_{ij} = a_{ji}$). Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of $A(H)$ of H . The subhypergraph centrality of a hypergraph H , firstly put forward by Estrada and Rodríguez-Velázquez in 2006, is defined as [21]

$$\langle C_{SH} \rangle = \frac{1}{n} \sum_{i=1}^n C_{SH}(i) = \frac{1}{n} \sum_{i=1}^n e^{\lambda_i}. \quad (2)$$

They revealed that the subhypergraph centrality provides a measure of the centrality of complex hypernetworks (social, reaction, metabolic, protein, food web, etc). For convenience, we call the subhypergraph centrality of a hypergraph its Estrada index and define the Estrada index as

$$EE(H) = \sum_{i=1}^n e^{\lambda_i}. \quad (3)$$

Thus far, results on the Estrada index of hypergraph seem to be few although the Estrada index of graph has numerous applications. So our main goal is to investigate the Estrada index of 3-uniform linear hypertrees. In this paper,

FIGURE 1: A 3-uniform linear hypertree H and its completely connected graph G_H .

we determine the unique 3-uniform linear hypertree with the maximum Estrada index among the set of 3-uniform linear hypertrees.

2. Preliminaries

For a hypergraph H of order n , its completely connected graph, denoted by G_H , is a graph which has the same order and in which two vertices are adjacent if they share one hyperedge. Obviously, G_H is a multigraph. For an h -uniform linear hypergraph H , G_H is a simple graph. According to the definition of adjacency matrix of hypergraph, it is easy to see that both a 3-uniform linear hypertree H and its completely connected graph G_H have the same adjacency matrix; see Figure 1. Then, they have the identical Estrada index. Thus, we investigate the Estrada index of its completely connected graphs instead of the 3-uniform linear hypertrees in this paper.

We use $M_k(G) = \sum_{i=1}^n \lambda_i^k$ to denote the k th spectral moment of the graph G . It is well-known [22] that $M_k(G)$ is equal to the number of closed walks of length k in G . Obviously, for any graph G , $M_0(G) = n$, $M_1(G) = 0$, $M_2(G) = 2m$, $M_3(G) = 6t$, and $M_4(G) = 2 \sum_{i=1}^n d_i^2 - 2m + 8q$, where t , q , and $d_i = d_G(v_i)$ are the number of triangles, the number of quadrangles, and the degree of vertex v_i in graph G , respectively. Then

$$EE(G) = \sum_{i=1}^n \sum_{k=0}^{\infty} \frac{\lambda_i^k}{k!} = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}. \quad (4)$$

For $u, v \in V(G)$, denote by $\mathcal{W}_k(G; u, v)$ the set of (u, v) -walks of length k in G . Obviously, $M_k(G; u, v) = |\mathcal{W}_k(G; u, v)|$. For convenience, let $\mathcal{W}_k(G; u) = \mathcal{W}_k(G; u, u)$ and $M_k(G; u) = M_k(G; u, u)$. Let W be a (u, v) -walk in graph G ; we denote by W^{-1} a (v, u) -walk obtained from W by reversing W .

For any two graphs G_1 and G_2 , if $M_k(G_1) \geq M_k(G_2)$ for all integers $k > 0$, then $EE(G_1) \geq EE(G_2)$. Moreover, if the strict inequality $M_k(G_1) > M_k(G_2)$ holds for at least one value $k > 0$, then $EE(G_1) > EE(G_2)$.

Denote by $\Gamma(n, m)$ the set of connected graphs on n vertices and m triangles such that any two triangles have a common vertex at most. Apparently, for a 3-uniform linear hypertree H on n vertices and m hyperedges, $G_H \in \Gamma(n, m)$. Now we study the Estrada index of a graph in $\Gamma(n, m)$.

FIGURE 2: The star S_m^3 on m triangles.

3. Maximum Estrada Index of 3-Uniform Linear Hypertrees

In this section, we determine the maximum value of Estrada index among the set of 3-uniform linear hypertrees.

Lemma 1. Let S_m^3 be star which is the completely connected graph of $\mathcal{S}_m^3$ with m hyperedges. It is easily found that the star S_m^3 has n vertices labeled $v_1, v_2, v_3, \dots, v_n$ and $m = (n-1)/2$ triangles. Let k be a positive integer; then there is an injection ξ from $\mathcal{W}_k(S_m^3; v_2)$ to $\mathcal{W}_k(S_m^3; v_1)$, and ξ is not surjective for $n \geq 5$, $2 \leq m \leq (n-1)/2$, and $k > 1$, where $\mathcal{W}_k(S_m^3; v_2)$ and $\mathcal{W}_k(S_m^3; v_1)$ are the sets of closed walks of length k of v_2 and v_1 in S_m^3 , respectively; see Figure 2.

