ON A POSET OF TREES

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Abstract. We will prove that the path minimizes the number of closed walks of length ℓ among the connected graphs for all ℓ. Indeed, we will prove that the number of closed walks of length ℓ and many other properties such as the spectral radius, Estada index increase or decrease along a certain poset of trees. This poset is a leveled poset with path as the smallest element and star as the greatest element.

1. Introduction

J. A. de la Peña, I. Gutnam and J. Rada [3] proved several inequality for the Estrada index [5],[6] of graphs, i.e., $\sum_{i=1}^{n} e^{\mu_i}$ where μ_i's are the eigenvalues of the adjacency matrix of the graph. In their paper they gave estimate to the minimal and maximal values of the Estrada index among the graphs on n vertices and m edges. They also conjecture that the minimum of the Estrada index is attained at the path among the connected graphs and the star has the maximum value of the Estrada index among the trees on n vertices. V. Nikiforov noticed that both conjecture would be true if the corresponding statement holds for closed walks (private communication). Indeed, we will prove this stronger result in our paper:

Theorem 4.6: The path has the minimum number of the closed walks of length ℓ among the connected graphs on n vertices for all ℓ and n. The star has the maximum number of closed walks of length ℓ among the trees on n vertices.

Our method will be as follows: we will generalize Kelmans's operation for trees. This new operation will induce a leveled poset on trees, on each level the number of leaves of the trees are the same, the greatest element of the poset is the star, the smallest element of the poset is the path. We will show that like the Kelmans operation, the generalized Kelmans operation for trees have many nice properties, it will increase the spectral radius, decrease the value $\sum_{x,y \in V(G)} d(x,y)$ ($d(x,y)$ is the distance between x and y), increase the number of closed walks of length ℓ. For the induced poset this will simply means that these properties increase or decrease along the poset and consequently, has the maximum for the star and minimum for the path.

The structure of this paper is the following: In the next section we introduce the concept of generalized tree shift (GTS) and the induced poset and we give the very basic facts about it. In Section 3. we will give an elementary

2000 *Mathematics Subject Classification.* Primary: 05C05. Secondary: 05C35.

Key words and phrases. Trees, walks, eigenvalues.

While this paper was carried out the author was the guest of the University of Memphis.

property of GTS, namely we will prove that this transformation decreases the $\sum_{x,y\in V(G)} d(x,y)$. In the next section we will study the number of walks in trees, and prove Theorem 4.6. In the last section we will give some open problems which naturally arise after studying this method.

Notation: We will follow the usual notation: G is a graph, $V(G)$ is the set of its vertices, $e(G)$ denotes the number of edges, $N(x)$ is the set of the neighbors of x, $\mu = \mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ is the set of adjacency eigenvalues of G, μ is also called spectral radius. W_ℓ will denote the number of closed walks of length ℓ.

2. Generalized tree shift and the induced poset

As far as our research shows Kelmans [7] was the first who studied the following operation on graphs. Let x, y be two vertices of some graph G and let G' be the graph obtained from G by erasing the edges between y and $N(y)\backslash(N(x)\cup\{x\})$ and adding the edges between x and $N(y)\backslash(N(x)\cup\{x\})$. This transformation has many nice properties: it increases the spectral radius and decreases the number of spanning trees [1],[13]. This transformation can be applied to any graph, but if we consider it as a transformation on trees we have to make a restriction on x and y, namely they should have distance at most 2 in order to obtain a connected G' as a result; in this case G' will be also a tree. Due to this restriction we cannot get any tree different from the path as an image of this transformation which we will see later has a crucial importance. To handle this problem we extend this transformation as follows.

Definition 2.1. Let G_2 be a tree and x and y be vertices such that all the interior points of the path xy (if they exist) have degree 2 in G_2. The generalized tree shift (GTS) of G_2 is the tree G_1 obtained from G_2 as follows: let z be the neighbor of y lying on the path xy, let us erase all the edges between y and $N(y)\backslash\{z\}$ and add the edges between x and $N(y)\backslash\{z\}$. See Figure 2.

