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MORE EXAMPLES AND COUNTEREXAMPLES FOR A CONJECTURE OF MERRIFIELD AND SIMMONS

Yong Wang, Xuelian Li, and Ivan Gutman

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ABSTRACT. Let $\sigma(G)$ be the number of independent–vertex sets of a graph G. Merrifield and Simmons conjectured that for any connected graph G and any pair of its non-adjacent vertices u and v, $\Delta_{uv}(G) := \sigma(G-u)\,\sigma(G-v) - \sigma(G)\,\sigma(G-u-v)$ is positive if the distance between u and v is odd, and negative otherwise. In earlier works by the authors the conjecture was shown to be true for trees, cycles and several other types of graphs, but a few counterexamples were discovered among dense graphs. We now prove that the conjecture is true for all bipartite and some non-bipartite connected unicyclic graphs, but not for all connected unicyclic graphs. Moreover, we find a graph G for which $\Delta_{uv}(G) = 0$.

1. Introduction

Two vertices of a graph G are said to be independent if they are not adjacent. The k-th independence number of G is denoted by $\sigma_k(G)$. By definition, for $k \geq 2$, $\sigma_k(G)$ is equal to the number of ways in which k pairwise independent vertices can be selected in the graph G. In addition to this, $\sigma_0(G) = 1$ and $\sigma_1(G) =$ number of vertices of G. Thus $\sigma(G) = \sum_{k \geq 0} \sigma_k(G)$ is the number of all independent–vertex sets of G.

On page 144 of the book [**5**], Merrifield and Simmons claimed without proof a property of $\sigma(G)$, which for non-adjacent vertices u and v of a connected graph G may be formulated as follows. Abbreviate $\sigma(G-u)\,\sigma(G-v) - \sigma(G)\,\sigma(G-u-v)$ by $\Delta_{uv}(G)$. Then

$$\Delta_{uv}(G) \begin{cases} < 0 & \text{if } d(u,v) \text{ is even} \\ > 0 & \text{if } d(u,v) \text{ is odd} \end{cases} \tag{1}$$

where $d(u,v)$ denotes the distance of u and v in G.

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Gutman [**1**] proved that the conjecture is true for all trees. Li [**4**] proved that the conjecture is true for all cycles and for many other kinds of graphs. Although Li [**4**] found two families of counterexamples for this conjecture, the respective graphs were very dense, i.e., had relatively many edges. On the other hand, the considerations in the book [**5**] were limited to sparse graphs, i.e., graphs having relatively few edges. Therefore, it may be understood that the property (1) was believed to hold only for sparse graphs. If so, then the counterexamples reported in [**4**] cannot be considered as fully satisfactory. What one would need to convincingly disprove the validity of the Merrifield–Simmons conjecture are counterexamples based on sparse graphs. In order to accomplish this task, we examined (connected) unicyclic graphs, which, apart from trees, have the least number of edges. We show that although the majority of connected unicyclic graphs satisfies the relation (1), counterexamples for the Merrifield–Simmons conjecture exist already within this class.

2. Preliminary considerations

We first state without proof some properties and lemmas, which are either given in [1–4] or are immediate consequences of results found in [1–4].

Property 1. If v is a vertex of G, then

$$\sigma(G) = \sigma(G - v) + \sigma(G - [v])$$

where $G - v$ is the subgraph obtained by deleting v from G, and $G - [v]$ is the subgraph obtained by deleting from G both v and the vertices adjacent to v.

Property 2. Let $G_1 \cup G_2$ denote a graph composed of disjoint components G_1 and G_2. Then

$$\sigma(G_1 \cup G_2) = \sigma(G_1)\, \sigma(G_2)$$

An immediate consequence of Property 2 is that if the graph G is disconnected and the vertices u and v belong to its different components, then $\Delta_{uv}(G) = 0$. If, in turn, $G = G_1 \cup G_2$ and both u and v belong to G_1, then $\Delta_{uv}(G) = \sigma^2(G_2)\, \Delta_{uv}(G_1)$. Therefore, without loss of generality the examination of the quantity $\Delta_{uv}(G)$ may be restricted to connected graphs.

In what follows, if it is not explicitly stated otherwise, it is assumed that the graph considered is connected.

Property 3. Let P_n be the path on n vertices. From Property 1 follows that

$$\sigma(P_n) = \sigma(P_{n-1}) + \sigma(P_{n-2})$$

with $\sigma(P_0) = 1$ and $\sigma(P_1) = 2$. Hence the σ-values of the path–graphs are just the Fibonacci numbers.

Label the vertices of P_n by $v_1, v_2, \ldots, v_n$ so that v_i and v_{i+1} are adjacent, $i = 1, \ldots, n-1$. Let $R_1, R_2, \ldots, R_n$ be distinct rooted graphs with mutually disjoint vertex sets. Then the compound graph $P_n(R_1, \ldots, R_n)$ is obtained by identifying the root r_i of R_i with the vertex v_i of P_n for $i = 1, 2, \ldots, n$.

