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Spectral Distances of Graphs Based on their Different Matrix Representations

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Abstract. The investigation of the spectral distances of graphs that started in [3] (I. Jovanović, Z. Stanić, *Spectral distances of graphs*, Linear Algebra Appl., 436 (2012) 1425–1435.) is continued by defining Laplacian and signless Laplacian spectral distances and considering their relations to the spectral distances based on the adjacency matrix of graph. Some separate results concerning the defined distances are given, and the initial spectral distances in certain sets of graphs are investigated. Computational data on Laplacian and signless Laplacian spectral distances are provided.

1. Introduction

Given a graph G on n vertices with the adjacency matrix A and the diagonal matrix of its vertex degrees D, then the Laplacian matrix of G is $L = D - A$, and the signless Laplacian matrix of G is $Q = D + A$. The M-*spectrum* of G is just the spectrum of the corresponding matrix M, where M is one of the matrices A, L, or Q (in the case of A-spectrum the matrix name will be usually suppressed). For $i = 1, \ldots, n$, the eigenvalues of A, L, and Q in non-increasing order will be denoted by $\lambda_i(G)$, $\mu_i(G)$, and $\kappa_i(G)$, respectively. In [3] we defined the A-*spectral distance* (where it is simply named spectral distance) of n-vertex graphs G_1 and G_2 as

$$\sigma_A(G_1, G_2) = \sum_{i=1}^{n} |\lambda_i(G_1) - \lambda_i(G_2)|.$$

This definition was earlier suggested by R.A. Brualdi (see [4]). If X is an arbitrary set of graphs on n vertices, then the *cospectrality* of $G \in X$ is defined as

$$\mathrm{cs}_X^A(G) = \min\{\sigma_A(G, H) : H \in X,\ H \neq G\}, \tag{1}$$

which is completed by the *cospectrality measure*

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$$\mathrm{cs}^A(X) = \max\{\mathrm{cs}_X^A(G) : G \in X\}.$$

We also introduced the *spectral eccentricity* of G and the *spectral diameter* of X by

$$\mathrm{secc}_X^A(G) = \max\{\sigma_A(G,H) : H \in X\}, \quad \text{and} \quad \mathrm{sdiam}^A(X) = \max\{\mathrm{secc}_X^A(G) : G \in X\},$$

respectively. All these quantities are closely related to the spectral distances and can be used for measuring how far apart the spectrum of a graph in X can be from the spectrum of any other graph belonging to the same set. Moreover, the L- and Q-spectral distances (between n-vertex graphs G_1 and G_2) are defined as

$$\sigma_L(G_1,G_2) = \sum_{i=1}^{n} |\mu_i(G_1) - \mu_i(G_2)|, \text{ and } \sigma_Q(G_1,G_2) = \sum_{i=1}^{n} |\kappa_i(G_1) - \kappa_i(G_2)|,$$

respectively. The quantities that are related to the A-spectral distances can be defined for the L- or Q-spectral distances in the same way. We just change the matrix name in the corresponding notation to indicate which spectrum we are dealing with (for example, we write cs_X^L to indicate that we use σ_L instead of σ_A in (1)). To avoid possible confusion we keep the matrix name in the A-spectral distances, while the term "spectral distance" will be used as a common name for all three kinds of spectral distances.

An n-vertex cycle is denoted by C_n, while the complete multipartite graph with k parts and n_i $(1 \leq i \leq k)$ vertices in each is denoted by $K_{n_1,n_2,\dots,n_k}$; if $n_1 = n_2 = \cdots = n_k = m$, we use the short expression $K_{k\times m}$. The disjoint union of two graphs G_1 and G_2 is denoted by $G_1 \dot{+} G_2$, while the complement of G is denoted by $\overline{G}$. The complete product $G_1 \nabla G_2$ is obtained by joining every vertex of G_1 with every vertex of G_2. For the remaining notation and terminology we refer the reader to [2].

The paper is organized as follows. In Section 2 we consider the relations between different spectral distances and give some particular results regarding the A-spectral distances. In Section 3 we consider the L- and Q-spectral distances, and in Section 4 we consider the A-spectral distances between graphs belonging to some specified sets of graphs. A computational data related to the L- and Q-spectral distances are given in Appendix.

2. Relations between different spectral distances and some particular results

Recall from [1] that if $r = \lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ is the spectrum of r-regular graph G, then its L-spectrum is $r-\lambda_n(G) \geq r-\lambda_{n-1}(G) \geq \cdots \geq r-\lambda_1(G) = 0$, its Q-spectrum is $\lambda_1(G)+r \geq \lambda_2(G)+r \geq \cdots \geq \lambda_n(G)+r$, while the spectrum of the complement $\overline{G}$ is $n-1-r \geq -1-\lambda_n(G) \geq \cdots \geq -1-\lambda_2(G)$. Finally, the line graph $L(G)$ is $(2r-2)$-regular with spectrum $2r-2 \geq \lambda_2(G)+r-2 \geq \cdots \geq \lambda_n(G)+r-2 \geq [-2]^{\frac{nr}{2}-n}$ (as usual, in the exponential notation the exponent stands for the multiplicity of the eigenvalue).