Proof. Firstly, we construct a mapping φ from $\mathcal{W}_k(S_m^3; v_2)$ to $\mathcal{W}_k(S_m^3; v_1)$. For $W \in \mathcal{W}_k(S_m^3; v_2)$, let $\varphi(W)$ be the closed walk obtained from W by replacing v_1 by v_2 and v_2 by v_1 . Obviously, $\varphi(W) \in \mathcal{W}_k(S_m^3; v_1)$ and φ is a bijection.

Secondly, we construct a mapping ξ from $\mathcal{W}_k(S_m^3; v_2)$ to $\mathcal{W}_k(S_m^3; v_1)$. For $W \in \mathcal{W}_k(S_m^3; v_2)$, we consider the following cases.

Case 1. Suppose W does not pass the edge $v_1 v_t$ for $t \geq 4$; then $\xi(W) = \varphi(W)$.

Case 2. Suppose W passes the edge $v_1 v_t$ for $t \geq 4$. For $W \in \mathcal{W}_k(S_m^3; v_2)$, we may uniquely decompose W into three sections $W_1 W_2 W_3$, where W_1 is the longest (v_2, v_1) -section of W without v_t , W_2 is the internal longest (v_t, v_t') -section of W for $t' \geq 4$, and the last W_3 is the remaining (v_1, v_2) -section of W not containing v_t . We consider the following three subcases.

FIGURE 3: Transformation I.

Case 2.1. If both W_1 and W_3 contain the vertex v_3 , we may uniquely decompose W_1 into two sections $W_{11}W_{12}$ and decompose W_3 into two sections $W_{31}W_{32}$, where W_{11} is the shortest (v_2, v_3) -section of W_1 , W_{12} is the remaining (v_3, v_1) -section of W_1 , W_{31} is the longest (v_1, v_3) -section of W_3 , and W_{32} is the remaining (v_3, v_2) -section of W_3 .

Let $\xi(W) = \xi(W_{11})\xi(W_{12})\xi(W_2)\xi(W_{31})\xi(W_{32})$, where $\xi(W_{12}) = W_{12}$, $\xi(W_2) = W_2$, $\xi(W_{31}) = W_{31}$, $\xi(W_{11})$ is a (v_1, v_3) -walk obtained from W_{11} replacing v_1 by v_2 and v_2 by v_1 , and $\xi(W_{32})$ is a (v_3, v_1) -walk obtained from W_{32} replacing v_1 by v_2 and v_2 by v_1 .

Case 2.2. If W_1 contains the vertex v_3 and W_3 does not contain v_3 , let $\xi(W) = \xi(W_1)\xi(W_2)\xi(W_3)$, where $\xi(W_2) = W_2$, $\xi(W_1)$ is a (v_1, v_1) -walk obtained from W_1 replacing its first vertex v_2 by v_1v_2 , and $\xi(W_3)$ is a (v_1, v_1) -walk obtained from W_3 replacing its last two vertices v_1v_2 by v_1 .

Case 2.3. If W_1 does not contain the vertex v_3 , let $\xi(W) = \xi(W_1)\xi(W_2)\xi(W_3)$, where $\xi(W_2) = W_2$, $\xi(W_1)$ is a (v_1, v_1) -walk obtained from W_1 replacing its first two vertices v_2v_1 by v_1 , and $\xi(W_3)$ is a (v_1, v_1) -walk obtained from W_3 replacing its last vertex v_2 by v_2v_1 .

For example, in star S_3^3 on 7 vertices and 3 triangles, $W = v_2v_3v_1v_2v_1v_3v_2$ is a closed walk of length 6 of v_2 not passing the edge v_1v_t . By Case 1, we have

$$\xi(W) = v_1v_3v_2v_1v_2v_3v_1. \quad (5)$$

$W' = v_2v_3v_1v_4v_5v_1v_6v_7v_1v_2$ is a closed walk of length 9 of v_2 passing the edge v_1v_t . By Case 2.2, we get

$$\xi(W') = v_1v_2v_3v_1v_4v_5v_1v_6v_7v_1. \quad (6)$$

$W'' = v_2v_1v_2v_1v_4v_5v_1v_2v_3v_1v_6v_7v_1v_3v_2$ is a closed walk of length 14 of v_2 passing the edge v_1v_t . By Case 2.3, we obtain

$$\xi(W'') = v_1v_2v_1v_4v_5v_1v_2v_3v_1v_6v_7v_1v_3v_2v_1. \quad (7)$$

Obviously, $\xi(W) \in \mathcal{W}_k(S_m^3; v_1)$, ξ is an injective and not a surjective for $n \geq 5$, and $k \geq 1$. $\square$

Lemma 2. Let u be a nonisolated vertex of a connected graph G . If G_1 and G_2 are the graphs obtained from G by identifying

an external vertex v_2 and the center vertex v_1 of the union of $S_m^3 \cup Q$ to u , respectively, where $|V(S_m^3)| = n$, Q is either empty graph or nonempty graph. Then $M_k(G_1) < M_k(G_2)$ for $n \geq 5$ and $k \geq 4$; see Figure 3.

