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SIGNLESS LAPLACIAN SPECTRAL MOMENTS OF GRAPHS AND ORDERING SOME GRAPHS WITH RESPECT TO THEM

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Abstract. Let $G = (V, E)$ be a simple graph. Denote by $D(G)$ the diagonal matrix $diag(d_1, \cdots, d_n)$, where d_i is the degree of vertex i and $A(G)$ the adjacency matrix of G. The signless Laplacian matrix of G is $Q(G) = D(G) + A(G)$ and the $k-$th signless Laplacian spectral moment of graph G is defined as $T_k(G) = \sum_{i=1}^{n} q_i^k$, $k \geqslant 0$, where q_1,q_2, $\cdots$, q_n are the eigenvalues of the signless Laplacian matrix of G. In this paper we first compute the $k-$th signless Laplacian spectral moments of a graph for small k and then we order some graphs with respect to the signless Laplacian spectral moments.

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1. Introduction

In this section we recall some definitions that will be used in the paper. Let G be a simple graph with vertex set $V(G) = \{v_1, \cdots, v_n\}$ and edge set $E(G) = \{e_1, \cdots, e_m\}$. The degree of a vertex $v \in V(G)$, denoted by $d(v)$, is the number of neighbors of v. The adjacency matrix of G is an $n \times n$ matrix $A(G)$ whose $(i, j)-$entry is the number of edges between v_i and v_j. The signless Laplacian matrix of G is the matrix $Q(G) = A(G) + D(G)$, where $D(G)$ is the diagonal matrix with $d(v_1), \cdots, d(v_n)$ on its main diagonal. It is well-known that $Q(G)$ is positive semidefinite and so their eigenvalues are nonnegative real numbers. The eigenvalues of $A(G)$ and $Q(G)$ are called the eigenvalues and signless Laplacian eigenvalues of G, and are denoted by $\lambda_1(G), \cdots, \lambda_n(G)$ and $q_1(G), \cdots, q_n(G)$, respectively.

A walk of length k in a graph G is an alternating sequence v_1, e_1, v_2, e_2, $\cdots$, v_k, e_k, v_{k+1}, of vertices $v_1, v_2, \cdots, v_{k+1}$ and edges $e_1, e_2, \cdots, e_k$ such that for any $i = 1, 2, \cdots, k$ the vertices v_i and v_{i+1} are distinct end-vertices of the edge e_i.

Lemma 1.1. [1] *Let A be the adjacency matrix of graph G. The $(i, j)-$entry of the matrix A^k is equal to the number of walks of length k starting at vertex i and terminating at vertex j.*

Suppose G is a graph with adjacency matrix $A(G)$ and $\lambda_1(G)$, $\lambda_2(G)$, $\cdots$ $\lambda_n(G)$ are eigenvalues in non-increasing order of G. The numbers $S_k(G) = \sum_{i=1}^{n} \lambda_i^k(G)$, $k \geqslant 0$ is called the $k-$th spectral moment of G.

We now recall some definitions that will be used in the paper. P_n, C_n, S_n and U_n stand for the path of length n, the cycle of size n, the star graph on n vertices and a graph obtained from C_{n-1} by attaching a leaf to one of its vertices, respectively. Our undefined terminology and notation can be found in [2].

Lemma 1.2. [2] *The $k-$th spectral moment of G is equal to the number of closed walks of length k.*

It is well-known that $S_0(G) = n$, $S_1(G) = 0$, $S_2(G) = 2m$ and $S_3(G) = 6t$, where n, m and t denote the number of vertices, edges and triangles, respectively (see [2]). The following results are crucial throughout this paper.

Let F be a graph. An $F-$subgraph of G is a subgraph of G which is isomorphic to the graph F. Let $\varphi_G(F)$ (or $\varphi(F)$) be the number of all $F-$subgraphs of G.

Lemma 1.3. *For every graph G, we have:*

(1) $S_4(G) = 2\varphi(P_2) + 4\varphi(P_3) + 8\varphi(C_4)$, ([3])
(2) $S_5(G) = 30\varphi(C_3) + 10\varphi(U_4) + 10\varphi(C_5)$. ([14])

Let n, m, R be the number of vertices, the number of edges and the vertex-edge incidence matrix of a graph G. The following relations can be found in [1]:

(1) $RR^t = A + D$,

(2) $R^tR = A_L + 2I$,

where D is the diagonal matrix $diag(d_1, \cdots, d_n)$ of vertex degrees and $A_{L(G)}$ is the adjacency matrix of the line graph $L(G)$ of G. Since the non-zero eigenvalues of RR^t and R^tR are the same, we deduce from the relations above that:

$$P_{L(G)}(\lambda) = (\lambda + 2)^{m-n} Q_G(\lambda + 2).$$

In [5], Cvetković and Rowlinson obtained the first and the last graphs in an $S-$order, in the classes of trees and unicyclic graphs with a given girth, respectively. Taghvaee and Ashrafi in [11, 12, 13], compute the spectral moments of some fullerene graphs, $I-$graphs and generalized Petersen graphs, respectively, and then they order that graphs with respect to the spectral moments. Also Fath-Tabar and Ashrafi in [6, 7, 8] obtained some results on Laplacian eigenvalues and Laplacian energy of graphs, new upper bounds for Estrada index of bipartite graphs and note on Estrada and $L-$Estrada indices of graphs, respectively.

2. Main Results

In this section, we find our description for the signless Laplacian spectral moments of graphs. At first, we define a new version of walks that is called semi-edge walk. Such a walk can be considered as a alternating sequence of vertices and edges of a graph such that end vertices of edges are not necessarily distinct. In the following the more formal definition of this concept is presented.

Definition 2.1. A semi-edge walk of length k in an undirected graph G is an alternating sequence $v_1, e_1, v_2, e_2, \cdots, v_k, e_k, v_{k+1}$, of vertices $v_1, v_2, \cdots, v_{k+1}$ and edges $e_1, e_2, \cdots, e_k$ such that for any $i = 1, 2, \cdots, k$, the vertices v_i and v_{i+1} are end vertices (not necessarily distinct) of the edge e_i.

Theorem 2.2. [4] *Let Q be the signless Laplacian matrix of a graph G. The $(i, j)-$entry of the matrix Q^k is equal to the number of semi-edge walks of length k starting at vertex i and terminating at vertex j.*

Definition 2.3. Suppose that G is a simple graph and $q_1(G), q_2(G), \cdots, q_n(G)$ are the eigenvalues of the signless Laplacian of G. The number $T_k(G) = \sum_{i=1}^{n} q_i^k(G)$, $k \geqslant 0$, is called the $k-$th signless Laplacian spectral moment of G.

Corollary 2.4. [4] *The $k-$th signless Laplacian spectral moment of G, $T_k(G)$, is equal to the number of closed semi-edge walks of length k.*

Definition 2.5. Let $T(G) = (T_0(G), T_1(G), \cdots, T_{n-1}(G))$ be the sequence of signless Laplacian spectral moments of G. For two graphs G_1 and G_2, we shall write $G_1 =_T G_2$ if $T_i(G_1) = T_i(G_2)$ for $i = 0, 1, \cdots, n-1$. Similarly, we have $G_1 \prec_T G_2$ (G_1 comes before G_2 in an $T-$ order) if for some k $(1 \leqslant k \leqslant n-1)$, we have $T_i(G_1) = T_i(G_2)(i = 0, 1, \cdots, k-1)$ and $T_k(G_1) < T_k(G_2)$. We shall also write $G_1 \preceq_T G_2$ if $G_1 \prec_T G_2$ or $G_1 =_T G_2$.

Theorem 2.6. [4] *Let G be a simple graph with n vertices, m edges and vertex degrees $d_1, d_2, \cdots, d_n$. Then we have:*

$$\begin{aligned} T_0(G) &= n, \\ T_1(G) &= \sum_{i=1}^{n} d_i = 2m, \\ T_2(G) &= S_2(G) + \sum_{i=1}^{n} d_i^2, \\ T_3(G) &= S_3(G) + 3\sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i^3. \end{aligned}$$

Theorem 2.7. *Let G be a simple graph. Then we have:*

$$\begin{aligned} T_4(G) &= S_4(G) + 8\sum_{i=1}^{n} t_i d_i + 4\sum_{i=1}^{n} d_i^3 + \sum_{i=1}^{n} d_i^4 + 4\sum_{ij\in E(G)} d_i d_j, \\ T_5(G) &= S_5(G) + 5\sum_{i=1}^{n}[d_i^2 + (d_i^* - 1) + 2q_i]d_i + 10\sum_{i=1}^{n} t_i d_i^2 + 5\sum_{i=1}^{n} d_i^4 \\ &+ \sum_{i=1}^{n} d_i^5 + 5\sum_{j=1}^{n}\sum_{i=1}^{n} d_i d_j^2 + 10\sum_{ij\in E(G)} d_i d_j t_{ij}, \end{aligned}$$

where d_i is the degree of ith vertex, d_i^* is the degree of its neighbors, q_i is the number of quadrangles containing the ith vertex, t_i is the number of triangles containing the ith vertex and t_{ij} is the number of triangles at edge ij.