We consider the relations between A-, L-, and Q-spectral distances in some specific cases.

Proposition 2.1. *Let G_1 and G_2 be n-vertex regular graphs of degree r_1 and r_2, respectively. If $r_1 \leq r_2$, then the following inequalities hold:*

(i) $\sigma_Q(G_1,G_2) \leq \sigma_A(G_1,G_2) + n(r_2 - r_1)$,

(ii) $\sigma_L(G_1,G_2) \leq \sigma_A(G_1,G_2) + n(r_2 - r_1)$.

Proof (i) We get

$$\sigma_Q(G_1,G_2) = \sum_{i=1}^{n} |\kappa_i(G_1) - \kappa_i(G_2)| = \sum_{i=1}^{n} |(\lambda_i(G_1) + r_1) - (\lambda_i(G_2) + r_2)| \leq$$
$$\sum_{i=1}^{n} |\lambda_i(G_1) - \lambda_i(G_2)| + \sum_{i=1}^{n} |r_1 - r_2| = \sigma_A(G_1,G_2) + n(r_2 - r_1).$$

The statement (ii) is proved in the similar way. □

Note that if G_1 and G_2 are regular graphs with the same degree, we have

$$\sigma_A(G_1, G_2) = \sigma_Q(G_1, G_2) = \sigma_L(G_1, G_2). \tag{2}$$

Moreover, we have the following result.

Proposition 2.2. *Let $O(G)$ stands for application of line and complement of regular graph G arbitrary number of times and in arbitrary order. Let G_1 and G_2 be r-regular graphs on n vertices. Then*

$$\sigma_A(O(G_1), O(G_2)) = \sigma_A(G_1, G_2) = \sigma_L(O(G_1), O(G_2)) = \sigma_L(G_1, G_2) = \sigma_Q(O(G_1), O(G_2)) = \sigma_Q(G_1, G_2).$$

Proof All equalities follow from the corresponding spectra given at the beginning of the section, and the equalities (2). □

We prove an inequality.

Proposition 2.3. *Given an r-regular graph G on n vertices, such that its degree is not greater than degree of $\overline{G}$. Then we have*

$$\sigma_L(G, \overline{G}) \leq \sigma_A(G, \overline{G}) + (n-2)(n-2r-1).$$

Proof We have $\mu_n(G) = \mu_n(\overline{G}) = 0$, and, by assumption, $n - 2r - 1 \geq 0$ holds. We compute

$$\begin{aligned}\sigma_L(G, \overline{G}) = &\sum_{i=1}^{n-1} |\mu_i(G) - \mu_i(\overline{G})| = \sum_{i=1}^{n-1} |(r - \lambda_{n-i+1}(G)) - (n - r + \lambda_{i+1}(G))| = \\ &\sum_{i=2}^{n} |\lambda_i(G) + \lambda_{n-i+2}(G) + n - 2r| \leq \sum_{i=2}^{n} |\lambda_i(G) + \lambda_{n-i+2}(G) + 1| + \sum_{i=2}^{n} |n - 2r - 1| = \\ &\sum_{i=2}^{n} |\lambda_i(G) - (-1 - \lambda_{n-i+2}(G))| + |\lambda_1(G) - (n-1-r)| + (n-2)(n-2r-1) = \\ &\sum_{i=2}^{n} |\lambda_i(G) - \lambda_i(\overline{G}))| + |\lambda_1(G) - \lambda_1(\overline{G})| + (n-2)(n-2r-1) = \\ &\sigma_A(G, \overline{G}) + (n-2)(n-2r-1). \quad \square\end{aligned}$$

Remark 2.1. *There can be found many graphs attaining the equality in the previous proposition. For example, if G is the Petersen graph then both sides of the inequality are equal to 30. Conversely, if G is a complete bipartite graph of even order n with a perfect matching removed, $K^-_{\frac{n}{2},\frac{n}{2}}$, then the equality is attained only if $n = 2$. Moreover, if $n \geq 8$ we have*

$$3n - 16 = \sigma_L\left(K^-_{\frac{n}{2},\frac{n}{2}}, \overline{K^-_{\frac{n}{2},\frac{n}{2}}}\right) < \sigma_A\left(K^-_{\frac{n}{2},\frac{n}{2}}, \overline{K^-_{\frac{n}{2},\frac{n}{2}}}\right) + (n-2)\left(n - 2\left(\frac{n}{2} - 1\right) - 1\right) = 3n - 10,$$

i.e. the corresponding values differ in 6.

We now turn the attention to the A-spectral distances.