Proof. Let $\mathcal{W}_k(G_i)$ ($\mathcal{W}_k(G)$, $\mathcal{W}_k(S_m^3 \cup Q)$, resp.) be the set of closed walks of length k of G_i (G , $S_m^3 \cup Q$, resp.) for $i = 1, 2$. Then $\mathcal{W}_k(G_i) = \mathcal{W}_k(G) \cup \mathcal{W}_k(S_m^3 \cup Q) \cup X_i$ is a partition, where X_i is the set of closed walks of length k of G_i ; each of them contains both at least one edge in $E(G)$ and at least one edge in $E(S_m^3 \cup Q)$. So $M_k(G_i) = |\mathcal{W}_k(G)| + |\mathcal{W}_k(S_m^3 \cup Q)| + |X_i| = M_k(G) + M_k(S_m^3 \cup Q) + |X_i|$. Thus we need to show the inequality $|X_1| < |X_2|$.

We construct a mapping η from X_1 to X_2 and consider the following four cases.

Case 1. Suppose W is a closed walk starting from $u \in V(G)$ in X_1 . For $W \in X_1$, let $\eta(W) = (W - W \cap (S_m^3 \cup Q)) \cup \xi(W \cap (S_m^3 \cup Q))$; that is, $\eta(W)$ is the closed walk in X_2 obtained from W by replacing its every section in $S_m^3 \cup Q$ with its image under the map ξ .

Case 2. Suppose W is a closed walk starting at v_1 in X_1 . For $W \in X_1$, we may uniquely decompose W into three sections $W_1W_2W_3$, where W_1 is the longest (v_1, v_2) -section of W without vertices $u_0, \dots, u_t'' \in V(G)$, W_2 is the internal longest (u_0, u_t'') -section of W (for which the internal vertices are some possible vertices in $V(G_1)$), and W_3 is the remaining (v_2, v_1) -section of W . Let $\eta(W) = \eta(W_1)\eta(W_2)\eta(W_3)$, where $\eta(W_1) = W_1^{-1}$, $\eta(W_3) = W_3^{-1}$, and $\eta(W_2) = (W_2 - W_2 \cap (S_m^3 \cup Q)) \cup \xi(W_2 \cap (S_m^3 \cup Q))$; that is, $\eta(W_2)$ is a (u_0, u_t'') -walk from W_2 by replacing its every section in $S_m^3 \cup Q$ with its image under the map ξ .

Case 3. Suppose W is a closed walk starting from v_3 or $w \in V(Q)$ in X_1 . For $W \in X_1$, we may uniquely decompose W into three sections $W_1W_2W_3$, where W_1 is the longest (v_3, v_2) (or (w, v_2))-section of W without vertices $u_0, \dots, u_t''$, W_2 is the internal longest (u_0, u_t'') -section of W (for which the internal vertices are some possible vertices in $V(G_1)$), and W_3 is the remaining (v_2, v_3) (or (v_2, w))-section of W without vertices $u_0, \dots, u_t''$. We have three subcases.

Case 3.1. If both W_1 and W_3 do not pass edge v_1v_t , let $\eta(W) = \eta(W_1)\eta(W_2)\eta(W_3)$, where $\eta(W_2) = (W_2 - W_2 \cap (S_m^3 \cup Q)) \cup \xi(W_2 \cap (S_m^3 \cup Q))$, $\eta(W_1)$ is a (v_3, v_1) (or (w, v_1))-walk obtained from W_1 replacing v_1 by v_2 and v_2 by v_1 , and $\eta(W_3)$ is a (v_1, v_3) (or (v_1, w))-walk obtained from W_3 replacing v_1 by v_2 and v_2 by v_1 .

Case 3.2. If both W_1 and W_3 pass edge v_1v_t , we may anew decompose W into five sections $W_1W_2W_3W_4W_5$, where W_1 is the longest (v_3, v_1) (or (w, v_1))-section of W (which do not contain vertices $u_0, \dots, u_t''$), W_2 is the second (v_1, v_2) -section of W (for which the internal vertices, if exist, are only possible $v_1, v_2, v_3, w \in V(Q)$), the third W_3 is the internal longest (u_0, u_t'') -section of W (for which the internal vertices are some possible vertices in $V(G_1)$), the fourth W_4 is the longest (v_2, v_1) -section of W (for which the internal vertices, if exist, are only possible $v_1, v_2, v_3, w \in V(Q)$), and the last W_5 is the remaining (v_t', v_3) (or (v_t, w))-section of W . We have three subsubcases.