Proof. The formulla for T_4 followes from

$$\begin{aligned} tr(Q)^4 &= tr(A+D)^4 = tr[(A+D)^2(A+D)^2] \\ &= tr(A^4) + 4tr(A^3D) + 4tr(A^2D^2) + 4tr(AD^3) + tr(D^4) + 2tr(ADAD). \end{aligned}$$

By Lemma 1.2 we have $tr(A^4) = S_4(G)$, where $S_4(G)$ is the 4-th spectral moments of G. Next we have $tr(AD^3) = 0$, $tr(D^4) = \sum_{i=1}^{n} d_i^4$, $tr(A^2D^2) = \sum_{i=1}^{n} d_i^3$, $tr(A^3D) = 2\sum_{i=1}^{n} t_i d_i$, where t_i is the number of triangles containing the ith vertex and d_i is the degree of ith vertex. By direction computation we get $tr(ADAD) = 2\sum_{ij\in E(G)} d_i d_j$. By substituting the values obtained we get $T_4(G) = S_4(G) + 8\sum_{i=1}^{n} t_i d_i + 4\sum_{i=1}^{n} d_i^3 + \sum_{i=1}^{n} d_i^4 + 4\sum_{ij\in E(G)} d_i d_j$.

Now assume that $k = 5$. Similar to above we have:

$$\begin{aligned} tr(Q)^5 &= tr(A+D)^5 = tr(A^5) + 5tr(A^4D) + 5tr(A^3D^2) + 5tr(A^2D^3) \\ &+ 5tr(AD^4) + tr(D^5) + 5tr(AD^2AD) + 5tr(A^2DAD). \end{aligned}$$

By direct computation, we have $tr(D^5) = \sum_{i=1}^{n} d_i^5$, $tr(A^2D^3) = \sum_{i=1}^{n} d_i^4$, $tr(A^3D^2) = 2\sum_{i=1}^{n} t_i d_i^2$, where t_i is the number of triangles containing the $i-$th vertex, and $tr(A^4D) = \sum_{i=1}^{n}[d_i^2 + d_i(d_i^* -$

$1) + 2q_i]d_i$, where d_i is the degree of ith vertex, d_i^* is the degree of its neighbors and q_i is the number of quadrangles containing the ith vertex. Consider now $tr(A^2DAD)$. By computing $(i,i)-$entry of the matrix A^2DAD, we obtain $tr(A^2DAD) = 2\sum_{ij\in E(G)} d_id_jt_{ij}$, where t_{ij} is the number of triangles containing the edge ij. Finally by computing $(i,i)-$enrty of matrix AD^2AD, we get $tr(AD^2AD) = \sum_{i=1}^n \sum_{j=1}^n d_id_j^2$, for any edge v_iv_j of G. By substituting the values obtained above, we have:

$$\begin{aligned} T_5(G) &= S_5(G) + 5\sum_{i=1}^n [d_i^2 + (d_i^* - 1) + 2q_i]d_i + 10\sum_{i=1}^n t_id_i^2 + 5\sum_{i=1}^n d_i^4 \\ &+ \sum_{i=1}^n d_i^5 + 5\sum_{j=1}^n\sum_{i=1}^n d_id_j^2 + 10\sum_{ij\in E(G)} d_id_jt_{ij}. \end{aligned}$$

In the following we order some graphs with respect to the signless Laplacian spectral moment. First consider the set of all trees of order n. Then by Theorem 2.6 we have the following result.

Corollary 2.8. *In an $T-$order of trees on n vertices, the first graph is the path P_n, and the last graph is the star $K_{1,n-1}$.*

Proof. Let G be a tree with n vertices. Since the number of edges of G is $n-1$, so $T_1(G) = 2(n-1)$. On the other hand $T_2(G) = \sum_{i=1}^n d_i + \sum_{i=1}^n d_i^2$. By [10] we know that $\sum_{i=1}^n d_i^2$ is minimal in P_n and is maximal in $K_{1,n-1}$. So for $i = 0, 1$ we have, $T_i(G) = T_i(P_n) = T_i(K_{1,n-1})$, and $T_2(P_n) < T_2(G) < T_2(K_{1,n-1})$. Therefore in an $T-$order we have, $P_n \prec_T G \prec_T K_{1,n-1}$ and this completes the proof.

Now we consider the generalized Petersen graphs. We first compute the signless Laplacian spectral moments of this graphs and then order them with respect to the signless Laplacian spectral moment. First we define the generalized Petersen graphs.