LEMMA 1. *If* $n \geq 2$ *, then*

$$\Delta_{v_1,v_n}(P_n(R_1,\ldots,R_n)) = (-1)^n \prod_{i=1}^{n} \sigma(R_i - r_i)\,\sigma(R_i - [r_i])$$

In order to proceed we need to fix our notation and terminology. Let U_n be a (connected) unicyclic graph, such that its (unique) cycle possess n vertices. Denote this cycle by C_n and label its vertices consecutively by $a_1, a_2, \ldots, a_n$. We call the subtree of U_n attached to the vertex a_i the a_i-tree; the vertex a_i belongs to the a_i-tree.

Denote by T_{a_i} the forest obtained by deleting a_i from the a_i-tree, and by $T_{i,n}$ the subgraph obtained by deleting from U_n the union of the a_1-tree, a_2-tree, ..., a_{i-1}-tree. Then we have

$$U_n - a_1 = T_{a_1} \cup T_{2,n}$$

Denote by $T_{[a_i]}$ the forest obtained by deleting from the a_i-tree both the vertex a_i and the vertices adjacent to it. Then we have

$$U_n - [a_1] = T_{[a_1]} \cup T_{3,n-1} \cup T_{a_2} \cup T_{a_n}$$

Note that $T_{3,n-1}$ is the subgraph obtained by deleting from U_{n-1} the union of the a_1- and a_2-trees. In harmony with the above specified notation, the graph U_{n-1} is unicyclic, containing a cycle on $n-1$ vertices. The vertices of this cycle are $a_1, \ldots, a_{n-1}$, and the subtrees attached to them are the same as in the case of U_n.

If u is a vertex of the a_i-tree and $d(u, a_i) \geq 2$, then we denote by $\overline{a_i}$ the vertex adjacent to a_i in the unique path of the a_i-tree, connecting u and a_i. The connected component of T_{a_i} containing the vertex u is denoted by T_u.

LEMMA 2. *Let* U *be a unicyclic graph,* u *a vertex of the* a_i*-tree, and* $d(u, a_i) \geq 2$*, then*

$$\sigma(T_{a_i} - u)\,\sigma(T_{[a_i]}) - \sigma(T_{a_i})\,\sigma(T_{[a_i]} - u) \begin{cases} > 0 & \text{if } d(u,a_i) \text{ is even} \\ < 0 & \text{if } d(u,a_i) \text{ is odd} \end{cases}$$

PROOF. By Properties 1 and 2,

$$\begin{aligned}
&\sigma(T_{a_i} - u)\,\sigma(T_{[a_i]}) - \sigma(T_{a_i})\,\sigma(T_{[a_i]} - u) \\
&= \sigma(T_u - u)\,\sigma(T_{a_i} - T_u)\,\sigma(T_u - \overline{a_i})\,\sigma(T_{[a_i]} - (T_u - \overline{a_i})) \\
&\quad - \sigma(T_u)\,\sigma(T_{a_i} - T_u)\,\sigma(T_u - \overline{a_i} - u)\,\sigma(T_{[a_i]} - (T_u - \overline{a_i})) \\
&= \sigma(T_{a_i} - T_u))\,\sigma(T_{[a_i]} - (T_u - \overline{a_i}))[\sigma(T_u - u)\,\sigma(T_u - \overline{a_i}) - \sigma(T_u)\,\sigma(T_u - \overline{a_i} - u)]
\end{aligned}$$

Because T_u is a tree, by Lemma 1 we have

$$\sigma(T_u - u)\,\sigma(T_u - \overline{a_i}) - \sigma(T_u)\,\sigma(T_u - \overline{a_i} - u) \begin{cases} < 0 & \text{if } d(u,\overline{a_i}) \text{ is even} \\ > 0 & \text{if } d(u,\overline{a_i}) \text{ is odd} \end{cases}$$

Since $\sigma(T_{a_i} - T_u)\,\sigma(T_{[a_i]} - (T_u - \overline{a_i})) > 0$, we have

$$\sigma(T_{a_i} - u)\,\sigma(T_{[a_i]}) - \sigma(T_{a_i})\,\sigma(T_{[a_i]} - u) \begin{cases} > 0 & \text{if } d(u,a_i) = d(u,\overline{a_i}) + 1 \text{ is even} \\ < 0 & \text{if } d(u,a_i) = d(u,\overline{a_i}) + 1 \text{ is odd} \end{cases}$$

The proof is complete. □

LEMMA 3. *Assume that T is a tree, and u and v are distinct vertices of T. Let P be the unique path connecting u and v. Then,*

$$\Delta_{uv}(T) = (-1)^{d(u,v)}\, \sigma(T-P)\, \sigma(T-[P])$$

where $T-[P]$ stands for the subgraph obtained by deleting from T the vertices of P and their first neighbors.

3. The main results

We start with two counterexamples.