Case 3.2.1. If both W_2 and W_4 contain the vertex v_3 , we may uniquely decompose W_2 into two sections $W_{21}W_{22}$ and W_4 into two sections $W_{41}W_{42}$, where W_{21} is the longest (v_1, v_3) -section of W_2 , W_{22} is the remaining shortest (v_3, v_2) of W_2 , W_{41} is the shortest (v_2, v_3) -section of W_4 , and W_{42} is the remaining longest (v_3, v_1) -section of W_4 .

Let $\eta(W) = \eta(W_1)\eta(W_{21})\eta(W_{22})\eta(W_3)\eta(W_{41})\eta(W_{42})\eta(W_5)$, where $\eta(W_1) = W_1$, $\eta(W_{21}) = W_{21}$, $\eta(W_3) = (W_3 - W_3 \cap (S_m^3 \cup Q)) \cup \xi(W_3 \cap (S_m^3 \cup Q))$, $\eta(W_{42}) = W_{42}$, $\eta(W_5) = W_5$, $\eta(W_{22})$ is a (v_3, v_1) -walk obtained from W_{22} replacing v_1 by v_2 and v_2 by v_1 , and $\eta(W_{41})$ is a (v_1, v_3) -walk obtained from W_{41} replacing v_1 by v_2 and v_2 by v_1 .

Case 3.2.2. If W_2 does not contain the vertex v_3 , let $\eta(W) = \eta(W_1)\eta(W_2)\eta(W_3)\eta(W_4)\eta(W_5)$, where $\eta(W_1) = W_1$, $\eta(W_3) = (W_3 - W_3 \cap (S_m^3 \cup Q)) \cup \xi(W_3 \cap (S_m^3 \cup Q))$, $\eta(W_5) = W_5$, $\eta(W_2)$ is a (v_1, v_1) -walk obtained from W_2 replacing its last two vertices v_1v_2 by v_1 , and $\eta(W_4)$ is a (v_1, v_1) -walk obtained from W_4 replacing its first vertex v_2 by v_1v_2 .

Case 3.2.3. If W_2 contains the vertex v_3 and W_4 does not contain vertex v_3 , let $\eta(W) = \eta(W_1)\eta(W_2)\eta(W_3)\eta(W_4)\eta(W_5)$, where $\eta(W_1) = W_1$, $\eta(W_3) = (W_3 - W_3 \cap (S_m^3 \cup Q)) \cup \xi(W_3 \cap (S_m^3 \cup Q))$, $\eta(W_5) = W_5$, $\eta(W_2)$ is a (v_1, v_1) -walk obtained from W_2 replacing its last vertex v_2 by v_2v_1 , and $\eta(W_4)$ is a (v_1, v_1) -walk obtained from W_4 replacing its first two vertices v_2v_1 by v_1 .

Case 3.3. If W_1 passes edge v_1v_t and W_3 does not pass edge v_1v_t , we may anew decompose W into four sections $W_1W_2W_3W_4$, where W_1 is the longest (v_3, v_t) (or (w, v_t))-section of W (which do not contain vertices $u_0, \dots, u_t''$), W_2 is the second (v_1, v_2) -section of W (for which the internal vertices, if exist, are only possible $v_1, v_2, v_3, w \in V(Q)$), the third W_3 is the internal longest (u_0, u_t'') -section of W (for which the internal vertices are some possible vertices in $V(G_1)$), and the last W_4 is the longest (v_2, v_3) (or (v_2, w))-section of W (for which the internal vertices, if exist, are only

possible $v_1, v_2, v_3, w \in V(Q)$). We consider the following two subsubcases.

Case 3.3.1. If W_2 contains vertex v_3 , we may uniquely decompose W_2 into two sections $W_{21}W_{22}$, where W_{21} is the longest (v_1, v_3) -section of W_2 and W_{22} is the remaining shortest (v_3, v_2) -section of W_2 .

Let $\eta(W) = \eta(W_1)\eta(W_{21})\eta(W_{22})\eta(W_3)\eta(W_4)$, where $\eta(W_1) = W_1$, $\eta(W_{21}) = W_{21}$, $\eta(W_3) = (W_3 - W_3 \cap (S_m^3 \cup Q)) \cup \xi(W_3 \cap (S_m^3 \cup Q))$, $\eta(W_{22})$ is a (v_3, v_1) -walk obtained from W_{22} replacing v_1 by v_2 and v_2 by v_1 , and $\eta(W_4)$ is a (v_1, v_3) (or (v_1, w))-walk obtained from W_4 replacing v_1 by v_2 and v_2 by v_1 .