The generalized Petersen graph $GP(n,k)$ is a graph with vertices and edges given by $V(GP(n,k)) = \{a_i, b_i \mid 1 \le i \le n\}$ and $E(GP(n,k)) = \{a_ib_i, a_ia_{i+1}, b_ib_{i+k} \mid 1 \le i \le n\}$, respectively. Here, $i+k$ are integers modulo n, $n > 6$. Since $GP(n,k) \cong GP(n, n-k)$, we can assume that $k \leqslant \lfloor \frac{n-1}{2} \rfloor$. Define $A(n,k)$ and $B(n,k)$ to be the induced subgraphs of $GP(n,k)$ consisting the vertices $\{a_1, \cdots, a_n\}$ and $\{b_1, \cdots, b_n\}$, respectively. The subgraphs $A(n,k)$ and $B(n,k)$ are called the outer and inner subgraphs of $GP(n,k)$, respectively. Gera and Stănică [9], in a recent paper computed the spectrum of this important class of cubic graphs. Taghvaee and Ashrafi [13] computed the spectral moments of $GP(n,k)$. In this section, the signless Laplacian spectral moment sequence of $GP(n,k)$ is computed.

Theorem 2.9. [13] *The spectral moments $S_i(GP(n,k))$, $2 \le i \le 5$, can be computed by the following formulas:*

$$S_2(GP(n,k)) = 6n, \qquad S_3((GP(n,k)) = \begin{cases} 2n & 3 \mid n,\ k = \frac{n}{3} \\ 0 & Otherwise, \end{cases}$$

$$S_4(GP(n,k)) = \begin{cases} 32n & 4 \mid n,\ k=\frac{n}{4} \\ 38n & k=1 \\ 30n & Otherwise, \end{cases} \qquad S_5(GP(n,k)) = \begin{cases} 2n & 5 \mid n,\ k=\frac{n}{5} \\ & or\ k=\frac{2n}{5}\ and\ n \neq 10 \\ 10n & k=2, n \neq 10 \\ 20n & 3 \mid n,\ k=\frac{n}{3} \\ 0 & Otherwise. \end{cases}$$

By using Theorems 2.6 and 2.7 we compute the signless Laplacian spectral moments of generalized Petersen graphs.

Theorem 2.10. *The signless Laplacian spectral moments of $GP(n,k)$ is equal to the followings:*

$$T_0(GP(n,k)) = 2n, \qquad T_1(GP(n,k)) = 6n, \qquad T_2(GP(n,k)) = 24n,$$

$$T_3(GP(n,k)) = \begin{cases} 110n & 3 \mid n,\ k=\frac{n}{3} \\ 108n & Otherwise, \end{cases}$$

$$T_4(GP(n,k)) = \begin{cases} 540n & 3 \mid n,\ k=\frac{n}{3} \\ 524n & k=1 \\ 518n & 4 \mid n, k=\frac{n}{4} \\ 516n & Otherwise, \end{cases}$$

$$T_5(GP(n,k)) = \begin{cases} 2558n & 5 \mid n,\ k=\frac{n}{5}\ or\ k=\frac{2n}{5} \\ 2756n & 3 \mid n,\ k=\frac{n}{3} \\ 2586n & 4 \mid n,\ k=\frac{n}{4} \\ 2676n & k=1 \\ 2566n & k=2 \\ 2556n & Otherwise. \end{cases}$$

Proof. Since $|V(GP(n,k))| = 2n$ and $|E(GP(n,k))| = 3n$, we get $T_0(GP(n,k)) = 2n$ and $T_1(GP(n,k)) = 6n$. By Theorem 2.6, we have $T_2(GP(n,k)) = 6n + 18n = 24n$. Now consider $T_3(GP(n,k))$. If $3 \mid n$ and $k = \frac{n}{3}$, then the number of triangles in $GP(n,k)$ is equal to $\frac{n}{3}$ and otherewise the number of triangles in $GP(n,k)$ is 0. Therefore in the first case we have $T_3(GP(n,k)) = 2n+54n+54n = 110n$ and the second case we have $T_3(GP(n,k)) = 54n+54n = 108n$.

Now we compute $T_4(GP(n,k))$. Suppose that $4 \mid n$ and $k = \frac{n}{4}$. Then by Theorem 2.9 $S_4(GP(n,k)) = 32n$, and since $t_i = 0$, we obtaine $T_4(GP(n,k)) = 32n + 216n + 162n + 108n = 518n$. If $3|n$ and $k = \frac{n}{3}$, then the number of triangles containing the outer subgraph of $GP(n,k)$ is 0 and the number of triangles containing the inner subgraph of $GP(n,k)$ is equal to n. On the other hand $S_4(GP(n,k)) = 30n$. Thus, in this case $T_4(GP(n,k)) = 30n + 24n + 216n + 162n + 108n = 540n$. If $k = 1$, by Theorem 2.9 we have $S_4(GP(n,k)) = 38n$ and so $T_4(GP(n,k)) = 38n+216n+162n+108n = 524n$. Otherwise,we have $S_4(GP(n,k)) = 30n$ and so $T_4(GP(n,k)) = 30n+216n+162n+108n = 516n$. Similarly for $T_5(GP(n,k))$ we get above relations and this completes the proof.

