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The Minimal Estrada Index of Trees with Two Maximum Degree Vertices

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Abstract

Let G be a simple graph with n vertices and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of its adjacency matrix. The Estrada index EE of G is the sum of the terms e^{λ_i}. In 2009 Ilić et al. obtained the trees with minimal Estrada index among trees with a given maximum vertex degree. In this paper, we give the trees with minimal Estrada index among the trees of order n with exactly two vertices of maximum degree.

1 Introduction

Let G be a simple graph with n vertices and m edges. A walk [1] in a simple graph G is a sequence $W := v_0 v_1 \cdots v_\ell$ of vertices, such that $v_{i-1}v_i$ is an edge in G. If $v_0 = x$ and $v_\ell = y$, we say that W connects x to y and refer to W as an *xy-walk*. The vertices x and

y are called the ends of the walk, x being its initial vertex and y its terminal vertex, while the vertices $v_1, \ldots, v_{\ell-1}$ are called its internal vertices. The integer ℓ is the length of W. If u and v are two vertices of a walk W, where u precedes v on W, the subsequence of W starting from u and ending at v is denoted by uWv and called the *segment* of W from u to v.

The spectrum of G is the spectrum of its adjacency matrix [2], and consists of the (real) numbers $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The Estrada index is defined as

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

Although invented in the year 2000 [6], the Estrada index has already found a large number of applications, such as in biochemistry [6, 7, 10] and in the theory of complex networks [8, 9]. Also numerous lower and upper bounds for the Estrada index have been communicated [5, 11, 12, 15].

Recently, Deng in [3] showed that the path P_n and the star S_n have the minimal and the maximal Estrada indices among n-vertex trees. Zhao and Jia in [14] determined also the trees with the second and the third maximal Estrada index. Then, Deng in [4] gave the first six trees with the maximal Estrada index. In 2009 Ilić et al. [13] obtained the trees with minimal Estrada index among trees of order n with a given maximum vertex degree. In this paper, we give the trees with minimal Estrada index among trees of order n with exactly two vertices of maximum degree.

2 Preliminaries

In our proofs, we will use a relation between EE and the spectral moments of a graph. For $k \geq 0$, we denote by M_k the k-th spectral moment of G,

$$M_k(G) = \sum_{i=1}^{n} \lambda_i^k.$$

We know from [2] that M_k is equal to the number of closed walks of length k of the graph G, and the first few spectral moments of a graph with m edges and n vertices satisfy the relations:

$$M_0 = n, \quad M_1 = 0, \quad M_2 = 2m, \quad M_3 = 6t,$$

where t is the number of triangles in G.

From the Taylor expansion of e^x, we have the following important relation between the Estrada index and the spectral moments of G:

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k}{k!}.$$

Thus, if for two graphs G and H we have $M_k(G) \geq M_k(H)$ for all $k \geq 0$, then $EE(G) \geq EE(H)$. Moreover, if the strict inequality $M_k(G) > M_k(H)$ holds for at least one value of k, then $EE(G) > EE(H)$.

3 The minimal Estrada index of trees with two maximum degree vertices

Let G_i be a graph with n vertices and m edges, in which there are exactly two vertices of maximum degree Δ. Let $W(G_i)$ denote the set of closed walks in G_i, and $W_{2k}(G_i)$ denote the set of closed walks of length $2k$ in G_i. We say a closed walks is at vertex v_j, if it is a closed walk from v_j to v_j.

Lemma 3.1 *[3] Let u be a non-isolated vertex of a simple graph H. If H_1 and H_2 are the graphs obtained from H by identifying an end vertex v_1 and an internal vertex v_t of the n-vertex path P_n, respectively, with u, see Figure 3.1, then $M_{2k}(H_1) < M_{2k}(H_2)$ for $n \geq 3$ and $k \geq 2$.*

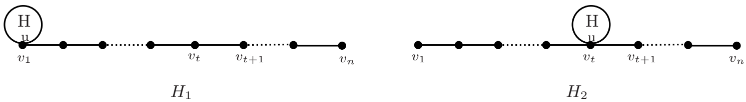

Figure 3.1 The transformation in Lemma 3.1.