Case 3.3.2. If W_2 does not contain vertex v_3 , let $\eta(W) = \eta(W_1)\eta(W_2)\eta(W_3)\eta(W_4)$, where $\eta(W_1) = W_1$, $\eta(W_3) = (W_3 - W_3 \cap (S_m^3 \cup Q)) \cup \xi(W_3 \cap (S_m^3 \cup Q))$, $\eta(W_2)$ is a (v_1, v_1) -walk obtained from W_2 replacing its last two vertices v_1v_2 by v_1 , and $\eta(W_4)$ is a (v_1, v_3) (or (v_1, w))-walk obtained from W_4 replacing its first vertex v_2 by v_1v_2 .

Case 3.4. If W_1 does not pass edge v_1v_t and W_3 passes edge v_1v_t , we may anew decompose W into four sections $W_1W_2W_3W_4$, where W_1 is the longest (v_3, v_2) (or (w, v_2))-section of W (which do not contain vertices $u_0, \dots, u_t''$ and must contain vertex v_3), the second W_2 is the internal longest (u_0, u_t'') -section of W (for which the internal vertices are some possible vertices in $V(G_1)$), W_3 is the third (v_2, v_1) -section of W (for which the internal vertices, if exist, are only possible $v_1, v_2, v_3, w \in V(Q)$), and the last W_4 is the longest (v_t, v_3) (or (v_t, w))-section of W . We have two subsubcases.

Case 3.4.1. If W_3 contains vertex v_3 , we may uniquely decompose it into two sections $W_{31}W_{32}$, where W_{31} is the shortest (v_2, v_3) -section of W_3 and W_{32} is the remaining longest (v_3, v_1) -section of W_3 .

Let $\eta(W) = \eta(W_1)\eta(W_2)\eta(W_{31})\eta(W_{32})\eta(W_4)$, where $\eta(W_2) = (W_2 - W_2 \cap (S_m^3 \cup Q)) \cup \xi(W_2 \cap (S_m^3 \cup Q))$, $\eta(W_{32}) = W_{32}$, $\eta(W_4) = W_4$, $\eta(W_1)$ is a (v_3, v_1) (or (w, v_1))-walk obtained from W_1 replacing v_1 by v_2 and v_2 by v_1 , and $\eta(W_{31})$ is a (v_1, v_3) -walk obtained from W_{31} replacing v_1 by v_2 and v_2 by v_1 .

Case 3.4.2. If W_3 does not contain vertex v_3 , let $\eta(W) = \eta(W_1)\eta(W_2)\eta(W_3)\eta(W_4)$, where $\eta(W_2) = (W_2 - W_2 \cap S_m^3) \cup \xi(W_2 \cap S_m^3)$, $\eta(W_4) = W_4$, $\eta(W_1)$ is a (v_3, v_1) (or (w, v_1))-walk obtained from W_1 replacing its last vertex v_2 by v_2v_1 , and $\eta(W_3)$ is a (v_1, v_1) -walk obtained from W_3 replacing its first two vertices v_2v_1 by v_1 .

Case 4. Suppose W is a closed walk starting from v_i for $i = 4, 5, 6, \dots, n$ in X_1 . For $W \in X_1$, we may uniquely decompose W into five sections $W_1W_2W_3W_4W_5$, where W_1 is the longest (v_i, v_t) -section of W (which do not contain vertices $u_0, \dots, u_t''$), W_2 is the second (v_1, v_2) -section of W (for which the internal vertices, if exist, are only possible $v_1, v_2, v_3, w \in V(G)$), the third W_3 is the internal longest (u_0, u_t'') -section of W (for which the internal vertices are some possible vertices in $V(G_1)$), the fourth W_4 is the longest

FIGURE 4: The procedure of transformation.

(v_2, v_1) -section of W (for which the internal vertices, if exist, are only possible $v_1, v_2, v_3, w \in V(G)$), and the last W_5 is the remaining (v'_t, v_i) -section of W . We have four subcases.

Case 4.1. If both W_2 and W_4 contain the vertex v_3 , we may uniquely decompose W_2 into two sections $W_{21}W_{22}$ and decompose W_4 into two sections $W_{41}W_{42}$, where W_{21} is the longest (v_1, v_3) -section of W_2 , W_{22} is the remaining shortest (v_3, v_2) of W_2 , W_{41} is the shortest (v_2, v_3) -section of W_4 , and W_{42} is the remaining longest (v_3, v_1) -section of W_4 .

