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On Maximal Energy of Trees with Fixed Weight Sequence

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Abstract

Let $W = \{w_1, w_2, \ldots, w_{n-1}\}$ be a sequence of positive numbers. Denote by $\mathcal{T}(n, W)$ the set of all weighted trees of order n with weight sequence W. We show that a weighted tree that has maximal energy in $\mathcal{T}(n, W)$, is a weighted path. For $n \leq 6$, we determine the unique path having maximal energy in $\mathcal{T}(n, W)$. For $n \geq 7$, we give a conjecture on the structure and distribution of weights of the unique maximum–energy tree in $\mathcal{T}(n, W)$. Some results supporting this conjecture are obtained.

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1 Introduction

In this paper we consider trees on n vertices, to each edge of which a positive weight is assigned. The sequence of weights of the edges in a weighted tree is referred to as its weight sequence. Let $W = \{w_1, w_2, \ldots, w_{n-1}\}$ be a sequence of positive numbers. Denote by $\mathcal{T}(n, W)$ the set of all weighted trees of order n with weight sequence W.

In general, the energy of a weighted graph G of order n is defined as

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the (real) eigenvalues of the (nonnegative, symmetric) adjacency matrix $\mathbf{A}$ of G. More information on (weighted) graph energy can be found in [2–6, 10, 12, 15, 17, 21].

In [3], Brualdi et al. investigated the extremal energy of a class of integral weighted graphs. Let $\mathcal{T}(n, m)$ be the set of all weighted trees of order n with the fixed total weight sum m. They stated the following conjecture pertaining to the maximal energy of all integral weighted trees with fixed weight:

Conjecture 1. [3, Conjecture 10] *Let $n \geq 5$ and $m \geq n$. The path with weight sequence $\{m - n + 2, 1, \ldots, 1\}$, where the weight of one of the pendent edges equals $m - n + 2$, is the unique integral weighted tree in $\mathcal{T}(n, m)$ with maximal energy.*

Let $\hat{\mathbb{E}}(n, W) = \max\{\mathcal{E}(T) : T \in \mathcal{T}(n, W)\}$ be the maximal energy of a tree in $\mathcal{T}(n, W)$. Motivated by the above conjecture, in this paper we consider the following problem:

Problem 2. *For a given weight sequence W, determine the tree(s) in $\mathcal{T}(n, W)$ whose energy achieves $\hat{\mathbb{E}}(n, W)$.*

We show that in $\mathcal{T}(n, W)$, a weighted tree with maximal energy is a weighted path. Further, for small order n (≤ 6), we determine the unique path having maximal energy in $\mathcal{T}(n, W)$. For larger order n, we give a conjecture on the structure and the distribution of weights of the unique tree in $\mathcal{T}(n, W)$. Finally, some results supporting this conjecture are obtained.

2 Preliminary results

We first introduce some terminology and notation. Let $G = (V(G), E(G))$ be a graph. For $V_1 = \{v_1, v_2, \ldots, v_s\} \subseteq V(G)$ and $E_1 = \{e_1, e_2, \ldots, e_k\} \subseteq E(G)$, denote by $G \backslash E_1$ the graph obtained from G by deleting all edges of E_1 and by $G \backslash V_1$ the graph obtained from G by removing all vertices of V_1 together with all incident edges. For convenience, we sometimes write $G \backslash e_1 e_2 \ldots e_k$ and $G \backslash v_1 v_2 \ldots v_s$ instead of $G \backslash E_1$ and $G \backslash V_1$, respectively. Denote by $P_n = u_1 e_1 u_2 \ldots u_{n-1} e_{n-1} u_n$ the path on n vertices, where u_i and u_{i+1} are the two endvertices of the edge e_i. For convenience, we sometimes denote by $P = u_1 w_1 u_2 w_2 u_3 \ldots u_{n-1} w_{n-1} u_n$ or $P = w_1 w_2 \ldots w_{n-1}$ a weighted path on n vertices, where w_i denotes the weight of the edge e_i for $i = 1, 2, \ldots, n-1$. We refer to Cvetković et al. [5] for terminology and notation not defined here.