Proposition 2.4. *Given an n-vertex graph G, and let H is obtained from G by replacing edges $uw_1, \ldots, uw_k$ with non-edges $vw_1, \ldots, vw_k$. If $\Lambda = \max\{\lambda_1(G), \lambda_1(H)\}$, and $\lambda = \min\{\lambda_n(G), \lambda_n(H)\}$ then*

$$\sigma_A(G, H) \leq \Lambda + \lambda_1(G) - \lambda_n(G) - \lambda.$$

Proof We have (see [5])

$$\lambda_{i-1}(G) \geq \lambda_i(H) \geq \lambda_{i+1}(G), \text{ for } i = 2, 3, \dots, n-1.$$

Using these inequalities and the eigenvalue interlacing ([2, Corollary 1.3.12]) we get

$$|\lambda_i(G) - \lambda_i(H)| \leq \lambda_{i-1}(G) - \lambda_{i+1}(G), \text{ for } i = 2, 3, \dots, n-1,$$

and we also have

$$|\lambda_1(G) - \lambda_1(H)| \leq \Lambda - \lambda_2(G), \text{ and } |\lambda_n(G) - \lambda_n(H)| \leq \lambda_{n-2}(G) - \lambda.$$

Putting together we get

$$\sigma_A(G,H) = \sum_{i=1}^{n} |\lambda_i(G) - \lambda_i(H)| \leq \Lambda + \lambda_1(G) - \lambda_n(G) - \lambda. \quad \square$$

Proposition 2.5. *Given an r-regular bipartite graph G on n vertices, such that its degree is not greater than degree of $\overline{G}$. If $|\lambda_i(G) - \lambda_{i+1}(G)| \leq 1$, $i = 1, ..., \lfloor \frac{n}{2} \rfloor$, then $\sigma_A(G, \overline{G}) = 2(n - 2r - 1)$.*

Proof We compute

$$\sigma_A(G,\overline{G}) = \sum_{i=1}^{n} |\lambda_i(G) - \lambda_i(\overline{G})| = (n-2r-1) + \sum_{i=2}^{n} |\lambda_i(G) + \lambda_{n-i+2}(G) + 1| =$$
$$(n-2r-1) + 2\sum_{i=1}^{\lfloor n/2 \rfloor} |\lambda_i(G) - \lambda_{i+1}(G) - 1|.$$

If n is odd, since $\lambda_{\frac{n+1}{2}} = 0$, we get

$$2\sum_{i=1}^{\lfloor n/2 \rfloor} |\lambda_i(G) - \lambda_{i+1}(G) - 1| = (n-1) - 2\left(\lambda_1(G) - \lambda_{\frac{n+1}{2}}\right) = n - 2r - 1,$$

while if n is even we get

$$2\sum_{i=1}^{\lfloor n/2 \rfloor} |\lambda_i(G) - \lambda_{i+1}(G) - 1| = (n-2) - 2\left(\lambda_1(G) - \lambda_{n/2}(G)\right) + 1 - 2\lambda_{n/2}(G) = n - 2r - 1,$$

and so in both cases we get $\sigma_A(G, \overline{G}) = 2(n - 2r - 1)$. $\square$

3. *L*- and *Q*-spectral distances

The results concerning only the L- and Q-spectral distances of graphs are separated in this short section. We first get a simple formula for the L- and Q-spectral distance between the graph and its edge-deleted subgraph.

Proposition 3.1. *Given an n-vertex graph G. If the graph H is obtained by deleting k edges from G, then $\sigma_L(G,H) = \sigma_Q(G,H) = 2k$.*

Proof Assume that G has m edges, then $k \leq m$ holds. Let H' be the graph obtained by deleting an edge from G. Then, by [2, Theorem 7.1.5], we have $\mu_i(G) \geq \mu_i(H')$ $(i = 1, 2, \ldots, n)$. Similarly, by [2, Theorem 7.8.13], we have $\kappa_i(G) \geq \kappa_i(H')$ $(i = 1, 2, \ldots, n)$.

Since H is obtained by deleting k edges, by successive application of the above inequalities, we get $\mu_i(G) \geq \mu_i(H)$ $(i = 1, 2, \ldots, n)$, and $\kappa_i(G) \geq \kappa_i(H)$ $(i = 1, 2, \ldots, n)$, an therefore we have

$$\sigma_L(G,H) = \sigma_L(G,H) = \sum_{i=1}^{n} |\mu_i(G) - \mu_i(H)| = \sum_{i=1}^{n} (\mu_i(G) - \mu_i(H)) = 2m - 2(m-k) = 2k,$$

and similarly, $\sigma_Q(G,H) = 2k$. □

Corollary 3.1. *Let G_1, G_2, G^+ and G^- be n-vertex graphs with m_1, m_2, m^+ and m^- edges, respectively. If G^+ (resp. G^-) is a common supergraph (resp. subgraph) of G_1 and G_2, then the following inequalities hold:*

$$\max\{\sigma_L(G_1,G_2), \sigma_Q(G_1,G_2)\} \leq 2(2m^+ - m_1 - m_2),$$

and

$$\max\{\sigma_L(G_1,G_2), \sigma_Q(G_1,G_2)\} \leq 2(m_1 + m_2 - 2m^-).$$

Proof We have $\sigma_L(G_1,G_2) \leq \min\{\sigma_L(G_1,G^+) + \sigma_L(G^+,G_2), \sigma_L(G_1,G^-) + \sigma_L(G^-,G_2)\}$, and similarly for $\sigma_Q(G_1,G_2)$. Then both inequalities follow from Proposition 3.1. □

