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On the Laplacian Szeged Spectrum of Paths

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ABSTRACT

We present explicit formulas for the Laplacian Szeged eigenvalues of paths, grids, C_4-nanotubes and of Cartesian products of paths with some other simple graphs. A number of open problems is listed.

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1. INTRODUCTION AND PRELIMINARIES

One of the most common ways of representing and manipulating graphs is via their adjacency matrices. The **adjacency matrix** $A(G)$ of a (simple, undirected) graph G is a square matrix whose rows and columns are indexed by the vertices of G such that $A(i,j) = 1$ if vertices i and j are adjacent in G and $A(i,j) = 0$ otherwise. A **topological index** of a graph is a number derived from the graph which remains invariant under graph isomorphisms. The number of topological indices introduced and investigated during the last couple of decades is vast, and quite a few of them have been defined either directly from the adjacency matrix of a graph or by using certain weightings. A good example is one of the oldest and best researched topological indices, the Wiener index, which was (implicitly) defined in [13] as the sum of elements of weighted adjacency matrices of trees, where the weight of an edge uv of a tree T was given as the product of the number of vertices closer to u than to v and the number of vertices closer to v than to u. The more

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familiar definition of $W(G)$ as the sum of all distances among pairs of vertices in graph appeared later. These two definitions coincide for trees, but not for general graphs. Applying the original definition to graphs with cycles resulted in definition of a novel topological index called the Szeged index [8, 9]. The adjacency matrix of a graph weighted in the described way is called its Szeged matrix. In this paper we consider the Laplacians of Szeged matrices of paths and compute their spectra. Such matrices were first considered in [5], where their spectra were computed for several families of graphs. However, paths were not among those families. We apply the results on Cartesian products of paths with other simple factors such as paths, cycles, and graphs whose spectra were computed in [5].

All graphs in this paper are finite, simple, undirected and connected. For terms not defined here we refer the reader to any of several standard monographs such as, e.g., [12].

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. The number of vertices of G is denoted by n and the degree of vertex i is denoted by $d(i)$. The adjacency matrix of a graph G is denoted by $A(G)$. The eigenvalues of a graph G are the eigenvalues of its adjacency matrix $A(G)$.

The **Szeged index** of a connected graph G is denoted by $Sz(G)$ and defined by

$$Sz(G) = \sum_{e=uv} n_u(e)n_v(e).$$

Here the sum is taken over all edges of G, and for a given edge $e = uv$, the quantity $n_u(e)$ denotes the number of vertices closer to u than to v; the quantity $n_v(e)$ is defined analogously.

It is obvious that an end-vertex of any edge is closer to itself than to the other end-vertex of that edge. Hence the product $n_u(e)n_v(e)$ is always positive, and the function $w: E(G) \to \mathbb{R}^+$ is a weight function on $E(G)$. We call such weight function **Szeged weighting** of G. The adjacency matrix of a graph G weighted by the Szeged weighting is called the **Szeged matrix** of G and denoted by $SzM(G) = [s_{i,j}]$. Its eigenvalues are called the **Szeged eigenvalues** of G and denoted by $\sigma_r(G)$, for $r = 1, \dots, n$. Obviously, the Szeged index of a graph G can be expressed as one half of the sum of all entries of $SzM(G)$.

Let G be a weighted graph with a weight function $w: E(G) \to \mathbb{R}^+$ and $W(G) = [w_{i,j}]$ its adjacency matrix. (We assume $w(uv) = w(vu)$ and hence $w_{i,j} = w_{j,i}$.) The **Laplacian matrix** of a weighted graph G is defined as $LW(G) = [l_{i,j}]$, where

$$l_{i,j} = \begin{cases} w_i = \sum_{j=1}^{n} w_{ij} & i = j \\ -w_{ij} & ij \in E(G) \\ 0 & 0therwise \end{cases}.$$

For unweighted graphs this definition gives us the usual Laplacian matrix of G defined as $L(G) = D(G) - A(G)$, where $D(G) = [d(i)\delta_{i,j}]$ is the degree matrix of G, and $\delta_{i,j}$ denotes the Kronecker delta. The Laplacian matrix of a graph G weighted by the Szeged weighting is denoted by $LSzM(G)$ and called the **Laplacian Szeged matrix** of G. Its eigenvalues are the Laplacian Szeged eigenvalues of G. We denote them by $\mu'_r(G)$, $r = 1, \dots, n$, while the eigenvalues of the Laplacian matrix of the underlying unweighted graph G are denoted by $\mu_r(G)$, $r = 1, \dots, n$.