Let $\eta(W) = \eta(W_1)\eta(W_{21})\eta(W_{22})\eta(W_3)\eta(W_{41})\eta(W_{42})\eta(W_5)$, where $\eta(W_1) = W_1$, $\eta(W_{21}) = W_{21}$, $\eta(W_3) = (W_3 - W_3 \cap (S_m^3 \cup Q)) \cup \xi(W_3 \cap (S_m^3 \cup Q))$, $\eta(W_{42}) = W_{42}\eta(W_5) = W_5$, $\eta(W_{22})$ is a (v_3, v_1) -walk obtained from W_{22} replacing v_1 by v_2 and v_2 by v_1 , and $\eta(W_{41})$ is a (v_1, v_3) -walk obtained from W_{41} replacing v_1 by v_2 and v_2 by v_1 .

Case 4.2. If W_2 contains the vertex v_3 and W_4 does not contain vertex v_3 , let $\eta(W) = \eta(W_1)\eta(W_2)\eta(W_3)\eta(W_4)\eta(W_5)$, where $\eta(W_1) = W_1$, $\eta(W_3) = (W_3 - W_3 \cap (S_m^3 \cup Q)) \cup \xi(W_3 \cap (S_m^3 \cup Q))$, $\eta(W_5) = W_5$, $\eta(W_2)$ is a (v_1, v_1) -walk obtained from W_2 replacing its last vertex v_2 by v_2v_1 , and $\eta(W_4)$ is a (v_1, v_1) -walk obtained from W_4 replacing its first two vertices v_2v_1 by v_1 .

Case 4.3. If W_2 does not contain the vertex v_3 , let $\eta(W) = \eta(W_1)\eta(W_2)\eta(W_3)\eta(W_4)\eta(W_5)$, where $\eta(W_1) = W_1$, $\eta(W_3) = (W_3 - W_3 \cap (S_m^3 \cup Q)) \cup \xi(W_3 \cap (S_m^3 \cup Q))$, $\eta(W_5) = W_5$, $\eta(W_2)$ is a (v_1, v_1) -walk obtained from W_2 by replacing its last two vertices v_1v_2 by v_1 , and $\eta(W_4)$ is a (v_1, v_1) -walk obtained from W_4 by replacing its first vertex v_2 by v_1v_2 .

For example,

$$\begin{aligned} & \eta_1(u_0u_1 \cdots u_rv_2v_3w_1 \cdots w_tv_3v_1v_2u'_1 \cdots \\ & \quad u'_sv_2v_1v_3v_2u''_1 \cdots u''_tu_0) \\ &= u_0u_1 \cdots u_rv_1v_3w_1 \cdots w_tv_3v_2v_1u'_1 \cdots \\ & \quad u'_sv_1v_2v_3v_1u''_1 \cdots u''_tu_0, \\ & \eta_1(u_0u_1 \cdots u_rv_2v_3w_1 \cdots w_tv_3v_1v_4v_5v_1v_2u'_1 \cdots \\ & \quad u'_sv_2v_3v_5v_4v_1v_3v_2u''_1 \cdots u''_tu_0) \\ &= u_0u_1 \cdots u_rv_1v_2v_3w_1 \cdots w_tv_3v_1v_4v_5v_1u'_1 \\ & \quad \cdots u'_sv_1v_3v_5v_4v_1v_3v_1u''_1 \cdots u''_tu_0, \end{aligned}$$

$$\begin{aligned} & \eta_1(v_3w_1 \cdots w_tv_3v_2u_1 \cdots u_rv_2v_1v_5v_4v_1v_2u'_1 \cdots u'_sv_2v_1v_3) \\ &= v_3w_1 \cdots w_tv_3v_1u_1 \cdots u_rv_1v_5v_4v_1v_2v_1u'_1 \cdots u'_sv_1v_2v_3, \\ & \eta_1(v_3v_2v_1v_7v_6v_1v_2v_1v_2u_1 \cdots u_rv_2v_1v_4v_5v_1v_3v_2u'_1 \cdots \\ & \quad u'_sv_2v_1v_7v_6v_1v_2v_3) \\ &= v_3v_2v_1v_7v_6v_1v_2v_1u_1 \cdots u_rv_1v_4v_5v_1v_3v_2v_1u'_1 \\ & \quad \cdots u'_sv_1v_2v_1v_7v_6v_1v_2v_3, \\ & \eta_1(v_1v_4v_5v_1v_3v_2u_1 \cdots u_rv_2v_3v_2v_1v_4v_5v_1v_3v_2u'_1 \cdots u'_sv_2v_1) \\ &= v_2v_3v_1v_5v_4v_1u_1 \cdots u_rv_1v_3v_2v_1v_4v_5v_1v_3v_1u'_1 \cdots u'_sv_1v_2, \\ & \eta_1(v_4v_5v_1v_3v_2u_1 \cdots u_rv_2v_3v_2v_1v_4v_5v_1v_3v_2u'_1 \\ & \quad \cdots u'_sv_2v_3v_2v_1v_5v_4) \\ &= v_4v_5v_1v_3v_1u_1 \cdots u_rv_1v_3v_2v_1v_4v_5v_1v_3v_1u'_1 \\ & \quad \cdots u'_sv_1v_3v_2v_1v_5v_4, \end{aligned} \tag{8}$$