Corollary 3.2. *Let $X = \{G_0, G_1, ..., G_{\binom{n}{2}}\}$ be the set of n-vertex graphs, where G_i is an edge-deleted subgraph of G_{i+1} $(i = 0, 1 \ldots, \binom{n}{2} - 1)$. We have*

(i) $\mathrm{cs}^L_X(G_i) = 2$, $0 \leq i \leq \binom{n}{2}$,

(ii) $\mathrm{cs}^L(X) = 2$,

(iii) $\mathrm{secc}^L_X(G_i) = \max\{2i, n(n-1) - 2i\}$,

(iv) $\mathrm{sdiam}^L(X) = n(n-1)$.

Proof If $i < j$ then by Proposition 3.1, we have $\sigma_L(G_i, G_j) = 2(j-i)$, and the proof follows. □

The statements of Corollary 3.2 remain valid for the Q-spectral distances.

4. *A*-spectral distances in certain sets of graphs

As we noted in [3], any spectral distance is much easier considered in some specific set of n-vertex graphs (compare [4], as well), and this is exactly what we do in this section. We take an appropriate set of graphs X and we compute the A-spectral distance between any two graphs in X, along with the remaining quantities defined in the opening section. As a set X we choose three different sets of graphs related to complete bipartite graphs: $X_l = \{G_0, G_1, ..., G_k\}$ $(l = 1, 2, 3)$, where

1. if $G_i \in X_1$ then $G_i = C_{n_1} \nabla C_{n_2} \nabla \cdots \nabla C_{n_i} \nabla K_{n_{i+1}, n_{i+2}, \ldots, n_k}$, with $n_j \geq 3$ $(1 \leq j \leq k)$ and $n_1 + n_2 + \cdots + n_k = n$.
2. if $G_i \in X_2$ then $G_i = K_{n_1+n_2+\cdots+n_i} \nabla K_{n_{i+1}, n_{i+2}, \ldots, n_k}$, with $n_1 + n_2 + \cdots + n_k = n$.
3. if $G_i \in X_3$ then $G_i = (K_{ip} \nabla K_{i\times(m-p)}) \nabla K_{(k-i)\times m}$, with $0 < p < m$ and $k \cdot m = n$.

In particular, G_0 is a complete k-partite graph with m vertices in each part when $G_0 \in X_3$, or n_i vertices in i^{th} part when $G_0 \in X_1$ or $G_0 \in X_2$. Then, in each case, G_i $(1 \leq i \leq k)$ is obtained by inserting appropriate edges into G_{i-1} (i.e. n_i edges if $G_i \in X_1$, $\frac{n_i(n_i-1)}{2}$ edges if $G_i \in X_2$ and $\frac{p}{2}(2m-p-1)$ edges if $G_i \in X_3$).

Using the notation above, we prove the following three propositions. Before we state the first of them, recall that the energy of a graph G, usually denoted by $E(G)$, is equal to the sum of the absolute values of the eigenvalues of G. In [3] we presented several situations in which the A-spectral distance is a function of the energy. The next proposition provides another similar result.

Proposition 4.1. *For X_1 we have $\sigma_A(G_i, G_j) = \sum_{p=i+1}^{j} E(C_{n_p})$ $(0 \leq i < j \leq k)$, and*

(i) $\mathrm{cs}^A_{X_1}(G_i) = \min\{E(C_{n_i}), E(C_{n_{i+1}})\}, \quad 1 \leq i \leq k-1,$

(ii) $\mathrm{cs}^A(X_1) \leq E(C_{n_i})$*, where* $n_i = \max\{n_i,\ 1 \leq i \leq k\}$,

(iii) $\mathrm{secc}^A_{X_1}(G_i) = \max\{\sum_{p=1}^{i} E(C_{n_p}), \sum_{p=i+1}^{k} E(C_{n_p})\}, \quad 1 \leq i \leq k-1,$

(iv) $\mathrm{sdiam}^A(X_1) = \sum_{p=1}^{k} E(C_{n_p})$.

Proof Denote $H_1 = C_{n_1} \nabla C_{n_2} \nabla \cdots \nabla C_{n_i}$ and $H_2 = K_{n_{i+1},\ldots,n_k}$. Then H_1 has $m_1 = \sum_{p=1}^{i} n_p$ vertices, while H_2 has $m_2 = \sum_{q=i+1}^{k} n_q$ vertices. To determine the characteristic polynomial of $G_i = H_1 \nabla H_2$ we use the following formula [1, Theorem 2.7]:

$$\begin{aligned} P_{H_1 \nabla H_2}(x) =& (-1)^{m_2} P_{H_1}(x) P_{\overline{H_2}}(-x-1) + (-1)^{m_1} P_{H_2}(x) P_{\overline{H_1}}(-x-1) - \\ & (-1)^{m_1+m_2} P_{\overline{H_1}}(-x-1) P_{\overline{H_2}}(-x-1). \end{aligned} \tag{3}$$