In what follows we call x the beneficiary and y the candidate (for being a leaf) of the generalized tree shift. Note that if x or y is a leaf in G_2 then $G_1 \cong G_2$, otherwise the number of leaves in G_1 is the number of leaves in G_2 plus one. In this latter case we call the generalized tree shift proper.

Remark 2.2. Note that x and y need not to have degree 2.

Notation: In the following we call the vertices of the path xy $1, 2, \ldots, k$ if the path consists of k vertices such way that x will be 1 and y will be k. The set $A \subset V(G_2)$ consists of the vertices which can be reached with a path from k only through 1, and similarly the set $B \subset V(G_2)$ consists of those vertices which can be reached with a path from 1 only through k. For the sake of simplicity we denote the corresponding sets in G_1 also A and B. The set of neighbors of 1 in A is called A_0, and similarly B_0 is the set of neighbors of 1 in $B \subset V(G_1)$ and set of neighbors of k in $B \subset V(G_2)$.

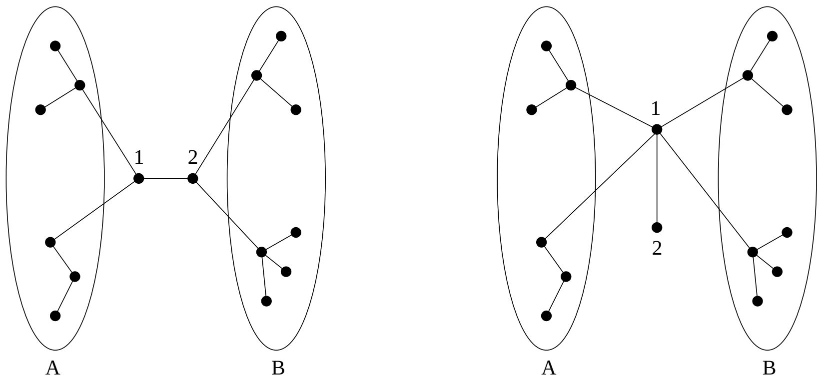

FIGURE 1. Original Kelmans's transformation applied to trees.

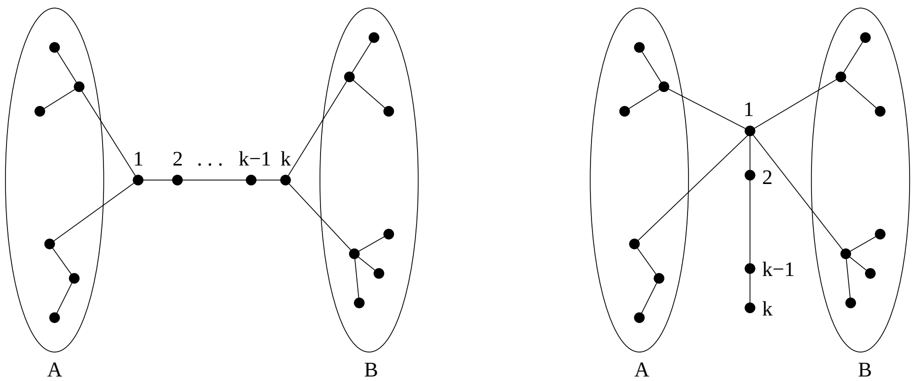

FIGURE 2. The generalized tree shift.

Definition 2.3. Let us say that $G_1 > G_2$ if G_1 can be obtained from G_2 by some proper generalized tree shift. The relation $>$ induces a poset on the trees on n vertices, since the number of leaves of G_1 is greater than the number of leaves of G_2, more precisely the two numbers differ by one. Hence the relation $>$ is indeed extendable.

One can always apply a proper generalized tree shift to any tree which has at least two vertices that are not leaves. This shows that the only maximal element of the induced poset is the star. The following theorem shows that the only minimal element of the induced poset, i. e., the smallest element is the path.