COUNTEREXAMPLE 1. Let G_a be the graph depicted in Figure 1. This graph is connected and the distance between its vertices u and v is 4. By direct calculation we check that $\sigma(G_a-u)=92$, $\sigma(G_a-v)=114$, $\sigma(G_a)=152$, $\sigma(G_a-u-v)=69$, and thus $\Delta_{uv}(G_a)=\sigma(G_a-u)\,\sigma(G_a-v)-\sigma(G_a)\,\sigma(G_a-u-v)=0$. It seems that the possibility that for a connected graph $\Delta_{uv}(G)$ may be equal to zero was not anticipated by Merrifield and Simmons [**5**].

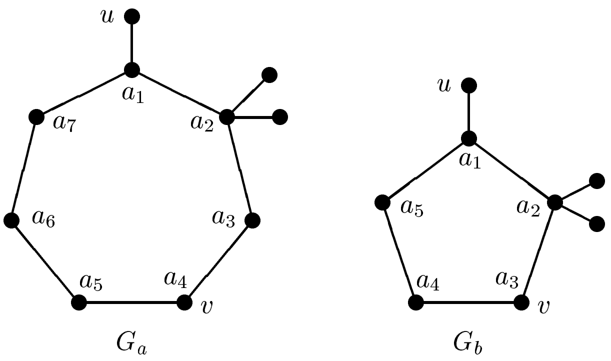

Figure 1

COUNTEREXAMPLE 2. Let G_b be the graph shown in Figure 1. Here $d(u,v)=3$, an odd number. It is not difficult to see that $\sigma(G_b-u)=35$, $\sigma(G_b-v)=38$, $\sigma(G_b)=58$, $\sigma(G_b-u-v)=23$, and thus $\Delta_{uv}(G_b)=-4<0$, contradicting to relation (1). This example shows that the Merrifield–Simmons conjecture is not generally valid already in the case of sparse graphs.

Our first theorem gives a family of counterexamples for the conjecture, including Counterexample 2 as a special case.

Let U_n be a unicyclic graph with a cycle C_n, such that e_i pendant vertices are attached to the vertex a_i of C_n , $i=1,2,\ldots,n$. In other words, the subtree of U_n attached to a_i is an (e_i+1)-vertex star.

Let u be a vertex of U_n, belonging to the a_1-tree, $u \neq a_1$, and let $v=a_3$. Therefore $d(u,v)=3$.

THEOREM 1. *If n is odd, $n \geq 5$, if $e_3 = e_4 = \cdots = e_n = 0$; $e_1, e_2 > 0$ and if*

$$1 + \sum_{i=1}^{n-4} \sigma(P_i)\,\sigma(P_{i-1}) \;<\; 2^{e_2} \tag{2}$$

then the above described graph U_n is a counterexample for the Merrifield–Simmons conjecture.

The structure of the graphs for which Theorem 1 applies is shown in Figure 2.

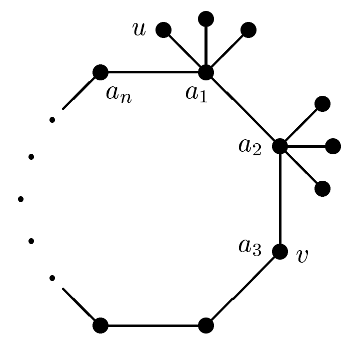

Figure 2

PROOF. Consider first the general case, when $e_i \geq 0$, $i = 1, 2, \ldots, n$. Denote by P the shortest path of U_n connecting a_2 and v. Then by Properties 1 and 2 and Lemma 3,

$$\begin{aligned}
\Delta_{uv}(U_n) &= \sigma(U_n - u)\,\sigma(U_n - v) - \sigma(U_n)\,\sigma(U_n - u - v) \\
&= [\sigma(U_n - a_1 - u) + \sigma(U_n - [a_1] - u)][\sigma(U_n - a_1 - v) + \sigma(U_n - [a_1] - v)] \\
&\quad - [\sigma(U_n - a_1) + \sigma(U_n - [a_1])][\sigma(U_n - a_1 - u - v) + \sigma(U_n - [a_1] - u - v)] \\
&= \Delta_{uv}(U_n - a_1) + \Delta_{uv}(U_n - [a_1]) + [\sigma(U_n - a_1 - u)\,\sigma(U_n - [a_1] - v) \\
&\quad + \sigma(U_n - a_1 - v)\,\sigma(U_n - [a_1] - u) - \sigma(U_n - a_1)\,\sigma(U_n - [a_1] - u - v) \\
&\quad - \sigma(U_n - [a_1])\,\sigma(U_n - a_1 - u - v)] \\
&= 0 + 0 + 2^{e_1 + e_n - 1}[\sigma(T_{2,n-1} - a_2)\,\sigma(T_{2,n} - v) - \sigma(T_{2,n})\,\sigma(T_{2,n-1} - a_2 - v)] \\
&= 2^{e_1 + e_n - 1}\,[2^{e_n}\,[\sigma(T_{2,n-1} - v)\,\sigma(T_{2,n-1} - a_2) - \sigma(T_{2,n-1})\,\sigma(T_{2,n-1} - a_2 - v)] \\
&\quad + 2^{e_{n-1}}\,[\sigma(T_{2,n-2} - v)\,\sigma(T_{2,n-1} - a_2) - \sigma(T_{2,n-2})\,\sigma(T_{2,n-1} - a_2 - v)]] \\
&= 2^{e_1 + e_n - 1}\,[2^{e_n}\,\sigma(T_{2,n-1} - P)\,\sigma(T_{2,n-1} - [P]) \\
&\quad + 2^{e_{n-1}}\,[\sigma(T_{2,n-2} - v)\,\sigma(T_{2,n-1} - a_2) - \sigma(T_{2,n-2})\,\sigma(T_{2,n-1} - a_2 - v)]] \\
&= 2^{e_1 + e_n - 1}\,[2^{e_n}\,\sigma(T_{2,n-1} - P)\,\sigma(T_{2,n-1} - [P]) \\
&\quad + 2^{2\,e_{n-1}}\,\sigma(T_{2,n-2} - P)\,\sigma(T_{2,n-2} - [P]) \\
&\quad + 2^{e_{n-1} + 2e_{n-2}}\,\sigma(T_{2,n-3} - P)\,\sigma(T_{2,n-3} - [P]) \\
&\quad + \cdots + 2^{e_{n-1} + e_{n-2} + \cdots + e_6 + 2e_5}\,\sigma(T_{2,4} - P)\,\sigma(T_{2,4} - [P])
\end{aligned}$$