where $u_0, u_1, \dots, u_r, u'_1, \dots, u'_s, u''_1, \dots, u''_t$ are vertices in G and $w_1, \dots, w_t$ are vertices in Q .

By Lemma 1, ξ is injective and not surjective. It is easily shown that η is also injective and not surjective. Thus $|X_1| < |X_2|$, $M_k(G_1) < M_k(G_2)$. $\square$

Theorem 3. Let G_H be an arbitrary graph on n vertices in set $\Gamma(n, m)$, where $n > 5$. Then $EE(G_H) \leq EE(S_m^3)$ with the equality holding if and only if $G_H \cong S_m^3$.

Proof. Determine a vertex v of the maximum degree Δ as a root in G_H , and let $k \geq 4$ be an integer. Let G_{H_i} be the completely connected graph of 3-uniform linear hypertree H_i attached at v , and let m_i be the number of triangles of G_{H_i} for $i = 1, 2, \dots, \Delta/2$, respectively. We can repeatedly apply this transformation from Lemma 2 at some vertices whose degrees are not equal to two or $2m_i$ in G_{H_i} till G_{H_i} becomes a star. From Lemma 2, it satisfies that each application of this transformation strictly increases the number of closed walks and also increases Estrada index.

When all G_{H_i} turn into stars, we can again use Lemma 2 at the vertex v as long as there exists at least one vertex whose degree is not equal to two or $2 \sum m_i$, further increasing the number of closed walks. In the end of this procedure, we get the star S_m^3 . The whole procedure of transformation is shown in Figure 4. $\square$

Lemma 4 (see [20]). *Let v be a vertex of a graph G , $G - \{v\} = G - v$ for $v \in V(G)$, and $\mathcal{C}(v)$ the set of cycles containing v . Consider*

$$P(G, \lambda) = \lambda \cdot P(G - v, \lambda) - \sum_{vw \in E(G)} P(G - v - w, \lambda) - 2 \sum_{Z \in \mathcal{C}(v)} P(G - V(Z), \lambda), \quad (9)$$

where $P(G - v - w, \lambda) = 1$ if G is a single edge and $P(G - V(Z), \lambda) = 1$ if G is a cycle.

Now, we calculate $EE(S_m^3)$. Applying Lemma 4, we have

$$P(S_m^3, \lambda) = (\lambda + 1)^{(n-1)/2} (\lambda - 1)^{(n-3)/2} (\lambda^2 - \lambda - n + 1). \quad (10)$$

By some simple calculating, we achieve the following eigenvalues:

$$\begin{aligned} \lambda_1 &= \lambda_2 = \dots = \lambda_{(n-1)/2} = -1, \\ \lambda_{(n+1)/2} &= \lambda_{(n+3)/2} = \dots = \lambda_{n-2} = 1, \\ \lambda_{n-1} &= \frac{1 - \sqrt{4n-3}}{2}, \quad \lambda_n = \frac{1 + \sqrt{4n-3}}{2}. \end{aligned} \quad (11)$$

Then, we obtain

$$EE(S_m^3) = \frac{(n-1)}{2e} + \frac{(n-3)}{2}e + e^{(1+\sqrt{4n-3})/2} + e^{(1-\sqrt{4n-3})/2}. \quad (12)$$

Theorem 3 shows that the star S_m^3 has the maximum Estrada index in set $\Gamma(n, m)$. Thus, according to previous definition, it is easy to show that the 3-uniform star $\mathcal{S}_m^3$ has the maximum Estrada index among the set of 3-uniform linear hypertrees; that is,

$$EE(H) \leq EE(\mathcal{S}_m^3), \quad (13)$$

where

$$EE(\mathcal{S}_m^3) = \frac{(n-1)}{2e} + \frac{(n-3)}{2}e + e^{(1+\sqrt{4n-3})/2} + e^{(1-\sqrt{4n-3})/2}. \quad (14)$$

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

Acknowledgments

This work was supported by Program for Changjiang Scholars and Innovative Research Team in University (PCSIRT)(no. ITR1068), Special 973 Program for Key Basic Research of the Ministry of Science and Technology, China (no. 2010CB334708), the National Natural Science Foundation of China (NSFC)(no. 60863006), Scientific Research Foundation of the Department of Science and Technology, Qinghai Province, China (no. 2012-Z-943).