The characteristic polynomial of H_1 we determine by using walk-generating functions [1, Theorem 1.11]:

$$H_{H_1}(x) = \frac{1}{x}\left((-1)^{m_1} \frac{P_{\overline{H_1}}(-\frac{x+1}{x})}{P_{H_1}(\frac{1}{x})} - 1\right), \tag{4}$$

wherefrom we directly get

$$P_{H_1}(x) = \frac{(-1)^{m_1} P_{\overline{H_1}}(-x-1)}{\frac{1}{x} H_{H_1}(\frac{1}{x}) + 1}. \tag{5}$$

Since $\overline{H_1} = \overline{C_{n_1} \nabla C_{n_2} \nabla \ldots \nabla C_{n_i}} = \overline{C_{n_1}} \dot{+} \overline{C_{n_2}} \dot{+} \ldots \dot{+} \overline{C_{n_i}}$ we have

$$P_{\overline{H_1}}(x) = \prod_{p=1}^{i} P_{\overline{C_{n_p}}}(x). \tag{6}$$

We next express the characteristic polynomial of $\overline{C_n}$

$$P_{\overline{C_n}}(x) = (-1)^n \frac{x-n+3}{x+3} P_{C_n}(-x-1),$$

and so the relation (6) begins

$$P_{\overline{H_1}}(x) = \prod_{p=1}^{i}\left((-1)^{n_p} \frac{x-n_p+3}{x+3}\left(-2 + \sum_{k=0}^{\lfloor n_p/2 \rfloor} (-1)^{n_p-k} \frac{n_p}{n_p-k}\binom{n_p-k}{k}(x+1)^{n_p-2k}\right)\right). \tag{7}$$

Using [1, Theorem 7.20] we get another formula for the walk-generating function of H_1

$$H_{H_1}(x) = \frac{\sum_{p=1}^{i} H_{\overline{C_{n_p}}}\left(-\frac{x}{x+1}\right)}{x+1-x\sum_{p=1}^{i} H_{\overline{C_{n_p}}}\left(-\frac{x}{x+1}\right)}, \tag{8}$$

as well as the walk-generating function of $\overline{C_{n_p}}$

$$H_{\overline{C_{n_p}}}(x) = \frac{H_{C_{n_p}}(-\frac{x}{x+1})}{x+1-x\cdot H_{C_{n_p}}(-\frac{x}{x+1})} = \frac{n_p}{1-x(n_p-3)},$$

where $H_{C_{n_p}}(x) = \frac{n_p}{1-2x}$. According to this, the relation (4) becomes

$$H_{H_1}(x) = \frac{\sum_{p=1}^{i} \frac{n_p}{x(n_p-2)+1}}{1-x\cdot\sum_{p=1}^{i} \frac{n_p}{x(n_p-2)+1}}. \tag{9}$$

Putting (7) and (9) into (5), we obtain the characteristic polynomial of H_1

$$\begin{aligned} P_{H_1}(x) =& \frac{1}{(2-x)^i}\prod_{p=1}^{i}(2-x-n_p)\left(1-\sum_{p=1}^{i}\frac{n_p}{n_p+x-2}\right)\cdot \\ & \prod_{p=1}^{i}\left(-2+\sum_{k=0}^{[n_p/2]}(-1)^k\frac{n_p}{n_p-k}\binom{n_p-k}{k}x^{n_p-2k}\right) \end{aligned} \tag{10}$$

On the other hand, the characteristic polynomial of H_2 is (cf. [1, p. 74])

$$P_{H_2}(x) = x^{m_2-(k-i)}\left(1-\sum_{q=i+1}^{k}\frac{n_q}{x+n_q}\right)\prod_{q=i+1}^{k}(x+n_q), \tag{11}$$

while of its complement

$$P_{\overline{H_2}}(x) = (x+1)^{m_2-(k-i)}\prod_{q=i+1}^{k}(x-n_q+1). \tag{12}$$

By substitution (7), (10), (11) and (12) into (3) we obtain the characteristic polynomial of G_i

$$\begin{aligned} P_{G_i}(x) =& x^{m_2-(k-i)}\frac{1}{(2-x)^i}\prod_{p=1}^{i}\left(-2+\sum_{k=0}^{\lfloor n_p/2\rfloor}(-1)^k\frac{n_p}{n_p-k}\binom{n_p-k}{k}x^{n_p-2k}\right)\cdot \\ & \prod_{p=1}^{i}(2-x-n_p)\prod_{q=i+1}^{k}(x+n_q)\left(1-\sum_{p=1}^{i}\frac{n_p}{n_p+x-2}-\sum_{q=i+1}^{k}\frac{n_q}{x+n_q}\right) \end{aligned}$$