Theorem 2.4. *Every tree different from the path is the image of some proper generalized tree shift.*

Proof. Let T be a tree different from the path, i. e., it has at least one vertex having degree greater or equal to 3. Let v be a vertex having degree one. Further let w be the closest vertex to v which has degree at least 3. Then the interior vertices (if they exist) of the path induced by v and w have degrees 2. The vertex w has at least two neighbors different from the one which lying on the path induced by v and w, so we can decompose these neighbors into two nonempty sets, A_0 and B_0. Let T' be the tree given by erasing the edges between w and B_0 and adding the edges between v and B_0. Then T

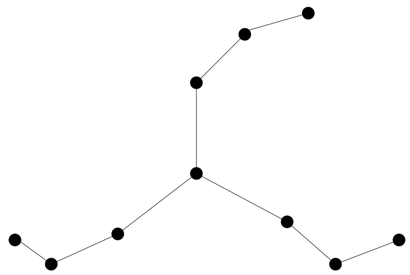

FIGURE 3. A tree which is not the image of the original Kelmans's transformation.

can be obtained from T' by the GTS, where w is the beneficiary and v is the candidate. Since A_0 and B_0 are nonempty this is a proper generalized tree shift. □

Corollary 2.5. *The star is the unique maximal, i.e., the greatest element, the path is the unique minimal, i.e., the smallest element of the induced poset of the generalized tree shift.*

Remark 2.6. This is a finite poset so the unique maximal really means greatest and the unique minimal really means smallest.

One can define the poset on trees induced by the original Kelmans transformation by the same way we defined the poset induced by GTS. Then it is true that star is the greatest element of the poset induced by the original Kelmans transformation, but it is not true that the path is the only minimal element of this poset. The graph in Figure 3 is not the image of any Kelman's shift. This explains why we needed to generalize this concept.

3. An elementary property of GTS

Theorem 3.1. *The proper generalized tree shift decreases the function $\sum_{x,y} d(x,y)$.*

Proof. Let G_2 be a tree and G_1 its image by a GTS. Let d_j be the distance in the corresponding graphs.

Clearly,

$$d_1(i,a) + d_1(k+1-i,a) = d_2(i,a) + d_2(k+1-i,a)$$

for all $a \in A$ and

$$d_1(i,b) + d_1(k+1-i,b) = d_2(i,b) + d_2(k+1-i,b)$$

for all $b \in B$.

Trivially $d_1(a,a') = d_2(a,a')$ for $a,a' \in A$, $d_1(b,b') = d_2(b,b')$ for $b,b' \in B$ and $d_2(a,b) = d_1(a,b) + (k-1)$ for $a \in A$ and $b \in B$.

Altogether we have

$$\sum_{x,y} d_2(x,y) = \sum_{x,y} d_1(x,y) + (k-1)|A||B|.$$

Hence the generalized tree shift decreases $\sum_{x,y} d(x,y)$. □

Corollary 3.2. *The path maximizes, the star minimizes $\sum_{x,y} d(x,y)$ among the trees on n vertices.*

Proof. It follows from the previous theorem and the fact that the path is the only minimal, the star is the only maximal element of the induced poset of the generalized tree shift. □

Remark 3.3. Corollary 3.2 was known [8].

4. Walks in trees

In this section we prove Theorem 4.6 on the number of closed walks which was already mentioned in the introduction. To do this we need some preparation.

Definition 4.1. Let $\hat{G}_1$ be the tree consisting of a path on k vertices and two vertices adjacent to one of the endpoints of the path. Let $\hat{G}_2$ be the tree consisting of a path on k vertices and two vertices which are adjacent to different endpoints of the path; this is simply a path on $k+2$ vertices. We will refer to these graphs as the reduced graphs of the generalized tree shift. (See Figure 4.)