References

- [1] E. Estrada, "Characterization of 3D molecular structure," *Chemical Physics Letters*, vol. 319, no. 5-6, pp. 713-718, 2000.
- [2] E. Estrada, "Characterization of the folding degree of proteins," *Bioinformatics*, vol. 18, no. 5, pp. 697-704, 2002.
- [3] E. Estrada, "Characterization of the amino acid contribution to the folding degree of proteins," *Proteins*, vol. 54, no. 4, pp. 727-737, 2004.
- [4] E. Estrada and J. A. Rodríguez-Velázquez, "Subgraph centrality in complex networks," *Physical Review E: Statistical, Nonlinear, and Soft Matter Physics*, vol. 71, no. 5, 9 pages, 2005.
- [5] E. Estrada, J. A. Rodríguez-Velázquez, and M. Randić, "Atomic branching in molecules," *International Journal of Quantum Chemistry*, vol. 106, no. 4, pp. 823-832, 2006.
- [6] K. C. Das and S. Lee, "On the Estrada index conjecture," *Linear Algebra and its Applications*, vol. 431, no. 8, pp. 1351-1359, 2009.
- [7] H. Deng, "A proof of a conjecture on the Estrada index," *MATCH, Communications in Mathematical and in Computer Chemistry*, vol. 62, no. 3, pp. 599-606, 2009.
- [8] Z. Du and B. Zhou, "The Estrada index of trees," *Linear Algebra and Its Applications*, vol. 435, no. 10, pp. 2462-2467, 2011.
- [9] Z. Du and B. Zhou, "The Estrada index of unicyclic graphs," *Linear Algebra and Its Applications*, vol. 436, no. 9, pp. 3149-3159, 2012.
- [10] Q. Deng and H. Chen, "On extremal bipartite unicyclic graphs," *Linear Algebra and Its Applications*, vol. 444, pp. 89-99, 2014.
- [11] A. Ilić and D. Stevanović, "The Estrada index of chemical trees," *Journal of Mathematical Chemistry*, vol. 47, no. 1, pp. 305-314, 2010.
- [12] W. Wang and W. Xu, "Graphs with the maximal Estrada indices," *Linear Algebra and its Applications*, vol. 446, pp. 314-328, 2014.
- [13] H. Zhao and Y. Jia, "On the Estrada index of bipartite graph," *MATCH: Communications in Mathematical and in Computer Chemistry*, vol. 61, no. 2, pp. 495-501, 2009.
- [14] B. Zhou and Z. Du, "Some lower bounds for Estrada index," *Iranian Journal of Mathematical Chemistry*, vol. 1, no. 2, pp. 67-72, 2010.
- [15] Z. Zhu, L. Tan, and Z. Qiu, "Tricyclic graph with maximal Estrada index," *Discrete Applied Mathematics*, vol. 162, pp. 364-372, 2014.
- [16] Z. Du, "An edge grafting theorem on the Estrada index of graphs and its applications," *Discrete Applied Mathematics*, vol. 161, no. 1-2, pp. 134-139, 2013.
- [17] J. A. de la Peña, I. Gutman, and J. Rada, "Estimating the Estrada index," *Linear Algebra and its Applications*, vol. 427, no. 1, pp. 70-76, 2007.

- [18] I. Gutman, H. Deng, and S. Radenković, "The Estrada index," in *Applications of Graph Spectra*, D. Cvetković and I. Gutman, Eds., pp. 155–174, Mathematics Institute, Beograd, Serbia, 2011.
- [19] J. Liu, X. Pan, and J. Cao, "Some properties on Estrada index of folded hypercubes networks," *Abstract and Applied Analysis*, vol. 2014, Article ID 167623, 6 pages, 2014.
- [20] C. Berge, *Graphs and Hypergraphs*, Elsevier, New York, NY, USA, 1973.
- [21] E. Estrada and J. A. Rodríguez-Velázquez, "Subgraph centrality and clustering in complex hyper-networks," *Physica A: Statistical Mechanics and Its Applications*, vol. 364, pp. 581–594, 2006.
- [22] D. Cvetkoic, M. Doob, and H. Sachs, *Spectra of Graphs. Theory and Application*, vol. 87 of *Pure and Applied Mathematics*, Academic Press, New York, NY, USA, 1980.