Lemma 3.2 *For the two trees G_1 and G_2 in Figure 3.2, we have $EE(G_1) > EE(G_2)$, where P_i are paths of length n_i, $n_i \geq 0$, $1 \leq i \leq s$, A and B are (connected) trees and $G_1 \ncong G_2$.*

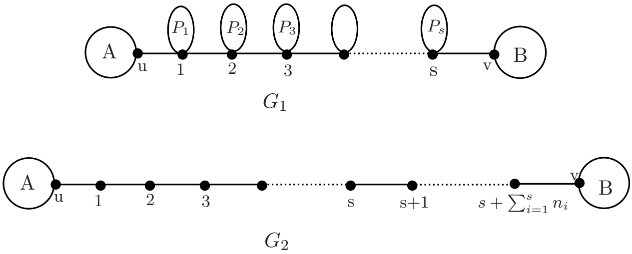

Figure 3.2 The graphs G_1 and G_2 in Lemma 3.2.

Proof. Suppose P_i is the first path with $n_i > 0$. Let $n_i = m$ and $i = i_0$. Then G_1 can be redrawn as in Figure 3.3. First we show that if $G_1 \ncong G_3$, then $EE(G_1) > EE(G_3)$. Consider the following correspondence:

$$\xi : W_{2k}(G_3) \to W_{2k}(G_1),\ \forall\, w \in W_{2k}(G_3).$$

Denote by A_1, B_1 the graphs in Figure 3.3. Since $W_{2k}(G_i) = W_{2k}(A_1) \cup W_{2k}(B_1) \cup W_i$, where W_i is the set of closed walks of length $2k$ of G_i, each of which contains at least one edge in $E(A_1)$ and at least one edge in $E(B_1)$. So $M_{2k}(G_i) = |W_{2k}(A_1)| + |W_{2k}(B_1)| + |W_i| = M_{2k}(A_1) + M_{2k}(B_1) + |W_i|$. Obviously, it is sufficient to show that $|W_1| > |W_3|$.

For any closed walk $w \in W_3$, it contains the segments $w_{1\ell}$ of the walk in $W(A_1)$, and the segments w_{2j} in $W(B_1)$, $1 \le \ell, j \le t$, $t = \max\{t_1, t_2\}$, where t_1 and t_2 are the numbers of segments of w in $W(A_1)$ and $W(B_1)$, respectively, and some of the segments may be empty. Then it can be written as $w = w_{11} \cup w_{21} \cup w_{12} \cup w_{22} \cdots \cup w_{1t} \cup w_{2t}$. For the segments $w_{1\ell} \in W(A_1)$, define $\xi(w_{1\ell}) = w_{1\ell}, 1 \le \ell \le t$. Now we define $\xi(w_{2j}), 1 \le j \le t$.

Let $f : \{i_0, i_1, \ldots, i_m\} \to \{i_0, i_1, \ldots, i_m\}$, $f(i_r) = i_{m-r}$, for $0 \le r \le m$.

Case 1. If w_{2j} does not pass the edge $e_{i_0,i+1}$, then define $\xi(w_{2j}) = f(w_{2j})$.

Case 2. If on the contrary, w_{2j} pass the edge $e_{i_0,i+1}$, then

- if w begins with a vertex in A_1, then w_{2j} is a closed walk at i_m. It contains the first segment w'_{2j} from the initial vertex i_m to the first i_0, the second segment w''_{2j} from the first i_0 to the last i_0, and the third segment w'''_{2j} from the last i_0 to the terminal vertex i_m. Then, define $\xi(w_{2j}) = f(w'_{2j}) \cup (w'''_{2j})^{-1} \cup w''_{2j}$, where $(w'''_{2j})^{-1}$ is the walk

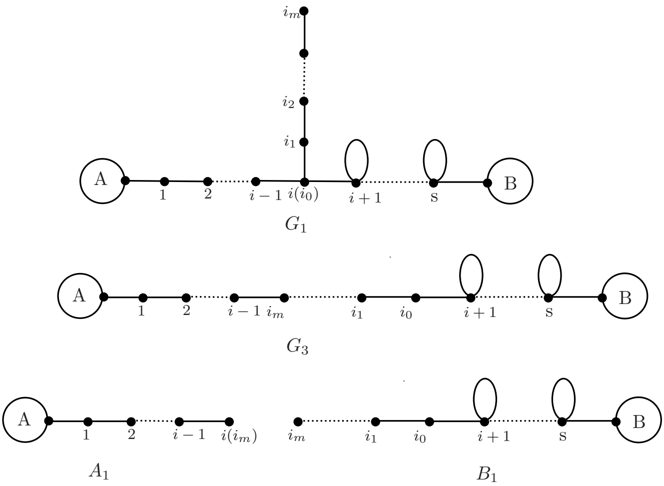

Figure 3.3 The graphs in the proof of Lemma 3.2.

from w'''_{2j} by reversing the order of all the vertices. It is the walk in G_1 that consists of the first segment from i_0 to the first i_m, the second segment from i_m to the next first i_0 and the third segment from i_0 to i_0.