Notation: The vertices of the path in each reduced graph will be denoted by $1, 2, \ldots, k$. The other two vertices are a and b. In $\hat{G}_1$ vertex 1 will be adjacent to a and b, in $\hat{G}_2$ vertex 1 will be adjacent to vertex a and vertex k will be adjacent to vertex b.

Definition 4.2. Let $\mathbf{R}(\ell, i, j, m, n)$ be the set of those walks of length ℓ in $\hat{G}_1$ which start at vertex i, finish at vertex j and visit vertex a exactly m times, vertex b exactly n times. Similarly let $\mathbf{D}(\ell, i, j, m, n)$ be the set of those walks of length ℓ in $\hat{G}_2$ which start at vertex i, finish at vertex j and visit vertex a exactly m times, vertex b exactly n times. The cardinality of $\mathbf{R}(\ell, i, j, m, n)$ and $\mathbf{D}(\ell, i, j, m, n)$ are denoted by $R(\ell, i, j, m, n)$ and $D(\ell, i, j, m, n)$, respectively.

Symmetry properties of the function R and D. Since we can "reflect" any walk of $\hat{G}_1$ in the "horizontal axis" of $\hat{G}_1$, i.e., we can exchange the a's and b's in any walk we have

$$R(\ell, i, j, m, n) = R(\ell, i, j, n, m)$$

for all ℓ, i, j, m, n.

Similarly we can "reflect" any walk of $\hat{G}_2$ in the "vertical symmetry axis" of $\hat{G}_2$ and so we have

$$D(\ell, i, j, m, n) = D(\ell, k+1-i, k+1-j, n, m)$$

for all ℓ, i, j, m, n.

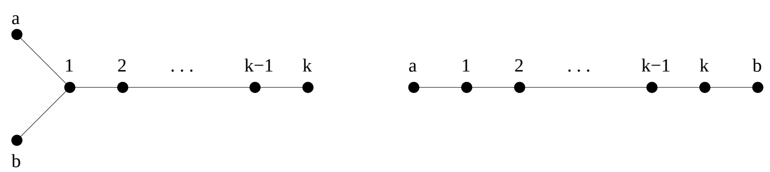

Figure 4. Reduced graphs of the generalized tree shift.

Lemma 4.3. *$R(\ell,1,j,m,n) \geq D(\ell,1,j,m,n)$ where $1 \leq j \leq k$.*

Proof. First we prove the statement in the case $m=0$, $j=k$. Let $w_1 w_2 \dots w_{\ell+1}$ be a walk from 1 to k in $\hat{G}_2$ in which b occurs n times. Let us define $v_i = f(w_i)$ as follows:

$$f(w_i) = \begin{cases} k+1-s \text{ if } w_{\ell+2-i} = s \\ \quad b \quad \text{if} \quad w_{\ell+2-i} = b \end{cases}$$

Then $v_1 v_2 \dots v_{l+1}$ is a walk of length ℓ from 1 to k in $\hat{G}_1$ which contains b exactly n times. Hence we have proved that

$$R(\ell,1,k,0,n) = D(\ell,1,k,0,n)$$

since this algorithm gives a bijection between $\mathbf{R}(\ell,1,k,0,n)$ and $\mathbf{D}(\ell,1,k,0,n)$.

Now let j arbitrary, but still $m=0$, i. e., the walks do not visit a. If $n=0$ then

$$R(\ell,1,j,0,0) = D(\ell,1,j,0,0)$$

trivially, because of the identical map between the vertices of $1,2\dots,k$ of $\hat{G}_1$ and $\hat{G}_2$. If $n \geq 1$ then a walk $w_1 w_2 \dots w_{\ell+1}$ in $\hat{G}_2$ surely visit the vertex k, let the time of the last visit of vertex k be t. Then let us encode $w_1 w_2 \dots w_t$ by the function f and let $v_1 v_2 \dots v_t w_{t+1} \dots w_{\ell+1}$ be the corresponding walk to $w_1 \dots w_{l+1}$ in $\hat{G}_1$. This way we managed to give an injection from $\mathbf{D}(\ell,1,j,0,n)$ to $\mathbf{R}(\ell,1,j,0,n)$. (Note: this mapping is no more bijective: those walks in $\hat{G}_1$ which do not visit k are not in the image of the mapping.)