Now, we can conclude about the spectrum of the graph G_i. The first factor in the previous equality gives $[0]^{m_2-(k-i)}$, and then the product of the next two factors gives the eigenvalues of the cycles $C_{n_1}, C_{n_2}, \ldots, C_{n_i}$ without eigenvalues equal to 2, respectively. The product of the last three factors gives the remaining k

eigenvalues, i.e. $\lambda_1(G_i)$, and $\lambda_{n-k+2}(G_i), \dots, \lambda_n(G_i)$, $1 \leq i \leq k$, where the positions of these eigenvalues in non-increasing spectrum are easily obtained by the eigenvalue interlacing. The sum of these eigenvalues is

$$\lambda_1(G_i) + \lambda_{n-k+2}(G_i) + \dots + \lambda_n(G_i) = 2i$$

(since the sum of eigenvalues of the cycle C_{n_p} $(1 \leq p \leq i)$ which is contained in the spectrum of G_i is equal to -2).

For computation of the A-spectral distance between two graphs G_i and G_j, $0 \leq i < j \leq k$ from the set X_1 we use the above sum of the corresponding eigenvalues and the following features of their spectra:

1. $\lambda_1(G_j) > \lambda_1(G_i)$ (follows directly),
2. $\lambda_l(G_j) \geq \lambda_l(G_i)$, $l = n-k+2, \dots, n$ (easily verified by the induction argumentation),
3. $|\lambda_l(G_j)| \geq |\lambda_l(G_i)|$, $l = 2, \dots, n-k+1$ (obvious, since these are the eigenvalues of the corresponding cycles).

The A-spectral distance between two graphs G_i and G_j, $0 \leq i < j \leq k$ is:

$$\begin{aligned}
\sigma_A(G_i, G_j) =& |\lambda_1(G_i) - \lambda_1(G_j)| + \sum_{l=2}^{n-k+1} |\lambda_l(G_i) - \lambda_l(G_j)| + \sum_{l=n-k+2}^{n} |\lambda_l(G_i) - \lambda_l(G_j)| = \\
& \lambda_1(G_j) - \lambda_1(G_i) + \sum_{l=2}^{n-k+1} (|\lambda_l(G_j)| - |\lambda_l(G_i)|) + \sum_{l=n-k+2}^{n} (\lambda_l(G_j) - \lambda_l(G_i)) = \\
& \lambda_1(G_j) - \lambda_1(G_i) + \sum_{l=n-k+2}^{n} (\lambda_l(G_j) - \lambda_l(G_i)) + \sum_{p=1}^{j} E(C_{n_p}) - 2j - \sum_{p=1}^{i} E(C_{n_p}) + 2i = \\
& \sum_{p=i+1}^{j} E(C_{n_p}) - 2(j-i) + \lambda_1(G_j) + \sum_{l=n-k+2}^{n} \lambda_l(G_j) - \lambda_1(G_i) - \sum_{l=n-k+2}^{n} \lambda_l(G_i) = \\
& \sum_{p=i+1}^{j} E(C_{n_p}) - 2(j-i) + 2j - 2i = \\
& \sum_{p=i+1}^{j} E(C_{n_p}).
\end{aligned}$$

Using the above equality we compute the quantities (i)–(iv) directly. □

Remark 4.1. *The L- and Q-spectral distances between the graphs in X_1 are simply computed. Namely, each graph G_i is an induced subgraph of G_j, so using Proposition 3.1, we get*

$$\sigma_L(G_i, G_j) = \sigma_Q(G_i, G_j) = 2 \sum_{p=i+1}^{j} n_p, \ 0 \leq i < j \leq k.$$

Forward, we have:

(i) $\mathrm{cs}^L_{X_1}(G_i) = \mathrm{cs}^Q_{X_1}(G_i) = \min\{2n_i, 2n_{i+1}\}$, $0 \leq i < j \leq k$, *and then* $\mathrm{cs}^L(X_1) = \mathrm{cs}^Q(X_1) \leq 2\max\{n_p, \ 1 \leq p \leq k\}$.

(ii) $\mathrm{secc}^L_{X_1}(G_i) = \mathrm{secc}^Q_{X_1}(G_i) = \max\{2\sum_{p=1}^{i} n_p, 2\sum_{p=i+1}^{k} n_p\}$, $0 \leq i < j \leq k$, *and then* $\mathrm{sdiam}^L(X_1) = \mathrm{sdiam}^Q(X_1) = 2\sum_{p=1}^{k} n_p = 2n$.