A graph is said to be *elementary* if it is isomorphic either to P_2 or to a cycle. The weight of P_2 is defined as the square of the weight of its unique edge. The weight of a cycle is the product of the weights of all its edges.

A graph $\mathscr{H}$ is called a *Sachs graph* if each component of $\mathscr{H}$ is an elementary graph [8, 9, 14]. The weight of a Sachs graph $\mathscr{H}$, denoted by $\mathscr{W}(\mathscr{H})$, is the product of the weights of all elementary subgraphs contained in $\mathscr{H}$.

Denote by $\phi(G, \lambda)$ the *characteristic polynomial* of a graph G, defined as

$$\phi(G, \lambda) = \det\left[\lambda\, \mathbf{I}_n - \mathbf{A}(G)\right] = \sum_{k=0}^{n} a_k(G)\, \lambda^{n-k} \tag{1}$$

where $\mathbf{A}(G)$ is the adjacency matrix of G and $\mathbf{I}_n$ the identity matrix of order n. The following well known result determines all coefficients of the characteristic polynomial of a weighted graph in terms of its Sachs subgraphs [1, 5, 7, 19, 20].

Theorem 3. *Let G be a weighted graph on n vertices with adjacency matrix $\mathbf{A}(G)$ and characteristic polynomial $\phi(G, \lambda) = \sum_{k=0}^{n} a_k(G)\, \lambda^{n-k}$. Then*

$$a_i(G) = \sum_{\mathscr{H}} (-1)^{p(\mathscr{H})}\, 2^{c(\mathscr{H})}\, \mathscr{W}(\mathscr{H})$$

where the summation is over all Sachs subgraphs $\mathscr{H}$ of G having i vertices, and where $p(\mathscr{H})$ and $c(\mathscr{H})$ are, respectively, the number of components and the number of cycles contained in $\mathscr{H}$.

Similarly, we have the following recursions for the characteristic polynomial of a weighted graph [11].

Theorem 4. *Let G be a weighted graph and $e = uv$ be a cut edge of G. Denote by $w(e)$ the weight of the edge e. Then*

$$\phi(G,\lambda) = \phi(G\backslash e,\lambda) - w(e)^2\,\phi(G\backslash uv,\lambda)\,.$$

From the Coulson integral formula for the energy (see [4,15–17] and the references cited therein), it can be shown [10] that if G is a weighted bipartite graph with characteristic polynomial as in Eq. (1), then

$$\mathcal{E}(G) = \frac{1}{\pi}\int\limits_{-\infty}^{+\infty} \lambda^{-2}\ln\left(\sum_{k=0}^{\lfloor n/2\rfloor} b_{2k}\,\lambda^{2k}\right)d\lambda$$

where $b_k = |a_k|$.

It follows that in the case of weighted trees, $\mathcal{E}(T)$ is a strict monotonically increasing function of the numbers b_{2i} , $i = 1,2,\ldots,\lfloor n/2\rfloor$. Thus, in analogy to comparing the energies of two non-weighted trees [10,22,23], we introduce a quasi-ordering relation $\preceq$ for weighted trees (see also [13,18]):

Definition 5. *Let T_1 and T_2 be two weighted trees of order n. If $b_{2k}(T_1) \le b_{2k}(T_2)$ for all k with $0 \le k \le \lfloor n/2\rfloor$, then we write $T_1 \preceq T_2$. Furthermore, if $T_1 \preceq T_2$ and there exists at least one index k such that $b_{2k}(T_1) < b_{2k}(T_2)$, then we write $T_1 \prec T_2$. If $b_{2k}(T_1) = b_{2k}(T_2)$ for all k, then we write $T_1 \sim T_2$.*

Note that there are non-isomorphic weighted graphs T_1 and T_2 with $T_1 \sim T_2$, which implies that in the general case $\preceq$ is a quasi-ordering, but not a partial ordering.