- if w begins with a vertex except i_m in B_1, and $j \neq 1, t$, then define $\xi(w_{2j})$ is the same as above.

- if w begins with a vertex except i_m in B_1, $j = 1, t$. We can see that w_{11} is empty, w_{21} contains the first segment w'_{21} from the initial vertex to the first i_0, the second segment w''_{21} from the first i_0 to the last i_0, and the third segment w'''_{21} from the last i_0 to the terminal vertex i_m. Then, define $\xi(w_{21}) = f(w'_{21}) \cup (w'''_{21})^{-1} \cup w''_{21}$. And w_{2t} contains the first segment w'_{2t} from i_m to the first i_0, the second segment w''_{2t} from the first i_0 to the last i_0, and the third segment w'''_{2t} from the last i_0 to the terminal vertex. Then, define $\xi(w_{2t}) = w''_{2t} \cup (w'_{2t})^{-1} \cup f(w'''_{2t})$.

We then define $\xi(w) = \xi(w_{11}) \cup \xi(w_{21}) \cup \xi(w_{12}) \cup \xi(w_{22}) \cdots \cup \xi(w_{1t}) \cup \xi(w_{2t})$, for $\xi(w) \in W_1$.

Now, for any closed walk $w \in W_3$, there is a unique walk $\xi(w)$ in W_1 corresponding to it. By the definition of ξ and the description above, we know that if there is a walk $\xi(w) \in W_1$, then $\xi(w)$ can be divided into some pieces in only one way, and ξ on each piece is bijective. We combine all the inverse images of the pieces according to the only order, so we can get the only $w \in W_3$. Therefore, if $w_1, w_2 \in W_3, w_1 \neq w_2$, then $\xi(w_1) \neq \xi(w_2)$. Thus, ξ is injective. But it is not surjective, since there is no $w \in W_{2k}(G_3)$ such that $\xi(w) = (i-1)i_0(i+1)i_0(i-1)$. Then clearly $|W_1| > |W_3|$.

Thus, $M_{2k}(G_1) > M_{2k}(G_3)$, that is, $EE(G_1) > EE(G_3)$.

Then, we can repeat the above process and finally get that $EE(G_1) > EE(G_2)$, as required. ∎

For any tree T of order n with exactly two vertices u, v of maximum degree Δ, by using the transformation in Lemma 3.1 repeatedly, we can easily get that $EE(T) \geq EE(G_1)$, where A denotes the union of the $\Delta - 1$ disjoint paths all of which have their end vertices adjacent to u, and B denotes the union of the $\Delta - 1$ disjoint paths all of which have the end vertices adjacent to v. Then from Lemma 3.2, $EE(T) \geq EE(G_1) \geq EE(G_2)$, and the equality holds if and only if $T \cong G_1 \cong G_2$.

The following is a very useful lemma from [13].

Lemma 3.3 *[13] Let w be a vertex of a nontrivial connected graph G, and for nonnegative integers p and q, let $G(p, q)$ denote the graph obtained from G by attaching pendent paths $P = wv_1v_2 \cdots v_p$ and $Q = wu_1u_2 \cdots u_q$ of lengths p and q, respectively, at w. If $p \geq q \geq 1$, then*

$$EE(G(p,q)) > EE(G(p+1, q-1)).$$

Then by applying the transformation in Lemma 3.3 repeatedly, we get that $EE(G_2) > EE(G_4)$ if $G_2 \ncong G_4$, where G_4 is the graph introduced in the following lemma.