$$
\begin{aligned}
&+ 2^{e_{n-1}+e_{n-2}+\cdots+e_4}\,[\sigma(T_{2,3}-v)\,\sigma(T_{2,4}-a_2)-\sigma(T_{2,3})\,\sigma(T_{2,4}-a_2-v)]]\\
&= 2^{e_1+e_n-1}\,[2^{e_n}\,\sigma(T_{4,n-1})\,\sigma(T_{5,n-1})\,2^{e_2+e_3+e_4}\\
&\quad + 2^{2e_{n-1}}\,\sigma(T_{4,n-2})\,\sigma(T_{5,n-2})\,2^{e_2+e_3+e_4}\\
&\quad + 2^{e_{n-1}+2e_{n-2}}\,\sigma(T_{4,n-3})\,\sigma(T_{5,n-3})\,2^{e_2+e_3+e_4}\\
&\quad + \cdots + 2^{e_{n-1}+e_{n-2}+\cdots+e_6+2e_5+e_4+e_3+e_2}\,(2^{e_4}+1)\\
&\quad + 2^{e_{n-1}+e_{n-2}+\cdots+e_5+2e_4+e_3+e_2} - 2^{e_{n-1}+e_{n-2}+\cdots+e_3+2e_2}]
\end{aligned}
$$

Now, in our case $e_n = e_{n-1} = \cdots = e_3 = 0$, and therefore

$$
\begin{aligned}
\Delta_{uv}(U_n) = 2^{e_2+e_1-1}[&\sigma(P_{n-4})\,\sigma(P_{n-5}) + \sigma(P_{n-5})\,\sigma(P_{n-6}) + \cdots + \sigma(P_2)\,\sigma(P_1)\\
&+ \sigma(P_1)\,\sigma(P_0) + 1 - 2^{e_2}]
\end{aligned}
$$

It is now evident that $\Delta_{uv}(U_n)$ will be negative–valued whenever the condition (2) is obeyed; this can be achieved by choosing e_2 sufficiently large. On the other hand, $d(u,v) = 3$ is odd, which contradicts to (1). □

The next two theorems show that, nevertheless, many unicyclic graphs obey the Merrifield–Simmons conjecture.

THEOREM 2. *Let U_n be the previously described (connected) unicyclic graph. Let the parameter n be even, i.e., U_n is bipartite. Let u and v be distinct vertices of U_n. Then relations (1) are satisfied.*

PROOF. have to distinguish between the following three cases.
Case 1. u and v belong to the same tree.
Case 2. u and v belong to different trees and at least one of them is not in C_n.
Case 3. u and v belong to C_n.

Case 1. Without loss of generality we may assume that u and v belong to the a_1-tree. From Lemma 1 we know that

$$
\Delta_{uv}(U_n) = (-1)^{d(u,v)+1}\prod_{i=1}^{n}\sigma(R_i - r_i)\,\sigma(R_i - [r_i])\begin{cases} <0 & \text{if } d(u,v) \text{ is even}\\ >0 & \text{if } d(u,v) \text{ is odd}\end{cases}
$$

Therefore, Theorem 2 is true in the Case 1.

Case 2 needs to be divided into two subcases:
Subcase 2.1. u belongs to the a_1-tree, $u \neq a_1$ and $v = a_i$;
Subcase 2.2. u belongs to the a_1-tree, $u \neq a_1$ and v is in the a_i-tree, $v \neq a_i$.