According to the integral formula above, we have for two weighted trees T_1 and T_2 of order n that

$$T_1 \preceq T_2 \Longrightarrow \mathcal{E}(T_1) \le \mathcal{E}(T_2) \qquad \text{and} \qquad T_1 \prec T_2 \Longrightarrow \mathcal{E}(T_1) < \mathcal{E}(T_2)\,. \tag{2}$$

3 Main results

An immediate consequence of Theorem 4 is:

Corollary 6. *Let G be a weighted bipartite graph with a cut edge $e = uv$. Suppose that the weight of the edge e is w_e. Then*

$$b_k(G) = b_k(G \backslash e) + w_e^2\, b_{k-2}(G \backslash uv)$$

where $b_k = |a_k|$, as defined as above.

Applying Corollary 6, we can deduce that a weighted tree with maximal energy in $\mathcal{T}(n, W)$ is a weighted path.

Theorem 7. *For $n \geq 2$, let $W = \{w_1, w_2, \ldots, w_{n-1}\}$ be a sequence of positive numbers. Let T be a weighted tree with maximal energy in $\mathcal{T}(n, W)$. Then, T is a weighted path.*

Proof. We prove the theorem by induction on n. Obviously, the result holds for $n = 2, 3$. Let $n \geq 4$ and suppose that the result is true for trees of orders less than n. For any $n \geq 4$, suppose that u_1 is a pendent vertex of T and $u_1u_2 = e_1$ has weight w_e. Then using Corollary 6, we have

$$b_k(T) = b_k(T \backslash u_1) + w_e^2\, b_{k-2}(T \backslash u_1u_2)\,.$$

Let W_1 be the weight sequence of $W \backslash w_e$ and W_2 the weight sequence obtained from W by removal of the weights of all edges incident with u_2. Then by the induction assumption, the trees achieving $\hat{\mathbb{E}}(n-1, W_1)$ and $\hat{\mathbb{E}}(n-2, W_2)$ are paths or union of paths. Moreover, in order to maximize $\hat{\mathbb{E}}(n-2, W_2)$, $T \backslash u_1u_2$ has to have $n-3$ edges. Consequently, both of $T \backslash u_1$ and $T \backslash u_1u_2$ are paths and hence the result follows. □

In view of Theorem 7, in order to determine the tree(s) having energy $\hat{\mathbb{E}}(n, W)$, we focus on discussing the weight distribution of the path P_n. For convenience, denote by $\mathcal{P}(n, W)$ the set of all weighted paths of order n with weight sequence W.

Lemma 8. *For $n \geq 4$, let $P' = u_1e_1u_2e_2 \ldots u_{n-1}e_{n-1}u_n \in \mathcal{P}(n, W)$. Let the weight of the edge e_i be denoted by w_i for $i = 1, 2, \ldots, n-1$. If $\mathcal{E}(P') = \hat{\mathbb{E}}(n, W)$, then* (**a**) *$w_1 \geq w_2$, and* (**b**) *$w_{n-1} \geq w_{n-2}$.*

Proof. (**a**) Let P'' be the weighted path obtained from P' by exchanging the edges e_1 and e_2, that is, $P'' = u_1e_2u_2e_1u_3\ldots u_{n-1}e_{n-1}u_n$. Then by the hypothesis that $\mathcal{E}(P') = \hat{\mathbb{E}}(n,W)$, we have

$$\mathcal{E}(P'') \leq \mathcal{E}(P')\,. \tag{3}$$

From Corollary 6,

$$\begin{aligned} b_k(P') &= b_k(P'\backslash e_1) + w_1^2\, b_{k-2}(P'\backslash u_1u_2) \\ &= b_k(P'\backslash e_1e_2) + w_2^2\, b_{k-2}(P'\backslash u_1u_2u_3) + w_1^2\, b_{k-2}(P'\backslash e_1e_2) \end{aligned}$$

and

$$\begin{aligned} b_k(P'') &= b_k(P''\backslash e_2) + w_2^2\, b_{k-2}(P''\backslash u_1u_2) \\ &= b_k(P''\backslash e_1e_2) + w_1^2\, b_{k-2}(P''\backslash u_1u_2u_3) + w_2^2\, b_{k-2}(P''\backslash e_1e_2)\,. \end{aligned}$$