In the following consider $GP(n)$ to be set of all generalized Petersen graphs of order $2n$. We order this graphs with respect to signless Laplacian spectral moments.

Theorem 2.11. *Let n be a positive integer such that only $3 \mid n$. Then in an $T-$order of the set of the generalized Petersen graphs of order $2n$,*

(1) *for any $G \in GP(n) \setminus GP(n, \frac{n}{3})$, we have:*

$$G \prec_T GP(n, \frac{n}{3}).$$

(2) *for any $G \in GP(n) \setminus \{GP(n, \frac{n}{3}), GP(n,1)\}$, we have:*

$$G \prec_T GP(n,1).$$

(3) *for any $G \in GP(n) \setminus \{GP(n, \frac{n}{3}), GP(n,1), GP(n,2)\}$, we have:*

$$G \prec_T GP(n,2).$$

Proof. By using Theorem 2.10 and Definition 2.5. First let $3 \mid n$. Then for $i = 0,1,2$, $T_i(G) = T_i(GP(n, \frac{n}{3}))$ and $T_3(G) < T_3(GP(n, \frac{n}{3}))$. So $G \prec_T GP(n, \frac{n}{3})$. Now let $G \in GP(n) \setminus \{GP(n, \frac{n}{3}), GP(n,1)\}$. Then for $i = 0,1,2,3$, $T_i(G) = T_i(GP(n,1))$ and $T_4(G) < T_4(GP(n,1))$ and so $G \prec_T GP(n,1)$.

If $G \in GP(n) \setminus \{GP(n, \frac{n}{3}), GP(n,1), GP(n,2)\}$, then $T_i(G) = T_i(GP(n,2))$, for $i = 0,1,2,3,4$, and $2556n = T_5(G) < T_5(GP(n,2)) = 2566n$. Thus $G \prec_T GP(n,2)$ and this completes the proof.

Theorem 2.12. *Let n be a positive integer such that only $4 \mid n$. Then in an $T-$order of the set of the generalized Petersen graphs of order $2n$,*

(1) *for any* $G \in GP(n) \setminus \{GP(n, \frac{n}{4}), GP(n, 1)\}$, *we have:*

$$G \prec_T GP(n, \frac{n}{4}) \prec_T GP(n, 1).$$

(2) *for any* $G \in GP(n) \setminus \{GP(n, \frac{n}{4}), GP(n, 1), GP(n, 2)\}$, *we have:*

$$G \prec_T GP(n, 2).$$

Proof. Suppose $G \in GP(n) \setminus \{GP(n, \frac{n}{4}), GP(n, 1)\}$. Then for $i = 0, 1, 2, 3$, $T_i(G) = T_i(GP(n, \frac{n}{4})) = T_i(GP(n, 1))$ and $516n = T_4(G) < T_4(GP(n, \frac{n}{4})) = 518n < T_4(GP(n, 1)) = 524n$. Therefore, in an $T-$order we have,

$$G \prec_T GP(n, \frac{n}{4}) \prec_T GP(n, 1).$$

Now let $G \in GP(n) \setminus \{GP(n, \frac{n}{4}), GP(n, 1), GP(n, 2)\}$. Then if $i = 0, 1, 2, 3, 4$, $T_i(G) = T_i(GP(n, 2))$ and $2556n = T_5(G) < T_5(GP(n, 2)) = 2566n$ and so $G \prec_T GP(n, 2)$. This completes the proof.

Theorem 2.13. *Let* n *be a positive integer such that only* $5 \mid n$. *Then in an* $T-$*order of the set of the generalized Petersen graphs of order* $2n$,

(1) *for any* $G \in GP(n) \setminus GP(n, 1)$, *we have:*

$$G \prec_T GP(n, 1).$$

(2) *for any* $G \in GP(n) \setminus \{GP(n, \frac{n}{5}), GP(n, \frac{2n}{5}), GP(n, 1), GP(n, 2)\}$, *we have:*

$$G \prec_T GP(n, \frac{n}{5}), GP(n, \frac{2n}{5}) \prec_T GP(n, 2).$$

Proof. By using Theorem 2.10, the proof of this theorem is similar to Theorems 2.11 and 2.12.

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