Now let us consider the general case. Let us do the following: repeat those sequences of the walk $w_1 \dots w_{\ell+1}$ of $\mathbf{D}(\ell,1,j,n,m)$ where the walk has the form $1a1a\dots a1$ and between two parts of this form we encode the way as in the previous case. Then it is trivially an injective mapping from $\mathbf{D}(\ell,1,j,m,n)$ to $\mathbf{R}(\ell,1,j,m,n)$.

Hence $R(\ell,1,j,m,n) \geq D(\ell,1,j,m,n)$. □

Lemma 4.4. *For all $1 \leq i,j \leq k$ and for all nonnegative integers ℓ, m, n we have*

$$R(\ell,i,j,m,n) + R(\ell,k+1-i,k+1-j,m,n) \geq$$
$$\geq D(\ell,i,j,m,n) + D(\ell,k+1-i,k+1-j,m,n).$$

Proof. We prove by induction on ℓ. The claim is trivial for $\ell = 0,1$.

We can assume that $i \leq k+1-i$. We distinguish two cases.

Case 1 Assume $i \geq 2$. Let $w_1 w_2 \dots w_{\ell+1}$ be a walk of $R(\ell,i,j,m,n)$, i.e., $w_1 = i$, $w_{\ell+1} = j$. Then $w_2 = i+1$ or $w_2 = i-1$, thus we can decompose the set $\mathbf{R}(\ell,i,j,m,n)$ into the sets $\mathbf{R}(\ell-1,i-1,j,m,n)$ and $\mathbf{R}(\ell-1,i+1,j,m,n)$ respected to $w_2 \dots w_{\ell+1}$ starting from $i-1$ or $i+1$. Similarly we can decompose the other sets respected to their first step.

$$R(\ell,i,j,m,n) + R(\ell,k+1-i,k+1-j,m,n) =$$
$$R(\ell-1,i-1,j,m,n) + R(\ell-1,i+1,j,m,n) +$$
$$+R(\ell-1,k-i,k+1-j,m,n) + R(\ell-1,k+2-i,k+1-j,m,n)$$

and similarly

$$D(\ell,i,j,m,n)+D(\ell,k+1-i,k+1-j,m,n)=$$
$$D(\ell-1,i-1,j,m,n)+D(\ell-1,i+1,j,m,n)$$
$$+D(\ell-1,k-i,k+1-j,m,n)+D(\ell-1,k+2-i,k+1-j,m,n).$$

By induction we have

$$R(\ell-1,i-1,j,m,n)+R(\ell-1,k+2-i,k+1-j,m,n)\geq$$
$$\geq D(\ell-1,i-1,j,m,n)+D(\ell-1,k+2-i,k+1-j,m,n)$$

and

$$R(\ell-1,i+1,j,m,n)+R(\ell-1,k-i,k+1-j,m,n)\geq$$
$$\geq D(\ell-1,i+1,j,m,n)+D(\ell-1,k-i,k+1-j,m,n).$$

By adding together the two inequalities we get the desired inequality

$$R(\ell,i,j,m,n)+R(\ell,k+1-i,k+1-j,m,n)\geq$$
$$\geq D(\ell,i,j,m,n)+D(\ell,k+1-i,k+1-j,m,n).$$

Case 2 Assume $i=1$. Then we see that

$$R(\ell,1,j,m,n)+R(\ell,k,k+1-j,m,n)=$$
$$=R(\ell-1,a,j,m,n)+R(\ell-1,b,j,m,n)+$$
$$+R(\ell-1,2,j,m,n)+R(\ell,k-1,k+1-j,m,n)$$

while

$$D(\ell,1,j,m,n)+D(\ell,k,k+1-j,m,n)=$$
$$=D(\ell-1,a,j,m,n)+D(\ell-1,2,j,m,n)$$
$$+D(\ell-1,b,k+1-j,m,n)+D(\ell-1,k-1,k+1-j,m,n).$$