Proposition 4.2. *For X_2 we have* $\sigma_A(G_i, G_j) = 2\sum_{p=i+1}^{j} n_p - 2(j-i)$ $(0 \leq i < j \leq k)$, *and* *(i)* $\mathrm{cs}^A_{X_2}(G_i) = \min\{2(n_i-1), 2(n_{i+1}-1)\}, \quad 1 \le i \le k-1,$

(ii) $\mathrm{cs}^A(X_2) = \max\{2(n_i-1), \quad 1 \le i \le k\},$

(iii) $\mathrm{secc}^A_{X_2}(G_i) = \max\{2\sum_{p=1}^{i} n_p - 2i, 2\sum_{p=i+1}^{k} n_p - 2(k-i)\}, \quad 1 \le i \le k-1,$

(iv) $\mathrm{sdiam}^A(X_2) = \sigma(G_0, G_k) = 2(n-k).$

Proof Similarly to the previous proposition we get the characteristic polynomial of G_i $(0 \le i \le k)$ as a characteristic polynomial of the complete product of two graphs:

$$P_{G_i}(x) = x^{\sum_{q=i+1}^{k} n_q-(k-i)}(x+1)^{\sum_{p=1}^{i} n_p-1}\prod_{s=i+1}^{k}(x+n_s)\cdot\left((x+1)\left(1-\sum_{l=i+1}^{k}\frac{n_l}{n_l+x}\right)-\sum_{p=1}^{i} n_p\right).$$

The first factor in the previous relation gives $[0]^{\sum_{q=i+1}^{k} n_q-(k-i)}$, while the second gives $[-1]^{\sum_{p=1}^{i} n_p-1}$. The last two factors give eigenvalue $\lambda_1(G_i)$ and the $(k-i)$ eigenvalues $\lambda_{n-(k-i)+1}, ..., \lambda_n$.

For computation of the A-spectral distance between two graphs G_i and G_j from the set X_2 for $0 \le i < j \le k$ we use the following feature of their spectra:

1. $\lambda_1(G_j) > \lambda_1(G_i)$ (follows directly),
2. $\lambda_l(G_j) \ge \lambda_l(G_i)$, $l = \sum_{q=1}^{k} n_q - (k-j)+1, ..., n$ (induction argument).

So we have:

$$\begin{aligned}\sigma_A(G_i,G_j) =& \lambda_1(G_j)-\lambda_1(G_i)+\sum_{p=i+1}^{k} n_p-\sum_{q=j+1}^{k} n_q+2(i-j)+\sum_{l=n-(k-j)+1}^{n}(\lambda_l(G_j)-\lambda_l(G_i)) = \\ & \lambda_1(G_j)-\lambda_1(G_i)+\sum_{p=i+1}^{k} n_p-\sum_{q=j+1}^{k} n_q+2(i-j)- \\ & \left(\sum_{p=1}^{i} n_p-1\right)+\lambda_1(G_i)+\left(\sum_{q=1}^{j} n_q-1\right)-\lambda_1(G_j) = \\ & 2\sum_{l=i+1}^{j} n_l-2(j-i).\end{aligned}$$

And the quantities (i)–(iv) are easily computed. □

Proposition 4.3. *For X_3 we have*

$$\sigma_A(G_0,G_i) = 2(ip-\lambda_{n-k+1}(G_i)-1), \quad 1 \le i \le k, \tag{13}$$

$$\sigma_A(G_i,G_j) = 2\Big(p(j-i)+\big(\lambda_{n-k+1}(G_i)-\lambda_{n-k+1}(G_j)\big)\Big), \quad 1 \le i < j \le k, \tag{14}$$

and

(i) $\mathrm{cs}^A_{X_3}(G_i) = \min\{\sigma(G_{i-1},G_i), \sigma(G_i,G_{i+1})\}, \quad 1 \le i \le k-1,$

(ii) $\mathrm{cs}^A(X_3) = \max\{\sigma(G_i,G_{i+1}), \quad 0 \le i \le k-1\},$

(iii) $\mathrm{secc}^A_{X_3}(G_i) = \max\{\sigma(G_0,G_i), \sigma(G_i,G_k)\}, \quad 1 \le i \le k-1,$

(iv) $\mathrm{sdiam}^A(X_3) = \sigma(G_0, G_k)$.

Proof Denote $H_1 = K_{ip}\nabla K_{i\times(m-p)}$ and $H_2 = K_{(k-i)\times m}$. We first determine the characteristic polynomial of H_1. According to the formula for the complete product of two regular graphs [1, Theorem 2.8]), we get

$$P_{H_1(x)} = (x+1)^{ip-1}x^{i(m-p-1)}(x+m-p)^{i-1}((x-ip+1)(x-(i-1)(m-p)) - i^2p(m-p)). \qquad (15)$$

Using (3) we compute the characteristic polynomial of $H_1\nabla H_2$

$$P_{G_i}(x) = P_{H_1\nabla H_2}(x) = x^{k(m-1)-ip}(x+1)^{ip-1}(x+m-p)^{i-1}(x+m)^{k-i-1}\cdot F$$

with $F = (x+m)F' + (x+1)(x+m-p)(x-m(k-i-1)) - (x+1)(x+m-p)(x+m)$, where F' denotes the last factor of the right hand side of (15).

From the last equality, we compute the eigenvalues of G_i ($1 \le i \le k$): $[0]^{k(m-1)-ip}$, $[-1]^{ip-1}$, $[-m+p]^{i-1}$, $[-m]^{k-i-1}$, while the factor F gives the three remaining eigenvalues: $\lambda_1(G_i)$ (G_i is a connected complete multipartite graph, so there is a unique positive eigenvalue), $\lambda_{n-k+1}(G_i)$ and $\lambda_{n-k+1+i}(G_i)$, where the positions of the last two eigenvalues are easily obtained by the fact that H_1 is an induced subgraph of G_i, and the eigenvalue interlacing. The sum of these three eigenvalues $\lambda_1(G_i) + \lambda_{n-k+1}(G_i) + \lambda_{n-k+1+i}(G_i) = m(k-2) + p - 1$ is used in the below computation.