Lemma 3.4 *Let G_4 and G_5 be two trees with n vertices, see Figure 3.4, we have $EE(G_4) > EE(G_5)$, where P_i are paths of length n_i, $n_i \geq 1, i = 1, 2, 3$, and u, v are vertices with maximum degree Δ, and $G_4 \ncong G_5$.*

Proof. We first show that if $G_4 \ncong G_6$, then $EE(G_4) > EE(G_6)$.

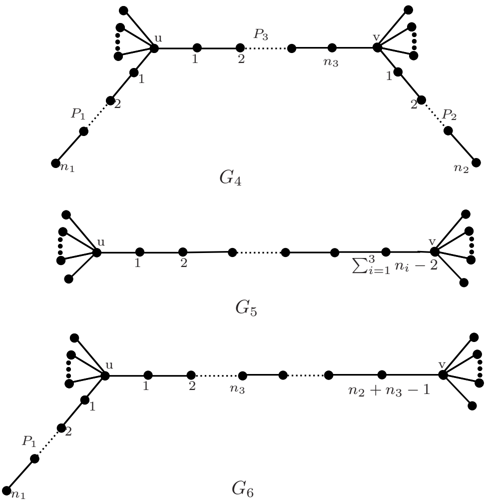

Figure 3.4 The graphs G_i, $i = 4, 5, 6$ in Lemma 3.4.

Since $M_{2k}(G_i) = |W_{2k}(A)| + |W_{2k}(B)| + |W_i| = M_{2k}(A) + M_{2k}(B) + |W_i|$, where W_i is the set of closed walks of length $2k$ of G_i containing at least one edge in $E(A)$ and at least one edge in $E(B)$, $i = 4, 6$. Similar to Lemma 3.2, we only need to show that $|W_4| > |W_6|$. For convenience, we relabel B as B', $m = n_2 + 2$, see Figure 3.5.

Now we show that for a closed walk $w \in W_6$, there is an injection ξ, such that $\xi(w) \in W_4$. For any closed walk $w \in W_6$, it contains the segments $w_{1\ell}$ of the walk in $W(A)$, and the segments w_{2j} in $W(B')$, $1 \le \ell, j \le s$, $s = \max\{s_1, s_2\}$, where s_1 and s_2 are the numbers of segments of w in $W(A)$ and $W(B')$, respectively, and some of the segments may be empty. Then it can be written as $w = w_{11} \cup w_{21} \cup w_{12} \cup w_{22} \cdots \cup w_{1s} \cup w_{2s}$. For the segments $w_{1\ell} \in W(A)$, define $\xi(w_{1\ell}) = w_{1\ell}, 1 \le \ell \le s$. Now we define $\xi(w_{2j}), 1 \le j \le s$.

Case 1. w_{2j} only uses edges on the path $P = v_1 v_2 \dots v_m$.

Let $f : \{v_1, v_2, \dots, v_m\} \to \{v_1, v_2, \dots, v_m\}$, $f(v_i) = v_{m+1-i}$, $\forall\, 1 \le i \le m$. Then, define $\xi(w_{2j}) = f(w_{2j})$.

Case 2. w_{2j} also uses other edges of B'.

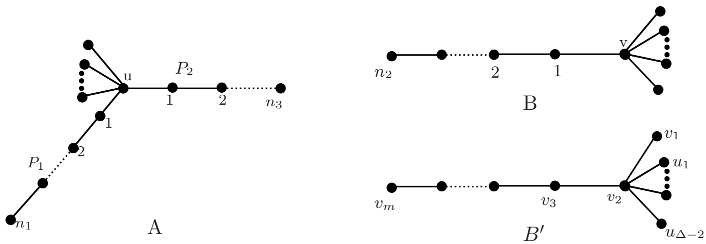

Figure 3.5 The trees in the proof of Lemma 3.4.

We first define the term *stable* segment S, it is a maximal consecutive subsequence of w_{2j} from u_i to v_2, $1 \leq i \leq \Delta - 2$, all the edges of the subsequence are of the form v_2u_k, $1 \leq k \leq \Delta - 2$. Now we consider the remaining subsequence w'_{2j} of w_{2j} by deleting all the stable segments.

Let $f' : \{v_2, v_3 \ldots, v_m\} \to \{v_1, v_2, \ldots, v_{m-1}\}$, $f'(v_i) = v_{i-1}$, $\forall\ 2 \leq i \leq m$. $f'' : \{v_2, \ldots, v_m\} \to \{v_2, \ldots, v_m\}$, $f''(v_i) = v_{m+2-i}$, $\forall\ 2 \leq i \leq m$. w^{-1} is the walk from w by reversing the order of all the vertices.