By induction we have

$$R(\ell-1,2,j,m,n)+R(\ell-1,k-1,k+1-j,m,n)\geq$$
$$\geq D(\ell-1,2,j,m,n)+D(\ell-1,k-1,k+1-j,m,n).$$

Further we have by Lemma 4.3

$$R(\ell-1,a,j,m,n)=R(\ell-2,1,j,m-1,n)\geq$$
$$\geq D(\ell-2,1,j,m-1,n)=D(\ell-1,a,j,m,n)$$

and by the symmetry properties and Lemma 4.3

$$R(\ell-1,b,j,m,n)=R(\ell-2,1,j,m,n-1)=R(\ell-2,1,j,n-1,m)\geq$$
$$D(\ell-2,1,j,n-1,m)=D(\ell-2,k,k+1-j,m,n-1)=D(\ell-1,b,k+1-j,m,n).$$

By adding together the three inequalities we obtain the required inequality

$$R(\ell,1,j,m,n)+R(\ell,k,k+1-j,m,n)\geq$$
$$\geq D(\ell,1,j,m,n)+D(\ell,k,k+1-j,m,n).$$

Hence we completed the proof of the inequality. $\square$

Corollary 4.5. *We have the following inequalities*

$$R(\ell,a,a,m,n) \geq D(\ell,a,a,m,n)$$

and

$$R(\ell,b,b,m,n) \geq D(\ell,b,b,m,n)$$

and

$$\sum_{i=1}^{k} R(\ell,i,i,m,n) \geq \sum_{i=1}^{k} D(\ell,i,i,m,n).$$

Proof. To obtain the first inequality we use Lemma 4.3.

$$R(\ell,a,a,m,n) = R(\ell-2,1,1,m-2,n) \geq$$
$$\geq D(\ell-2,1,1,m,n) = D(\ell,a,a,m,n).$$

Similarly, using Lemma 4.3 and the symmetry properties we have

$$R(\ell,b,b,m,n) = R(\ell-2,1,1,m,n-2) = R(\ell-2,1,1,n-2,m) \geq$$
$$\geq D(\ell-2,1,1,n-2,m) = D(\ell-2,k,k,m,n-2) = D(\ell,b,b,m,n).$$

To obtain the third inequality we put $i=j$ into the previous lemma

$$R(\ell,i,i,m,n) + R(\ell,k+1-i,k+1-i,m,n) \geq$$
$$\geq D(\ell,i,i,m,n) + D(\ell,k+1-i,k+1-i,m,n).$$

Summing these inequalities for $i = 1,\dots,k$, after dividing by two we get

$$\sum_{i=1}^{k} R(\ell,i,i,m,n) \geq \sum_{i=1}^{k} D(\ell,i,i,m,n).$$

□

Theorem 4.6. *The proper generalized tree shift increases the number of closed walks of length t.*

Proof. Let G_2 be a tree and G_1 a tree obtained from G_2 by a generalized tree shift. We give an injective mapping from the closed walks of length t of G_2 to the closed walks of length t of G_1. We can decompose a closed walk of G_2 into parts which are entirely in A, entirely in B or entirely in the path $\{1,2,\dots,k\}$ of G_2. By substituting a or b instead of the parts walking in A, respectively in B we get a walk of $\hat{G}_2$. By the previous corollary we know that there is an injective mapping from the closed walks of length ℓ with given number of a's and b's of $\hat{G}_2$ to the closed walks of length ℓ with given number of a's and b's of $\hat{G}_1$, moreover we can ensure that those walks which start with a or b have the image starting with a or b, respectively. Now by substituting back the a's and b's by the parts of walks going in A or B, respectively, we get an injective mapping from the closed walks of length t of G_2 to the closed walks of length t of G_1. □

Vladimir Nikiforov observed (private communication) that Theorem 4.6 already implies known and new results in a simple manner.