For $1 \le i < j \le k-1$ we get

$$\sigma_A(G_i, G_j) = \sum_{l=1}^{n} |\lambda_l(G_i) - \lambda_l(G_j)| = \sum_{\substack{l\notin\{1,n-k+1,\\ n-k+1+i,n-k+1+j\}}} |\lambda_l(G_i) - \lambda_l(G_j)| + |\lambda_1(G_i) - \lambda_1(G_j)| +$$
$$|\lambda_{n-k+1}(G_i) - \lambda_{n-k+1}(G_j)| + |\lambda_{n-k+1+i}(G_i) - (p-m)| + |-m - \lambda_{n-k+1+j}(G_j)|.$$

Using $\lambda_1(G_j) > \lambda_1(G_i), \lambda_{n-k+1}(G_j) < \lambda_{n-k+1}(G_i)$, and $\lambda_{n-k+1+i}(G_i) \le p-m, \lambda_{n-k+1+j}(G_j) \ge -m$ (follows from the eigenvalue interlacing), and computing the first sum of the right hand side of the above equality we get (13). Further, including the spectrum of G_0, and the eigenvalues $n-m$, $[0]^{n-k}$, $[-m]^{k-1}$, we get (14).

Finally, the quantities (i)–(iv) are computed directly. □

Appendix

We compute the L- and Q-spectral distances between every two graphs with specific order n. Some data obtained are presented in Table 1. There, the 1st column contains the total number of graphs with n vertices, the 2nd column contains the least spectral distance (distinct from zero), the 3rd column contains the largest spectral distance, the 4th column involves the number of pairs of (non-isomorphic) cospectral graphs, while the remaining three columns contain the number of spectral distances belonging to the specific numerical ranges.

In Table 2 we present similar computational results for the L-spectral distances of graphs that belong to the following 3 classes:

1. connected regular graphs,
2. connected bipartite graphs,
3. trees.

Since the L- and Q-spectral distances coincide whenever both corresponding graphs belong to one of the above classes, the same results hold for the Q-spectral distances.

The similar data on the A-spectral distances are given in [3].

n	♯ graphs	min $\sigma_L \neq 0$	max σ_L	$\sigma_L = 0$	$0 < \sigma_L \leq 0.5$	$0 < \sigma_L \leq 1$	$0 < \sigma_L \leq 2$
3	4	2	6	0	0	0	3
4	11	2	12	0	0	0	20
5	34	0.83	20	0	0	2	124
6	156	0.47	30	2	4	48	1357
7	1044	0.36	42	74	26	976	25813
8	12346	0.16	56	1112	1582	55148	1515175
n	♯ graphs	min $\sigma_Q \neq 0$	max σ_Q	$\sigma_Q = 0$	$0 < \sigma_Q \leq 0.5$	$0 < \sigma_Q \leq 1$	$0 < \sigma_Q \leq 2$
3	4	2	6	0	0	0	3
4	11	2	12	1	0	0	20
5	34	0.78	20	2	0	5	129
6	156	0.34	30	8	9	85	1450
7	1044	0.25	42	54	119	1813	30720
8	12346	0.13	56	694	3397	93430	2064027

Table 1: L- and Q-spectral distances of graphs with n ($3 \leq n \leq 8$) vertices.

n	♯ graphs	min $\sigma_L \neq 0$	max σ_L	$\sigma_L = 0$	$0 < \sigma_L \leq 0.5$	$0 < \sigma_L \leq 1$	$0 < \sigma_L \leq 2$
				connected regular graphs			
6	5	4	18	0	0	0	0
7	4	4	28	0	0	0	0
8	17	2.64	40	0	0	0	0
9	22	0.93	54	0	0	2	16
10	167	0.90	70	4	0	14	471
11	539	0.52	88	28	0	204	8636
				connected bipartite graphs			
4	3	2	2	0	0	0	3
5	5	1.38	4	0	0	0	4
6	17	0.47	8	0	1	2	47
7	44	0.68	12	2	0	12	201
8	182	0.50	18	6	1	102	1903
9	730	0.31	24	54	22	777	16585
10	4032	0.15	32	216	267	9009	243043
11	25598	0.09	40	1718	2077	114346	5051403
				trees			
5	3	1.38	4	0	0	0	1
6	6	0.92	6	0	0	1	7
7	11	0.98	8.49	0	0	2	20
8	23	0.52	10.83	0	0	7	87
9	47	0.42	13.06	0	1	37	294
10	106	0.24	15.59	0	3	126	1249
11	235	0.23	17.98	3	19	472	5222

Table 2: L (and Q)-spectral distances for some particular classes of graphs.

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