Both subcases need to be further divided into:
Subcase 2.1.1. u belongs to the a_1-tree, $d(u,a_1) \geq 2$ and $v = a_i$ $(3 \leq i \leq n/2+1)$;
Subcase 2.1.2. u belongs to the a_1-tree, v is in the unique cycle, and $v = a_2$, $d(u,a_1) \geq 2$;
Subcase 2.1.3. u belongs to the a_1-tree and $v = a_2$, $d(u,a_1) = 1$, $d(u,v) = 2$;
Subcase 2.1.4. u belongs to the a_1-tree, v is in the unique cycle and $d(u,a_1) = 1$, $v = a_i$, $3 \leq i \leq n/2+1$;
Subcase 2.2.1. u belongs to the a_1-tree, $d(u,a_1) \geq 2$ and v belongs to the a_i-tree,

$3 \le i \le n/2+1$, $v \ne a_i$;
Subcase 2.2.2. u belongs to the a_1-tree, $d(u,a_1) \ge 2$ and v belongs to the a_2-tree, $d(v,a_2) \ge 2$;
Subcase 2.2.3. u belongs to the a_1-tree, $d(u,a_1) = 1$ and v belongs to the a_2-tree, $d(v,a_2) \ge 2$;
Subcase 2.2.4. u belongs to the a_1-tree, $d(u,a_1) = 1$ and v belongs to the a_2-tree, $d(v,a_2) = 1$.

Proof of Subcase 2.1.1. Under the conditions specified in Subcase 2.1.1 we have

$$\begin{aligned}
\Delta_{uv}(U_n) &= \sigma(U_n-u)\,\sigma(U_n-v) - \sigma(U_n)\,\sigma(U_n-u-v)\\
&= [\sigma(U_n-a_1-u)+\sigma(U_n-[a_1]-u)][\sigma(U_n-a_1-v)+\sigma(U_n-[a_1]-v)]\\
&\quad - [\sigma(U_n-a_1)+\sigma(U_n-[a_1])][\sigma(U_n-a_1-u-v)+\sigma(U_n-[a_1]-u-v)]\\
&= \Delta_{uv}(U_n-a_1)+\Delta_{uv}(U_n-[a_1]) + [\sigma(U_n-a_1-u)\,\sigma(U_n-[a_1]-v)\\
&\quad + \sigma(U_n-a_1-v)\,\sigma(U_n-[a_1]-u) - \sigma(U_n-a_1)\,\sigma(U_n-[a_1]-u-v)\\
&\quad - \sigma(U_n-[a_1])\,\sigma(U_n-a_1-u-v)]\\
&= [\sigma(T_{a_1}-u)\,\sigma(T_{2,n})\,\sigma(T_{a_1})\,\sigma(T_{2,n}-v)\\
&\quad - \sigma(T_{a_1})\,\sigma(T_{2,n})\,\sigma(T_{a_1}-u)\,\sigma(T_{2,n}-v)]\\
&\quad + [\sigma(T_{[a_1]}-u)\,\sigma(T_{3,n-1})\,\sigma(T_{a_2})\,\sigma(T_{a_n})\,\sigma(T_{[a_1]})\,\sigma(T_{3,n-1})\,\sigma(T_{a_2})\,\sigma(T_{a_n})\\
&\quad - \sigma(T_{[a_1]})\,\sigma(T_{3,n-1})\,\sigma(T_{a_2})\,\sigma(T_{a_n})\,\sigma(T_{[a_1]}-u)\,\sigma(T_{3,n-1}-v)\,\sigma(T_{a_2})\,\sigma(T_{a_n})]\\
&\quad + [\sigma(T_{a_1}-u)\,\sigma(T_{2,n})\,\sigma(T_{[a_1]})\,\sigma(T_{3,n-1}-v)\,\sigma(T_{a_2})\,\sigma(T_{a_n})\\
&\quad + \sigma(T_{[a_1]}-u)\,\sigma(T_{3,n-1})\,\sigma(T_{a_2})\,\sigma(T_{a_n})\,\sigma(T_{a_1})\,\sigma(T_{2,n}-v)\\
&\quad - \sigma(T_{a_1})\,\sigma(T_{2,n})\,\sigma(T_{[a_1]}-u)\,\sigma(T_{3,n-1}-v)\,\sigma(T_{a_2})\,\sigma(T_{a_n})\\
&\quad - \sigma(T_{[a_1]})\,\sigma(T_{3,n-1})\,\sigma(T_{a_2})\,\sigma(T_{a_n})\,\sigma(T_{a_1}-u)\,\sigma(T_{2,n}-v)]\\
&= 0+0+\sigma(T_{a_2})\,\sigma(T_{a_n})\,\sigma(T_{2,n})\,\sigma(T_{3,n-1}-v)\\
&\quad \times [\sigma(T_{a_1}-u)\,\sigma(T_{a_1}) - \sigma(T_{a_1})\,\sigma(T_{[a_1]}-u)]\\
&\quad + \sigma(T_{a_2})\,\sigma(T_{a_n})\,\sigma(T_{3,n-1})\,\sigma(T_{2,n}-v)\\
&\quad \times [\sigma(T_{[a_1]}-u)\,\sigma(T_{a_1}) - \sigma(T_{[a_1]})\,\sigma(T_{a_1}-u)]\\
&= \sigma(T_{a_2})\,\sigma(T_{a_n})[\sigma(T_{2,n})\,\sigma(T_{3,n-1}-v) - \sigma(T_{3,n-1})\,\sigma(T_{2,n}-v)]\\
&\quad \times [\sigma(T_{a_1}-u)\,\sigma(T_{[a_1]}) - \sigma(T_{a_1})\,\sigma(T_{[a_1]}-u)]\\
&= \sigma(T_{a_2})[\sigma(T_{2,n})\,\sigma(T_{3,n}-a_n-v) - \sigma(T_{3,n}-a_n)\,\sigma(T_{2,n}-v)]\\
&\quad \times [\sigma(T_{a_1}-u)\,\sigma(T_{[a_1]}) - \sigma(T_{a_1})\,\sigma(T_{[a_1]}-u)]\\
&= \sigma(T_{a_2})\,X_1\,X_2
\end{aligned}$$