As an example, we demonstrate the relations between the four types of spectra for cycles on n vertices.

Example 1. Let C_n be the cycle graph on n vertices. The spectrum of C_n is given by $\lambda_r = 2\cos\frac{2r\pi}{n}$ (see, e.g. [4], p. 72), and the Laplacian eigenvalues are given by $\mu_r = 4\sin^2\frac{2r\pi}{n}$. For each edge $e = uv$ of C_n, the product $n_u(e)n_v(e)$ depends only on the parity of n and it is given by

$$n_u(e)n_v(e) = \begin{cases} \left(\frac{n}{2}\right)^2 & n \text{ is even} \\ \left(\frac{n-1}{2}\right)^2 & n \text{ is odd} \end{cases}.$$

Now the Szeged matrix of C_n is given by $SzM(C_n) = \left(\frac{n}{2}\right)^2 A(C_n)$ for n even and by $SzM(C_n) = \left(\frac{n-1}{2}\right)^2 A(C_n)$ for n odd. Hence $LSzM(C_n) = \left(\frac{n}{2}\right)^2 L(C_n)$ for n even and by $LSzM(C_n) = \left(\frac{n-1}{2}\right)^2 L(C_n)$ for n odd. Finally, $\mu'_r(C_n) = \frac{n^2\sin^2 r\pi}{n}$ and $\mu'_r(C_n) = \frac{(n-1)^2\sin^2 r\pi}{n}$ for n even and odd, respectively.

2. Main Results

2.1 Paths

Paths usually serve as first examples in papers dealing with topological indices. They owe this prominence to their simple and regular structure that is chemically realizable and hence relevant. Stars and other trees usually follow, before considering graphs with more elaborate connectivity patterns. The paper by Fath-Tabar *et al.* [5] is a notable exception: the only trees considered there are stars, and they were included only as special cases of complete bipartite graphs. In this section we fill this gap and determine the Laplacian Szeged eigenvalues of paths and of some graphs that arise as Cartesian products with path factors.

Theorem 2. The Laplacian Szeged spectrum of P_n is given by

$$\mu'_r = r(r-1), \qquad r = 1, \dots, n.$$

Proof. The Laplacian Szeged matrix of P_n conserves the tridiagonal structure of the adjacency matrix of P_n. If the vertices of P_n are labeled by $1,2, \dots, n$, then it is easy to see that the Szeged weights of the edges are symmetric and appear as the elements of the $(n-1)$-st anti-diagonal of the multiplication table (see Figure 1), but

1	2	3	4	5	6	7	8	9	…..
2	4	6	8	10	12	14	16	18	…..
3	6	9	12	15	18	21	24	27	…..
4	8	12	16	20	24	28	32	36	…..
5	10	15	20	25	30	35	40	45	…..
6	12	18	24	30	36	42	48	54	…..
7	14	21	28	35	42	49	56	63	…..
8	16	24	32	40	48	56	64	72	…..
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	

Figure 1: Super- and sub-diagonal of $LSzM(P_8)$ in the multiplication table.

with negative sign. Hence, the sub- and the super-diagonal of $LSzM(P_n)$ are equal. Further, the value in the m-th row on the main diagonal is equal to $n + 2m(n-m)$ for a given fixed n. The main diagonals of $LSzM(P_n)$ are, in fact, the rows of a triangular array that appears as sequence $A141387(n)$ in [11]. In spite of its simplicity, this array seems to have many physically relevant interpretations. For example, it is connected with infinite-dimensional matrix representations of angular momentum operators (J_1, J_2, J_3) in Jordan-Schwinger form [10]. Also, tridiagonal matrices with the same main diagonal appear in a paper by Bruschi et al. [3] concerned with some Diophantine problems for some classes of orthogonal polynomials arising in the context of isochronous many-body problems. In this last paper the authors show, in a rather elaborate way, that the eigenvalues of their matrices U_n are $r(r-1)$ for $r = 1, \dots, n$. By a closer look at their matrices U_n one can see that the elements of the sub-diagonal of U_n are given by $(m-1)^2$ for $2 \le m \le n$, while on the super-diagonal the elements are $(n-m)^2$ for $1 \le m \le n-1$. As U_n is a tridiagonal matrix, elements of its sub- and super-diagonals enter its characteristic polynomial only in products of the form $U_n(m, m-1)U_n(m-1, m)$ for $2 \le m \le n$. But

$$U_n(m, m-1)U_n(m-1, m) = LSzM(P_n)(m, m-1)LSzM(P_n)(m-1, m)$$
$$= [(m-1)\,(n-m)]^2.$$

Since the elements on the main diagonals of U_n and $LSzM(P_n)$ are equal, it follows that U_n and $LSzM(P_n)$ must have the same characteristic polynomials, and hence the same spectra.