Assume to the contrary that $w_1 < w_2$. Note that $P'\backslash u_1u_2u_3 = P''\backslash u_1u_2u_3$, $P'\backslash e_1e_2 = P''\backslash e_1e_2$, and that $P'\backslash u_1u_2u_3$ is a proper subgraph of $P\backslash e_1e_2$. Then

$$b_k(P') - b_k(P'') \;=\; (w_1^2 - w_2^2)\big[b_{k-2}(P'\backslash e_1e_2) - b_{k-2}(P'\backslash u_1u_2u_3)\big] \leq 0$$

and there exists at least one index k such that $b_k(P') - b_k(P'') < 0$ as $P\backslash e_1e_2$ contains at least one edge. Thus $P' \prec P''$, a contradiction to conditions (2) and (3). Consequently, the result (**a**) follows.

The proof of (**b**) is analogous. □

Lemma 9. *For $n \geq 5$, let $P' = u_1e_1u_2e_2u_3e_3u_4\ldots u_{n-1}e_{n-1}u_n \in \mathcal{P}(n,W)$. Let the weight of the edge e_i be denoted by w_i for $i = 1,2,\ldots,n-1$. If $\mathcal{E}(P') = \hat{\mathbb{E}}(n,W)$, then* (**a**) *$w_1 \geq w_3$, and* (**b**) *$w_{n-1} \geq w_{n-3}$.*

Proof. (**a**) Let P'' be the weighted path obtained from P' by exchanging the edges e_1 and e_3, that is, $P'' = u_1e_3u_2e_2u_3e_1u_4\ldots u_{n-1}e_{n-1}u_n$. Then

$$\mathcal{E}(P'') \leq \mathcal{E}(P')\,. \tag{4}$$

By Corollary 6,

$$\begin{aligned} b_k(P') &= b_k(P'\backslash e_1) + w_1^2\, b_{k-2}(P'\backslash u_1u_2) \\ &= b_k(P'\backslash e_1e_3) + w_3^2\, b_{k-2}(P'\backslash u_2u_3u_4) \\ &+ \; w_1^2\, b_{k-2}(P'\backslash u_1u_2u_3) + w_1^2\, w_3^2\, b_{k-4}(P'\backslash u_1u_2u_3u_4) \end{aligned}$$

and

$$\begin{aligned} b_k(P'') &= b_k(P''\backslash e_3) + w_3^2\, b_{k-2}(P''\backslash u_1u_2) \\ &= b_k(P''\backslash e_3e_1) + w_1^2\, b_{k-2}(P''\backslash u_2u_3u_4) \\ &+ w_3^2\, b_{k-2}(P''\backslash u_1u_2u_3) + w_1^2\, w_3^2\, b_{k-4}(P''\backslash u_1u_2u_3u_4)\,. \end{aligned}$$

Assume to the contrary that $w_1 < w_3$. Note that $P'\backslash u_1u_2u_3 = P''\backslash u_1u_2u_3$ and $P'\backslash u_2u_3u_4 = P''\backslash u_2u_3u_4$, and that $P'\backslash u_2u_3u_4$ is the union of the isolated vertex u_1 and a proper subgraph of $P'\backslash u_1u_2u_3$. Then

$$b_k(P') - b_k(P'') = (w_3^2 - w_1^2)\big[b_{k-2}(P''\backslash u_2u_3u_4) - b_{k-2}(P''\backslash u_1u_2u_3)\big] \le 0$$

and there exists at least one integer k such that $b_k(P') - b_k(P'') < 0$. Thus $P' \prec P''$, a contradiction to condition (4). Consequently, the result (**a**) follows.

The proof of (**b**) is analogous. □

For small order n, applying Lemmas 8 and 9, we can determine the paths having maximal energy among the weighted paths in $\mathcal{P}(n, W)$.