Subcase 2.1. If w begins with a vertex in A, or w begins with a vertex in B' and $j \neq 1, s$, then w_{2j} is a closed walk at v_m. We only need to show that $\xi(w_{2j})$ is a closed walk at v_1. Actually, it is easy to see that w'_{2j} is also a closed walk at v_m.

- If w_{2j} passes the vertex v_1, so is w'_{2j}. Then w'_{2j} consists of four segments: the first segment $\hat{w}'_1$ from the initial vertex v_m to the first v_2, the second segment $\hat{w}'_2$ from the first v_2 to the v_2 that is just before the first v_1, the third segment $\hat{w}'_3 = v_2v_1$, where the v_1 is the first v_1 in w'_{2j}, and the forth segment $\hat{w}'_4$ from the first v_1 to the terminal vertex of w'_{2j}. Actually, some of the segments may be empty.

  Let S_i^t be the stable segment after the i-th v_2 of $\hat{w}'_t$, $1 \leq t \leq 4$. Let $\xi(\hat{w}'_1) = f''(\hat{w}'_1)$, it is a walk from v_2 to v_m, no internal vertices is v_1 or v_m. And $\xi(\hat{w}_1)$ is the walk from $\xi(\hat{w}'_1)$ by inserting S_1^1 (if it exists) after the first v_2 in it. Let $\xi(\hat{w}'_2) = f'(\hat{w}'_2)$, it is a walk from v_1 to v_1, and no internal vertices is v_m. Since in $\hat{w}'_2$, there must be a v_3 before each v_2 except the first one, and $f'(v_3) = v_2, f'(v_2) = v_1$. So we can define $\xi(\hat{w}_2)$ to be the walk from $\xi(\hat{w}'_2)$ by inserting S_i^2 after the v_2 that is just before the i-th v_1, $i \geq 2$. Let $\xi(\hat{w}_3) = \xi(\hat{w}'_3) = (\hat{w}'_3)^{-1} = v_1v_2$. Finally, let $\xi(\hat{w}'_4) = (\hat{w}'_4)^{-1}$, it is a walk from v_m to v_1, and $\xi(\hat{w}_4)$ is the walk from $\xi(\hat{w}'_4)$ by inserting all S_i^4 to the original place in w_{2j}. Thus, we define $\xi(w_{2j}) = \xi(\hat{w}_2) \cup \xi(\hat{w}_3) \cup \xi(\hat{w}_1) \cup \xi(\hat{w}_4)$, it is a closed walk at v_1. On the other hand, if $\xi(w_{2j})$ is given, we can get the four parts uniquely according to the features we described above.

- If w_{2j} does not pass the vertex v_1, it must pass the vertex v_2, and so is w'_{2j}. Then w'_{2j} consists of three segments: the first segment $\hat{w}'_1$ from the initial vertex v_m to the first v_2, the second segment $\hat{w}'_2$ from the first v_2 to the last v_2, and the third segment $\hat{w}'_3$ from the last v_2 to the terminal vertex of w'_{2j}.

  Let S_i^t be the stable segment after the i-th v_2 of $\hat{w}'_t$, $1 \leq t \leq 3$. Let $\xi(\hat{w}'_1) = f(\hat{w}'_1)$, it is a walk from v_1 to v_{m-1}, no internal vertices is v_{m-1}. And $\xi(\hat{w}_1)$ is the walk from $\xi(\hat{w}'_1)$ by inserting S_1^1 (if it exists) after the first v_2 in it. Let $\xi(\hat{w}'_2) = f'(\hat{w}'_2)$, it is a walk from v_1 to v_1. Since in $\hat{w}'_2$, there must be a v_3 before each v_2 except the first one, and $f'(v_3) = v_2, f'(v_2) = v_1$. So we can define $\xi(\hat{w}_2)$ to be the walk from $\xi(\hat{w}'_2)$ by inserting S_i^2 after the v_2 that is just before the i-th v_1, $i \geq 2$. Finally, let $\xi(\hat{w}_3) = \xi(\hat{w}'_3) = (f'(\hat{w}'_3))^{-1}$, it is a walk from v_{m-1} to v_1, no internal vertices is v_1. Thus, we define $\xi(w_{2j}) = \xi(\hat{w}_1) \cup \xi(\hat{w}_3) \cup \xi(\hat{w}_2)$, it is a closed walk at v_1. On the other hand, if $\xi(w_{2j})$ is given, we can get the three parts uniquely according to the features we described above.