■

It is worth mentioning that the characteristic polynomials of $LSzM(P_n)$ form a system of orthogonal polynomials whose coefficients seem to be the Legendre-Stirling numbers of the first kind [1].

As an immediate application of the above result, we have an explicit expression for the Laplacian Szeged energy of paths. (Here the Laplacian Szeged energy of a graph G, denoted by $LSzE(G)$, is defined in the usual way, as the sum of absolute values of all eigenvalues of its Laplacian Szeged matrix, $LSzE(G) = \sum_{r=1}^{n} |\mu_r'|$.)

Corollary 3. $LSzE(P_n) = 2\binom{n+1}{3}$.

2.2 Cartesian Products

Let us consider two graphs G_1 and G_2. Their **Cartesian product** $G_1 \square G_2$ is a graph on the vertex set $V(G_1) \square V(G_2)$ and the vertices (u_1, u_2) and (v_1, v_2) are adjacent in $G_1 \square G_2$ if and only if either ($u_1 = v_1$ and $u_2 v_2 \in E(G_2)$) or ($u_1 v_1 \in E(G_1)$ and $u_2 = v_2$). The adjacency matrix of $G_1 \square G_2$ is given by

$$A(G_1 \square G_2) = I_{n_1} \otimes A(G_2) + A(G_1) \otimes I_{n_2}$$

[4], where n_1 and n_2 denote the number of vertices of G_1 and G_2, respectively, and $A \otimes B$ is the tensor product of matrices A and B (see, e.g., [7], p. 430). The Laplacian matrix of $G_1 \square G_2$ is then given by analogous formula

$$L(G_1 \square G_2) = I_{n_1} \otimes L(G_2) + L(G_1) \otimes I_{n_2}.$$

If the eigenvalues of G_1 are denoted by $\lambda_{1r}, r = 1, \dots, n_1$ and the eigenvalues of G_2 by λ_{2s}, $s = 1, \dots, n_2$, then the eigenvalues of $G_1 \square G_2$ are given by

$$\lambda_{r,s}(G_1 \square G_2) = \lambda_{1r}(G_1) + \lambda_{2s}(G_2),$$

for $r = 1, \dots, n_1$, $s = 1, \dots, n_2$ ([4], Ch. 2).

We start by recalling the basic result on the Laplacian Szeged spectra of Cartesian products [5] and then we combine it with our Theorem 2.

Theorem 4. The Laplacian Szeged eigenvalues of $G_1 \square G_2$ are given by

$$\mu_{r,s}'(G_1 \quad G_2) = n_2^2 \mu_r'(G_1) + n_1^2 \mu_s'(G_2), \quad for\ r = 1, \dots, n_1, \quad s = 1, \dots, n_2.$$

■

Cartesian products with path factors give rise to many interesting classes of graphs. The most obvious examples are rectangular grids $P_m \square P_n$ and C_4-nanotubes $P_m \square C_n$. Their Laplacian Szeged eigenvalues are given in the following corollary.

Corollary 5.

1. $\mu_{r,s}'(P_m \square P_n) = n^2 r(r-1) + m^2 s(s-1)$;
2. $\mu_{r,s}'(P_m \square C_{2n}) = 4n^2 \left[r(r-1) + m^2 \sin^2 \frac{s\pi}{2n} \right]$;

3. $\mu_{r,s}{}'(P_m \square C_{2n+1}) = (2n+1)^2 r(r-1) + 4m^2n^2\sin^2\frac{s\pi}{2n+1}$.

In all cases above r and s run from 1 to the number of vertices in the first and in the second factor, respectively. ■

Numerous other results could be obtained by combining Theorem 2 with results established in [5] for circulant and strongly regular graphs. We present here only the case of Cartesian products of paths and complete bipartite graphs, leaving the rest to the interested reader. Recall that the Laplacian Szeged eigenvalues of $K_{m,n}$ are 0, m^2n, mn^2 and $mn(m+n)$ with multiplicities 1, $n-1$, $m-1$ and 1, respectively [5].