Theorem 10. *For $n \le 6$, let $W = \{w_1, w_2, \ldots, w_{n-1}\}$ be a sequence of positive numbers such that $w_1 \ge w_2 \ge \cdots \ge w_{n-1}$, and let $P = u_1e_1u_2e_2 \ldots u_{n-1}e_{n-1}u_n \in \mathcal{P}(n, W)$ be the path having energy $\hat{\mathbb{E}}(n, W)$. Suppose $w(e_1) \ge w(e_{n-1})$. Then for $i = 1, 2, \ldots, n-1$,*

$$w(e_i) = \begin{cases} w_i & \text{if either } i \le \lceil \frac{n-1}{2} \rceil \text{ and } i \text{ is odd, or } i > \lceil \frac{n-1}{2} \rceil \text{ and } n-i \text{ is even,} \\ w_{n+1-i} & \text{otherwise.} \end{cases}$$

Proof. Bearing in mind Lemma 8 and the hypothesis that $w(e_1) \ge w(e_{n-1})$, the result follows for $n \le 4$.

For $n = 5$, from Lemmas 8 and 9, we have that the desired path is either $P_1 = w_1w_3w_4w_2$ or $P_2 = w_1w_4w_3w_2$. By a direct calculation, we have

$$\begin{aligned} b_2(P_1) &= b_2(P_2) \\ b_4(P_1) &= w_1^2\, w_4^2 + w_1^2\, w_2^2 + w_3^2\, w_2^2 \\ b_4(P_2) &= w_1^2\, w_3^2 + w_1^2\, w_2^2 + w_4^2\, w_2^2 \end{aligned}$$

from which we conclude that $P_2 \succeq P_1$. Then P_2 is the desired path and the result follows.

For $n = 6$, since $w(e_1) \geq w(e_5)$, we first show that $w(e_2) \leq w(e_4)$. Let P' be the weighted path obtained from P by exchanging the edges e_1 and e_5, that is, $P' = u_1e_5u_2e_2u_3e_3u_4e_4u_5e_1u_6$. Then

$$\mathcal{E}(P') \leq \mathcal{E}(P)\,. \tag{5}$$

By Corollary 6,

$$\begin{aligned} b_k(P) &= b_k(P\backslash e_1) + w(e_1)^2\, b_{k-2}(P\backslash u_1u_2) \\ &= b_k(P\backslash e_1e_5) + w(e_5)^2\, b_{k-2}(P\backslash e_1u_5u_6) \\ &+ w(e_1)^2\, b_{k-2}(P\backslash u_1u_2e_5) + w(e_1)^2\, w(e_5)^2\, b_{k-4}(P\backslash u_1u_2u_5u_6) \end{aligned}$$

and

$$\begin{aligned} b_k(P') &= b_k(P'\backslash e_5) + w(e_5)^2\, b_{k-2}(P'\backslash u_1u_2) \\ &= b_k(P'\backslash e_5e_1) + w(e_1)^2\, b_{k-2}(P'\backslash e_5u_5u_6) \\ &+ w(e_5)^2\, b_{k-2}(P'\backslash u_1u_2e_1) + w(e_1)^2\, w(e_5)^2\, b_{k-4}(P'\backslash u_1u_2u_5u_6) \end{aligned}$$

Hence,

$$b_k(P) - b_k(P') = \big(w(e_5)^2 - w(e_1)^2\big)\big[b_{k-2}(P\backslash e_1u_5u_6) - b_{k-2}(P\backslash u_1u_2e_5)\big].$$

So, we have

$$\begin{aligned} b_2(P) - b_2(P') &= 0 \\ b_4(P) - b_4(P') &= \big(w(e_5)^2 - w(e_1)^2\big)\big[\big(w(e_2)^2 + w(e_3)^2\big) - \big(w(e_3)^2 + w(e_4)^2\big)\big] \\ b_6(P) - b_6(P') &= 0\,. \end{aligned}$$

Since $\mathcal{E}(P') \leq \mathcal{E}(P)$, we have that $b_4(P) - b_4(P') \geq 0$. From $w(e_1) \geq w(e_5)$, it follows that $w(e_2) \leq w(e_4)$.