where

$$\begin{aligned}
X_1 &= \sigma(T_{2,n})\,\sigma(T_{3,n}-a_n-v) - \sigma(T_{3,n}-a_n)\,\sigma(T_{2,n}-v)\\
X_2 &= \sigma(T_{a_1}-u)\,\sigma(T_{[a_1]}) - \sigma(T_{a_1})\,\sigma(T_{[a_1]}-u)
\end{aligned}$$

Since u is in the a_1-tree and $d(u,a_1)\geq 2$, by Lemma 2,

$$X_2\begin{cases} >0 & \text{if } d(u,a_1) \text{ is even}\\ <0 & \text{if } d(u,a_1) \text{ is odd}\end{cases}$$

When $i=2k$, $3\leq i\leq n/2+1$ and $v=a_i$, we have

$$\begin{aligned}
X_1 &= \sigma(T_{2,n})\,\sigma(T_{3,n}-a_n-v)-\sigma(T_{3,n}-a_n)\,\sigma(T_{2,n}-v)\\
&= \sigma(T_{3,n}-a_n-v)\,[\sigma(T_{3,n})\,\sigma(T_{a_2})+\sigma(T_{4,n})\,\sigma(T_{[a_2]})\,\sigma(T_{a_3})]\\
&\quad -\sigma(T_{3,n}-a_n)\,[\sigma(T_{3,n}-v)\,\sigma(T_{a_2})+\sigma(T_{4,n}-v)\,\sigma(T_{[a_2]})\,\sigma(T_{a_3})]\\
&= [\sigma(T_{3,n}-a_n-v)\,\sigma(T_{3,n})-\sigma(T_{3,n}-a_n)\,\sigma(T_{3,n}-v)]\,\sigma(T_{a_2})\\
&\quad +\sigma(T_{a_3})\sigma(T_{[a_2]})\,[\sigma(T_{3,n}-a_n-v)\,\sigma(T_{4,n})-\sigma(T_{3,n}-a_n)\,\sigma(T_{4,n}-v)]\\
&= q_1\,\sigma(T_{a_2})+\sigma(T_{a_3})\,\sigma(T_{[a_2]})\,[\sigma(T_{3,n}-a_n-v)\,\sigma(T_{4,n})\\
&\quad -\sigma(T_{3,n}-a_n)\,\sigma(T_{4,n}-v)]\\
&= q_1\,\sigma(T_{a_2})+\sigma(T_{a_3})\,\sigma(T_{[a_2]})\,[[\sigma(T_{4,n}-a_n-v)\,\sigma(T_{a_3})\\
&\quad +\sigma(T_{5,n}-a_n-v)\,\sigma(T_{[a_3]})\,\sigma(T_{a_4})]\sigma(T_{4,n})\\
&\quad -\sigma(T_{4,n}-v)\,[\sigma(T_{4,n}-a_n)\,\sigma(T_{a_3})+\sigma(T_{5,n}-a_n)\,\sigma(T_{[a_3]})\,\sigma(T_{a_4})]]\\
&= q_1\,\sigma(T_{a_2})+(\sigma(T_{a_3}))^2\,\sigma(T_{[a_2]})\,[\sigma(T_{4,n}-a_n-v)\,\sigma(T_{4,n})\\
&\quad -\sigma(T_{4,n}-v)\,\sigma(T_{4,n}-a_n)]\\
&\quad +\sigma(T_{[a_2]})]\,\sigma(T_{a_3})\,\sigma(T_{[a_3]})\,\sigma(T_{a_4})\,[\sigma(T_{4,n})\,\sigma(T_{5,n}-a_n-v)\\
&\quad -\sigma(T_{4,n}-v)\,\sigma(T_{5,n}-a_n)]\\
&= q_1\,\sigma(T_{a_2})+q_2\,(\sigma(T_{a_3}))^2\,\sigma(T_{[a_2]})+q_3\,(\sigma(T_{a_4}))^2\,\sigma(T_{[a_2]})\\
&\quad \times[\sigma(T_{a_3})\,\sigma(T_{[a_3]})+\sigma(T_{[a_2]})]\,\sigma(T_{a_3})\,\sigma(T_{[a_3]})\,\sigma(T_{a_4})\,\sigma(T_{[a_4]})\,\sigma(T_{a_5})\\
&\quad \times[\sigma(T_{5,n}-a_n-v)\,\sigma(T_{6,n})-\sigma(T_{5,n}-a_n)\,\sigma(T_{6,n}-v)]\\
&= q_1\,\sigma(T_{a_2})+q_2\,(\sigma(T_{a_3}))^2\,\sigma(T_{[a_2]})+\cdots+q_{2k-3}\,(\sigma(T_{a_{2k-2}}))^2\,\sigma(T_{[a_2]})]\\
&\quad \times\sigma(T_{a_3})\,\sigma(T_{[a_3]})\cdots\sigma(T_{[a_{2k-3}]})+\sigma(T_{[a_2]})\,\sigma(T_{a_3})\,\sigma(T_{[a_3]})\cdots\\
&\quad \times\sigma(T_{a_{2k-2}})\,\sigma(T_{[a_{2k-2}]})\,\sigma(T_{a_{2k-1}})[\sigma(T_{2k-1,n}-a_n-v)\,\sigma(T_{2k,n})\\
&\quad -\sigma(T_{2k-1,n}-a_n)\,\sigma(T_{2k,n}-v)]\\
&= q_1\,\sigma(T_{a_2})+\cdots+q_{2k-2}\,(\sigma(T_{a_{2k-1}}))^2\,\sigma(T_{[a_2]})\,\sigma(T_{a_3})\,\sigma(T_{[a_3]})\cdots\sigma(T_{[a_{2k-2}]})\\
&\quad +\sigma(T_{[a_2]})\,\sigma(T_{a_3})\,\sigma(T_{[a_3]})\cdots\sigma(T_{[a_{2k-1}]})\,\sigma(T_{a_{2k}})\\
&\quad \times[\sigma(T_{2k+1,n}-a_n)\,\sigma(T_{2k,n})-\sigma(T_{2k+1,n}-a_n)\,\sigma(T_{2k,n}-v)]
\end{aligned}$$