Corollary 6. Let $K_{m,n}$ be a complete bipartite graph with $m \leq n$. Then

1. $\mu'_{r,1}(P_k \square K_{m,n}) = (m+n)^2 r(r-1)$;
2. $\mu'_{r,s}(P_k \square K_{m,n}) = (m+n)^2 r(r-1) + k^2m^2n$ for $2 \leq s \leq n$;
3. $\mu'_{r,s}(P_k \square K_{m,n}) = (m+n)^2 r(r-1) + k^2mn^2$ for $n+1 \leq s \leq m+n-1$;
4. $\mu'_{r,m+n}(P_k \square K_{m,n}) = (m+n)[r(r-1)(m+n) + k^2mn]$.

In all cases above r runs from 1 to k.

3. CONCLUDING REMARKS

In this note we have extended the line of research of reference [5] by providing explicit expressions for the Laplacian Szeged eigenvalues of paths. Now we know the Laplacian spectra of paths and stars, but for other trees they still remain unknown. There are also other interesting open questions. For example, both paths and stars have integral Laplacian Szeged spectra; are they the only such trees? If not, how to characterize trees with integral Laplacian Szeged spectrum? Then, the Laplacian Szeged eigenvectors of paths exhibit interesting structure; the one corresponding to the largest eigenvalue $n(n-1)$ is the alternating $(n-1)$-st row of the Pascal triangle. What can be said about other eigenvectors? Further, apparently simpler task of determining the Szeged eigenvalues of paths remains unsolved, in spite of very simple structure and weighting of $SzM(P_n)$. This matrix is of the so called Kac-Sylvester type [6]. Unlike in the Laplacian Szeged case, computer experiments have so far failed to reveal a clear pattern in the spectra. Similarly, coefficients of the characteristic polynomials of $SzM(P_n)$ form a triangular array that does not appear in [11]. There is a chance, however, that the coefficients appear in older literature. We list here characteristic polynomials $SzP_n(x)$ of the Szeged matrices of P_n for $1 \leq n \leq 5$.

$SzP_1(x) = -x$

$SzP_2(x) = x^2 - 1$

$SzP_3(x) = -x^3 + 8x$

$SzP_4(x) = x^4 - 34x^2 + 81$
$SzP_5(x) = -x^5 + 104x^3 - 1408x$

It can be easily seen that the free coefficients in the polynomials of even degree n behave as $[(n-1)!!]^4$. Also, the coefficients of x^{n-2} seem to be given by $n(n^4-1)/30$, but we cannot explain the pattern.

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REFERENCES

1. G. E. Andrews, W. Gawronski and L. L. Littlejohn, The Legendre-Stirling numbers, *Discrete Math.* **311** (2011) 1255–1272.
2. N. Biggs, *Algebraic Graph Theory*, Cambridge Univ. Press, Cambridge, 1974.
3. M. Bruschi, F. Calogero and R. Droghei, Proof of certain Diophantine conjectures and identification of remarkable classes of orthogonal polynomials, *J. Phys. A: Math. Theor.* **40** (2007) 3815–3829.
4. D. M. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs*, Academic Press, New York, 1980.
5. G. H. Fath-Tabar, T. Došlić andA. R. Ashrafi, On the Szeged and the Laplacian Szeged spectrum of a graph, *Linear Algebra Appl.* **433** (2010) 662–671.
6. C. M. da Fonseca and E. Kiliç, A new type of Sylvester–Kac matrix and its spectrum, *Linear Multilinear Algebra*, to appear.
7. C. D. Godsil, *Algebraic Combinatorics*, Chapman and Hall, New York, 1993.
8. I. Gutman, A formula for the Wiener number of trees and its extension to the graphs containing cycles, *Graph Theory Notes of New York* **XVII** (1994) 9–15.
9. I. Gutman, A. A. Dobrynin, The Szeged index-a success story, *Graph Theory Notes New York* **34** (1998) 37–44.
10. J. Schwinger, *On Angular Momentum*, Unpublished Report, Harvard University, Nuclear Development Associates, Inc., United States Department of Energy (through predecessor agency the Atomic Energy Commission), Report Number NYO-3071 (January 26, 1952).
11. N. J. A. Sloane, (ed.), *The On-Line Encyclopedia of Integer Sequences*, published electronically at http://oeis.org.
12. D. B. West, *Introduction to Graph Theory*, Prentice Hall, Upper Saddle River, 1996.
13. H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.