Corollary 4.7. *The proper generalized tree shift increases the spectral radius and the Estrada index.*

Proof. Let G_2 be a tree and G_1 a tree obtained from G_2 by a generalized tree shift. Then

$$\mu(G_1) = \lim_{k\to\infty} W_{2k}(G_1)^{1/(2k)} \geq \lim_{k\to\infty} W_{2k}(G_2)^{1/(2k)} = \mu(G_2)$$

by the identity $W_{2k} = \sum_{i=1}^n \mu_i^{2k}$ and Theorem 4.6.

Similarly, we have

$$\sum_{i=1}^n e^{\mu_i} = \sum_{i=1}^n \sum_{t=0}^\infty \frac{\mu_i^t}{t!} = \sum_{t=0}^\infty \frac{1}{t!} \sum_{i=1}^k \mu_i^t = \sum_{t=0}^\infty \frac{W_t}{t!}$$

proving the second statement. □

Corollary 4.8. *(a)The path minimizes the spectral radius and the Estrada index among all connected graphs on n vertices.*

(b) The star maximizes the spectral radius and the Estrada index among all trees on n vertices.

Proof. (a) The statement concerning the spectral radius is obvious since by the monotonicity of the spectral radius it is enough to find the minimizing graph among the trees. Since the only minimal element of the induced poset of the generalized tree shift is the path, the claim immediately follows from Corollary 4.7.

Similarly, it is enough to find the graph minimizing the Estrada index among the trees, because of the identity

$$\sum_{i=1}^n e^{\mu_i} = \sum_{t=0}^\infty \frac{W_t}{t!}.$$

This implies the minimality property of path the same way as before.
(b) Again it follows from the previous corollary and the fact that the star is the only maximal element of the induced poset of the generalized tree shift. □

Remark 4.9. The statement in Corollary 4.8 concerning the Estrada index was conjectured in the paper [3]. While both statements concerning the spectral radius are well-known in the previous corollary [9]. We mention that Nikiforov's inequality [10]

$$\mu(G) \leq \sqrt{2e(G)\left(1 - \frac{1}{\omega(G)}\right)}$$

also implies the second inequality concering the star and the spectral radius since for trees we have $e(G) = n - 1$, $\omega(G) = 2$ and the greatest eigenvalue of the star is exactly $\sqrt{n-1}$. (It was Nosal who proved that for triangle-free graphs $\mu \leq \sqrt{e(G)}$ holds, later Nikiforov [11] proved that in Nosal's inequality equality holds if and only if the graph is complete bipartite with some isolated vertices.)

Remark 4.10. The author recently learnt that H. Deng [4] also proved the conjecture concerning the Estrada index. His proof goes in a very similar fashion. He uses two different transformations for proving the minimality of the path and the maximality of the star; both transformations are special cases of the generalized tree shift.

5. Open problems

We have seen that several properties increase or decrease along the poset induced by the generalized tree shift. Such property was the number of leaves, the $\sum_{x,y} d(x,y)$, the greatest eigenvalue or the number of closed walks of length ℓ. Is it true that one of them implies another? For example, is it true that if trees the G_1, G_2 satisfy

$$\sum_{x,y\in V(G_1)} d_{G_1}(x,y) > \sum_{x,y\in V(G_2)} d_{G_2}(x,y)$$

then

$$W_\ell(G_1) \leq W_\ell(G_2)$$

for all ℓ?

We have seen that the star maximizes, path minimizes the number of closed walks of length ℓ among the connected graphs with $n-1$ edges. What is the truth for general m instead of $n-1$, i.e., which graphs maximizes and minimizes the number of closed walks of length ℓ among the (connected) graphs on n vertices and m edges? Is there a universal graph for all ℓ as in the case of $m = n-1$ for both the minimizing and maximizing problem?

Acknowledgement. The author is very grateful to Vladimir Nikiforov and László Lovász for their numerous advice and comments.

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