Subcase 2.2. If w begins with a vertex in B', and $j = 1, s$, the for the two cases that $w_{2j}, j = 1, s$ passes the vertex v_1 or does not pass v_1, both can be defined similarly as above. Thus, If w begins and ends with vertex $v_t, 2 \leq t \leq m-1$, $\xi(w_{21})$ can be defined uniquely to be a walk from v_{m+1-t} to v_1, $\xi(w_{2s})$ can be defined uniquely to be a walk from v_1 to v_{m+1-t}. If w begins and ends with vertex $u_t, 1 \leq t \leq \Delta - 2$, $\xi(w_{21})$ can be defined uniquely to be a walk from v_{m-1} to v_1, $\xi(w_{2s})$ can be defined uniquely to be a walk from v_1 to v_{m-1}.

Then we define $\xi(w) = \xi(w_{11}) \cup \xi(w_{21}) \cup \xi(w_{12}) \cup \xi(w_{22}) \cdots \cup \xi(w_{1s}) \cup \xi(w_{2s})$, for $\xi(w) \in W_4$.

Now, for any closed walk $w \in W_6$, there is a unique walk $\xi(w)$ in W_4 corresponding to it. By the definition of ξ and the description above, we know if there is a walk $\xi(w) \in W_4$, $\xi(w)$ can be divided into some pieces in only one way, and ξ on each piece is bijective. We combine all the inverse images of the pieces according to the only order, so we can get the only $w \in W_6$. Therefore, if $w_1, w_2 \in W_6, w_1 \neq w_2$, then $\xi(w_1) \neq \xi(w_2)$. Thus, ξ is injective. But it is not surjective, since there is no $w \in W_6$, such that there is a segment $\xi(w_{2j}) \subseteq \xi(w)$ with $\xi(w_{2j}) = v_1v_2u_1v_2v_1, 1 \leq j \leq s$.

Thus, $|W_4| > |W_6|$, and consequently, $M_{2k}(G_4) > M_{2k}(G_6)$, that is, $EE(G_4) > EE(G_6)$.

Analogously, we can get that $EE(G_6) > EE(G_5)$ if $G_5 \ncong G_6$. Thus $EE(G_4) > EE(G_5)$, as required. ∎

The above lemma is true for the case $n_3 \geq 1$, which means that u and v are not adjacent. Actually the lemma is also true when u and v are adjacent. We can prove it similarly.

From Lemmas 3.1 through 3.4, we finally get the result below.

Theorem 3.5 *For all trees T of order n with exactly two vertices of maximum degree, the graph G_5 has the minimal Estrada index.*

With one more restriction that the two maximum degree vertices of the trees must be adjacent, we give the following conjecture.

Conjecture 3.6 *For all trees T of order n with two adjacent vertices of maximum degree, the graph G_7 has the minimal Estrada index, see Figure 3.6, where u, v are vertices with maximum degree.*

Theorem 3.5 can be generalized to trees with one maximum and one second maximum degree vertex as follows.

Theorem 3.7 *For all trees T of order n with exactly one maximum and one second maximum degree vertex, the graph G_8 has the minimal Estrada index, see Figure 3.7, where u, v are vertices with the maximum and second maximum degree, respectively.*

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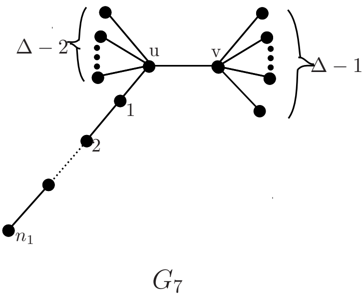

Figure 3.6 The graph G_7 in Conjecture 3.6.

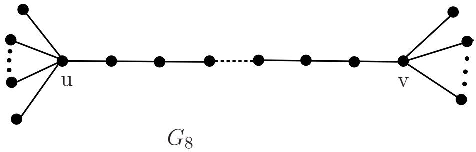

Figure 3.7 The graph G_8 in Theorem 3.7

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