Taking into account Lemmas 8 and 9, we get that the desired path is $P_1 = w_1w_4w_5w_3w_2$, or $P_2 = w_1w_5w_4w_3w_2$, or $P_3 = w_1w_5w_3w_4w_2$. Direct calculation yields that

$$b_2(P_1) = b_2(P_2) = b_2(P_3)$$

$$\begin{aligned}
b_4(P_1) &= w_1^2 w_5^2 + w_1^2 w_3^2 + w_1^2 w_2^2 + w_4^2 w_3^2 + w_4^2 w_2^2 + w_5^2 w_2^2 \\
b_4(P_2) &= w_1^2 w_4^2 + w_1^2 w_3^2 + w_1^2 w_2^2 + w_5^2 w_3^2 + w_5^2 w_2^2 + w_4^2 w_2^2 \\
b_4(P_3) &= w_1^2 w_3^2 + w_1^2 w_4^2 + w_1^2 w_2^2 + w_5^2 w_4^2 + w_5^2 w_2^2 + w_3^2 w_2^2 \\
b_6(P_1) &= w_1^2 w_5^2 w_2^2 \\
b_6(P_2) &= w_1^2 w_4^2 w_2^2 \\
b_6(P_3) &= w_1^2 w_3^2 w_2^2
\end{aligned}$$

which implies $P_3 \succeq P_2 \succeq P_1$. Then P_3 is the desired path and the result follows. □

For general case $n \geq 7$, we cannot solve the problem; but we think that the following conjecture is true.

Conjecture 11. *For $n \geq 3$, let $W = \{w_1, w_2, \ldots, w_{n-1}\}$ be a sequence of positive numbers such that $w_1 \geq w_2 \geq \cdots \geq w_{n-1}$. Let $P = u_1 e_1 u_2 e_2 \ldots u_{n-1} e_{n-1} u_n \in \mathcal{P}(n, W)$ be the path having energy $\hat{\mathbb{E}}(n, W)$. Suppose $w(e_1) \geq w(e_{n-1})$. Then for $i = 1, 2, \ldots, n-1$,*

$$w(e_i) = \begin{cases} w_i & \text{if either } i \leq \lceil \frac{n-1}{2} \rceil \text{ and } i \text{ is odd, or } i > \lceil \frac{n-1}{2} \rceil \text{ and } n-i \text{ is even,} \\ w_{n+1-i} & \text{otherwise.} \end{cases}$$

Though we cannot prove the conjecture, we get the following results to support it.

Theorem 12. *For $n \geq 3$, let $W = \{x, \overbrace{y, \ldots, y}^{n-2}\}$ be a sequence of positive numbers such that $x > y$. Then, up to isomorphism, $P = x\overbrace{y \ldots y}^{n-2}$ is the unique path having energy $\hat{\mathbb{E}}(n, W)$.*

Theorem 12 can be considered as a generalized version of Theorem 11 from Ref. [3], and therefore its proof is omitted.

Theorem 13. *For $n \geq 3$, let $W = \{x, y, \overbrace{z, \ldots, z}^{n-3}\}$ be a sequence of positive numbers such that $x \geq y > z$. Then, up to isomorphism, $P = x\overbrace{z \ldots z}^{n-3}y$ is the unique path having energy $\hat{\mathbb{E}}(n, W)$.*

Proof. By Theorem 10, the result follows for $n \leq 6$. Therefore, suppose $n \geq 7$.

Denote by $P^* = u_1 e_1 u_2 e_2 u_3 \ldots u_{n-1} e_{n-1} u_n$ the path having energy $\hat{\mathbb{E}}(n, W)$. Since there are exactly two edges in P^* whose weights are not z, we suppose that $w(e_i) \neq z$ and $w(e_{i+t}) \neq z$ for $1 \leq i \leq n-2, 1 \leq t \leq n-2$. Then it is sufficient to show that $t = n-2$.