where for $j=1,2,\dots,2k-2$,

$$\begin{aligned}
q_j &= \sigma(T_{j+2,n}-a_n-v)\,\sigma(T_{j+2,n})-\sigma(T_{j+2,n}-a_n)\,\sigma(T_{j+2,n}-v)\\
&= -[\sigma(T_{j+2,n}-a_n)\,\sigma(T_{j+2,n}-v)-\sigma(T_{j+2,n}-a_n-v)\,\sigma(T_{j+2,n})]
\end{aligned}$$

Note that the last term in the above expression for X_1 is equal to

$$\begin{aligned}
&\sigma(T_{[a_2]})\,\sigma(T_{a_3})\,\sigma(T_{[a_3]})\cdots\sigma(T_{[a_{2k-1}]})\,\sigma(T_{a_{2k}})\,[\sigma(T_{2k+1,n}-a_n)\,\sigma(T_{2k,n})\\
&\quad -\sigma(T_{2k+1,n}-a_n)\,\sigma(T_{2k,n}-v)]\;>\;0
\end{aligned}$$

Since $T_{j+2,n}$ is a tree, by Lemma 1 we know that

$$q_j \begin{cases} > 0 & \text{if } d(v, a_n) \text{ is even} \\ < 0 & \text{if } d(v, a_n) \text{ is odd} \end{cases}$$

Because $d(v, a_n) = d(a_{2k}, a_n)$ is even, it must be $q_j > 0$ for $j = 1, 2, \ldots, 2k-2$. So we have $X_1 > 0$ when $i = 2k$, $3 \le i \le n/2+1$ and $v = a_i$.

The conclusions obtained so far can be summarized in the following table.

$d(u,a_1)$	X_1	X_2	$d_{U_n}(u,v) = d(u,a_1) + 2k - 1$	$\Delta_{uv}(U_n) = \sigma(T_{a_2})\, X_1\, X_2$
odd	> 0	< 0	even	< 0
even	> 0	> 0	odd	> 0

Hence, when $i = 2k$, $3 \le i \le n/2+1$ and $v = a_i, d(u, a_1) \ge 2$, Theorem 2 is true.