If $t \geq 2$ and $t \neq n-2$, then there exists a pendent edge, say e_1, having weight z. Without loss of generality, suppose $w(e_{i+t}) = x$. Then $w(e_i) = y$. Applying Corollary 6 to the edge e_{i+t}, we have

$$b_k(P^*) = b_k(P^* \backslash e_{i+t}) + x^2\, b_{k-2}(P^* \backslash u_{i+t} u_{i+t+1})\,.$$

Let P^{**} be the weighted path obtained from P^* by exchanging the edges e_i and e_1. Then,

$$b_k(P^{**}) = b_k(P^{**} \backslash e_{i+t}) + x^2\, b_{k-2}(P^{**} \backslash u_{i+t} u_{i+t+1})\,.$$

One can show that both $P^* \backslash e_{i+t}$ and $P^{**} \backslash e_{i+t}$ contain a component which is a weighted path belonging to $\mathcal{P}(i+t, W_1)$, where $W_1 = \{y, \overbrace{z, \ldots, z}^{i+t-2}\}$. Applying Theorem 12, we have $P^* \backslash e_{i+t} \prec P^{**} \backslash e_{i+t}$. Similarly, we have $P^* \backslash u_{i+t} u_{i+t+1} \prec P^{**} \backslash u_{i+t} u_{i+t+1}$. Consequently, $P^* \prec P^{**}$, which yields a contradiction.

If $t = 1$, then there exists a pendent edge, say e_1, having weight z. Without loss of generality, suppose $w(e_{i+1}) = x$. Then $w(e_i) = y$. Applying Corollary 6 to the edge e_{i+1}, we have

$$b_k(P^*) = b_k(P^* \backslash e_{i+1}) + x^2\, b_{k-2}(P^* \backslash u_{i+1} u_{i+2})\,.$$

Let P^{**} be the weighted path obtained from P^* by exchanging the edges e_i and e_1. Then,

$$b_k(P^{**}) = b_k(P^{**} \backslash e_{i+1}) + x^2\, b_{k-2}(P^{**} \backslash u_{i+1} u_{i+2})\,.$$

One can show that $P^* \backslash e_{i+1} \sim P^{**} \backslash e_{i+1}$, and both $P^* \backslash u_{i+1} u_{i+2}$ and $P^{**} \backslash u_{i+1} u_{i+2}$ contain a component, denoted respectively by P_1^* and P_1^{**}, having i vertices. However, $P_1^* = \overbrace{z \ldots z}^{i-1}$ and $P_1^{**} \in \mathcal{P}(i, W_1)$, where $W_1 = \{y, \overbrace{z, \ldots, z}^{i-2}\}$. Hence, $P_1^* \prec P_1^{**}$. Consequently, $P^* \prec P^{**}$, which also yields a contradiction.

The result thus follows. $\square$

Theorem 14. *For $n \geq 3$, let $W_{n-1} = \{\overbrace{x, \dots, x}^{n-2}, y\}$ be a sequence of positive numbers such that $x > y$. Then, up to isomorphism, $\hat{P}_n = xy\overbrace{x \dots x}^{n-3}$ is the unique path having energy $\hat{\mathbb{E}}(n, W_{n-1})$.*

Proof. We prove Theorem 14 by induction on n. From Theorem 10, the result follows for $n \leq 6$. Suppose that the result is true for smaller n. For $n \geq 7$, denote the path having energy $\hat{\mathbb{E}}(n, W)$ by $P^* = u_1 e_1 u_2 e_2 u_3 \dots u_{n-1} e_{n-1} u_n$. By Lemma 8, $w(e_1) = w(e_{n-1}) = x$. Since P^* has exactly one edge having weight y, we suppose that $w(e_{n-2}) = x$. Applying Corollary 6, we have

$$b_k(P^*) = b_k(P^* \backslash e_{n-1}) + x^2\, b_{k-2}(P^* \backslash u_{n-1} u_{n-2})\,.$$

Then, $P^* \backslash e_{n-1} \in \mathcal{P}(n, W_{n-2})$ and $P^* \backslash u_{n-1} u_{n-2} \in \mathcal{P}(n, W_{n-3})$. By the induction assumption, $P^* \backslash e_{n-1} \preceq \hat{P}_{n-1}$ with equality holding if and only if $P^* \backslash e_{n-1} = \hat{P}_{n-1}$. In addition, $P^* \backslash u_{n-1} u_{n-2} \preceq \hat{P}_{n-2}$ with equality holding if and only if $P^* \backslash u_{n-1} u_{n-2} = \hat{P}_{n-2}$. Hence, the result follows. $\square$

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