If $i = 2k+1$, $3 \le i \le n/2+1$ and $v = a_i$, then we have

$$\begin{aligned} X_1 &= \sigma(T_{2,n})\, \sigma(T_{3,n} - a_n - v) - \sigma(T_{3,n} - a_n)\, \sigma(T_{2,n} - v) \\ &= q_1\, \sigma(T_{a_2}) + q_2\, (\sigma(T_{a_3}))^2\, \sigma(T_{[a_2]}) + q_3\, (\sigma(T_{a_4}))^2\, \sigma(T_{[a_2]})]\, \sigma(T_{a_3})\, \sigma(T_{[a_3]}) + \cdots \\ &\quad + q_{2k-2}\, (\sigma(T_{a_{2k-2}}))^2\, \sigma(T_{[a_2]})]\, \sigma(T_{a_3})\, \sigma(T_{[a_3]}) \cdots \sigma(T_{[a_{2k-2}]}) \\ &\quad + \sigma(T_{[a_2]})\, \sigma(T_{a_3})\, \sigma(T_{[a_3]}) \cdots \sigma(T_{a_{2k-1}})\, \sigma(T_{a_{2k}}) \\ &\quad \times [\sigma(T_{2k+1,n} - a_n - v)\, \sigma(T_{2k,n}) - \sigma(T_{2k,n} - a_n)\, \sigma(T_{2k,n} - v)] \\ &= q_1\, \sigma(T_{a_2}) + q_2\, (\sigma(T_{a_3}))^2\, \sigma(T_{[a_2]}) \\ &\quad + q_3\, (\sigma(T_{a_4}))^2\, \sigma(T_{[a_2]})]\, \sigma(T_{a_3})\, \sigma(T_{[a_3]}) \\ &\quad + \ \cdots \ + q_{2k-2}\, (\sigma(T_{a_{2k-2}}))^2\, \sigma(T_{[a_2]})]\, \sigma(T_{a_3})\, \sigma(T_{[a_3]}) \cdots \sigma(T_{[a_{2k-2}]}) \\ &\quad + q_{2k-1}\, (\sigma(T_{a_{2k}}))^2\, \sigma(T_{[a_2]})]\, \sigma(T_{a_3})\, \sigma(T_{[a_3]}) \cdots \sigma(T_{a_{2k-1}})\, \sigma(T_{[a_{2k-1}]}) + \\ &\quad + \sigma(T_{[a_2]})\, \sigma(T_{a_3})\, \sigma(T_{[a_3]}) \cdots \sigma(T_{a_{2k}})\, \sigma(T_{[a_{2k}]})\, \sigma(T_{a_{2k+1}})\, \sigma(T_{2k+2,n}) \\ &\quad \times [\sigma(T_{2k+1,n} - a_n - v) - \sigma(T_{2k+1,n} - a_n)] \end{aligned}$$

where for $j = 1, 2, \ldots, 2k-1$,

$$\begin{aligned} q_j &= \sigma(T_{j+2,n} - a_n - v)\, \sigma(T_{j+2,n}) - \sigma(T_{j+2,n} - a_n)\, \sigma(T_{j+2,n} - v) \\ &= -[\sigma(T_{j+2,n} - a_n)\, \sigma(T_{j+2,n} - v) - \sigma(T_{j+2,n} - a_n - v)\, \sigma(T_{j+2,n})] \end{aligned}$$

Note that the last term in the above expression for X_1 is:

$$\begin{aligned} &\sigma(T_{[a_2]})\, \sigma(T_{a_3})\, \sigma(T_{[a_3]}) \cdots \sigma(T_{a_{2k}})\, \sigma(T_{[a_{2k}]})\, \sigma(T_{a_{2k+1}})\, \sigma(T_{2k+2,n}) \\ &\quad \times [\sigma(T_{2k+1,n} - a_n - v) - \sigma(T_{2k+1,n} - a_n)] \ < \ 0 \end{aligned}$$

Since $T_{j+2,n}$ is a tree, by Lemma 1,

$$q_j \begin{cases} > 0 & \text{if } d(v, a_n) \text{ is even} \\ < 0 & \text{if } d(v, a_n) \text{ is odd} \end{cases}$$

Because $d(v, a_n) = d(a_{2k+1}, a_n)$ is odd, it must be $q_j < 0$ for $j = 1, 2, \ldots, 2k-1$. So we have $X_1 < 0$ when $i = 2k+1$, $3 \le i \le n/2+1$ and $v = a_i$. Now we have the following table:

$d(u,a_1)$	X_1	X_2	$d_{U_n}(u,v) = d(u,a_1) + 2k$	$\Delta_{uv}(U_n) = \sigma(T_{a_2})\, X_1\, X_2$
odd	< 0	< 0	odd	> 0
even	< 0	> 0	even	< 0

Hence, when $v = a_i$, $i = 2k+1$, $3 \leq i \leq n/2+1$, $d(u,a_1) \geq 2$, Theorem 2 is also true.

This completes the analysis of Subcase 2.1.1. □

Based on a suggestion by the referee, we omit the equally lengthy and to a great extent analogous considerations needed to verify the validity of Theorem 2 in the remaining subcases. For the same reason we also skip the proof of Theorem 2 for Case 3. These omitted parts of the proof are available from the authors (X. L.) upon request.

By a reasoning similar to that used in the proof of Theorem 2, we obtain the following result.

Let U_n be as before and let n be odd. Let u and v be distinct, nonadjacent vertices of U_n .

THEOREM 3. *If $e_1 = e_2 = \cdots = e_n = e$, a positive integer, then for the above described graph U_n the relations (1) are satisfied.*

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Yong Wang and Xueliang Li
Department of Applied Mathematics
Northwestern Polytechnical University
X'ian, Shaanxi 710072
P.R. China

iamlxl@nwpu.edu.cn

Prirodno-matematički fakultet
34000 Kragujevac, p.p. 60
Yugoslavia

gutman@knez.uis.kg.ac.yu

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