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A FEW EXAMPLES AND COUNTEREXAMPLES IN SPECTRAL GRAPH THEORY

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Dedicated to the memory of Professor Slobodan Simić.

Abstract

We present a small collection of examples and counterexamples for selected problems, mostly in spectral graph theory, that have occupied our minds over a number of years without being completely resolved.

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1. Introduction

In the forthcoming sections we review selected problems, mostly in spectral graph theory, that were either posed in literature or that we came across in our research. Their common property is that they are all only partially resolved, despite our best efforts. Hopefully, readers of this special issue will find them interesting and will help to solve them completely.

To avoid repetition in the following sections, we give here some common definitions. All graphs considered are simple and connected. The vertex and edge sets of a simple graph G are denoted by $V(G)$ and $E(G)$, respectively, while the adjacency matrix of G is denoted by $A(G)$. If the graph G is known from the context, we will drop it as the argument and write just V, E, A, etc. The degree of a vertex $v \in V$ is denoted by d_v, with δ and Δ denoting the minimum and the maximum vertex degree in G, respectively. For a graph G with n vertices, we denote by $\lambda_1 \geq \cdots \geq \lambda_n$ the eigenvalues of A, and with $x_1, \ldots, x_n$ corresponding eigenvectors which form an orthonormal basis. The largest eigenvalue λ_1 is also the spectral radius of A. We denote by K_n, P_n and S_n the complete graph, the path and the star on n vertices, respectively. The *broom* graph $B_{r,s}$ is obtained by identifying an endvertex of the path P_r with the center of the star S_{s+1}, so that $B_{r,s}$ has $r + s$ vertices.

2. Communicability Distance

Let us deal with counterexamples first. With $e^A = \sum_{k\geq 0} \frac{A^k}{k!}$, Estrada [13] defined the *communicability distance* between vertices u and v of a graph G as

$$\xi_{uv} = \sqrt{(e^A)_{uu} + (e^A)_{vv} - 2(e^A)_{uv}}$$

and further introduced the *communicability distance sum* Υ, an analogue of the Wiener index, as

$$\Upsilon(G) = \frac{1}{2} \sum_{u \neq v} \xi_{uv}.$$

Estrada then posed the following conjectures.

Conjecture 1 [13]**.** *If $G \ncong K_n$ is a simple connected graph on n vertices, then $\Upsilon(K_n) < \Upsilon(G)$.*

Conjecture 2 [13]**.** *If T is a tree on n vertices, then $\Upsilon(S_n) \leq \Upsilon(T) \leq \Upsilon(P_n)$.*

The *lollipop* graph $L_{r,s}$ is obtained by identifying a vertex of the complete graph K_r and an endvertex of the path P_{s+1}, so that the resulting graph has $r+s$ vertices.

Conjecture 3 [13]**.** *If G is a simple connected graph on $n > 5$ vertices, then* $\Upsilon(G) \leq \Upsilon(L_{n-2,2})$.

We will disprove Conjecture 2 by showing that $\Upsilon(P_n) < \Upsilon(S_n)$ holds for all sufficiently large n. To show this, we first need to represent $\Upsilon(G)$ more directly in terms of the eigenvalues and the eigenvectors of G. Let $\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_n)$ and $Q = [x_1 \cdots x_n]$, so that $A = Q\Lambda Q^T$ is a spectral decomposition of A. Since $e^A = Qe^\Lambda Q^T$ we have

$$\left(e^A\right)_{uv} = \sum_{j=1}^{n} x_{j,u} x_{j,v} e_j^\lambda \tag{1}$$

for all $u, v \in V$, so that

$$\begin{aligned}\Upsilon(G) = \frac{1}{2}\sum_{u \neq v} \xi_{u,v} &= \frac{1}{2}\sum_{u \neq v} \sqrt{(e^A)_{uu} + (e^A)_{vv} - 2(e^A)_{uv}} \\ &= \frac{1}{2}\sum_{u \neq v} \sqrt{\sum_{j=1}^{n} \left(x_{j,u}^2 + x_{j,v}^2 - 2x_{j,u}x_{j,v}\right) e^{\lambda_j}} \\ &= \frac{1}{2}\sum_{u \neq v} \sqrt{\sum_{j=1}^{n} (x_{j,u} - x_{j,v})^2 e^{\lambda_j}}.\end{aligned} \tag{2}$$

This representation enables us to get bounds on $\Upsilon(G)$ in terms of λ_1.

Theorem 4. *If G is a simple connected graph on n vertices, then*

$$\Upsilon(G) \leq \frac{n(n-1)\sqrt{2n}}{2} e^{\frac{\lambda_1}{2}}. \tag{3}$$

Proof. Since the eigenvectors $x_1, \dots, x_n$ are normalized, for each $u, v \in V$ we have $2|x_{j,u}x_{j,v}| \leq x_{j,u}^2 + x_{j,v}^2 \leq 1$, so that

$$\left(x_{j,u} - x_{j,v}\right)^2 \leq x_{j,u}^2 + x_{j,v}^2 + 2|x_{j,u}x_{j,v}| \leq 1 + 1 = 2.$$

Then

$$\Upsilon(G) \leq \frac{1}{2}\sum_{u \neq v} \sqrt{\sum_{j=1}^{n} 2e^{\lambda_j}} \leq \frac{n(n-1)}{2} \sqrt{\sum_{j=1}^{n} 2e^{\lambda_1}} = \frac{n(n-1)\sqrt{2n}}{2} e^{\frac{\lambda_1}{2}},$$

where in the second inequality above we used $e^{\lambda_j} \leq e^{\lambda_1}$ for $j = 1, \dots, n$. ∎

Theorem 5. *If G is a simple connected graph on n vertices, then*

$$\Upsilon(G) \geq \left(\frac{1}{\sqrt{n-1+\frac{\delta}{\Delta}}} - \frac{1}{\sqrt{n}} \right) e^{\frac{\lambda_1}{2}}. \tag{4}$$

If G is not regular, then further

$$\Upsilon(G) \geq \frac{1}{2n^2\sqrt{n}} e^{\frac{\lambda_1}{2}}. \tag{5}$$

Proof. By dropping nonnegative summands for $j = 2, \dots, n$ in the expression (3) for $\Upsilon(G)$ we get

$$\begin{aligned} \Upsilon(G) &= \frac{1}{2} \sum_{u \neq v} \sqrt{\sum_{j=1}^{n} (x_{j,u} - x_{j,v})^2 e^{\lambda_j}} \\ &\geq \frac{1}{2} \sum_{u \neq v} \sqrt{(x_{1,u} - x_{1,v})^2 e^{\lambda_1}} = \frac{e^{\frac{\lambda_1}{2}}}{2} \sum_{u \neq v} |x_{1,u} - x_{1,v}|. \end{aligned}$$

If $x_{1,\min} = \min_{u \in V} x_{1,u}$ and $x_{1,\max} = \max_{u \in V} x_{1,u}$ denote the minimum and the maximum principal eigenvector component of G, respectively, then we can drop further nonnegative summands from the above inequality to obtain

$$\Upsilon(G) \geq (x_{1,\max} - x_{1,\min}) e^{\frac{\lambda_1}{2}}. \tag{6}$$

Since $1 = \sum_{j=1}^{n} x_{1,j}^2 \geq n x_{1,\min}^2$, we have $x_{1,\min} \leq \frac{1}{\sqrt{n}}$. Cioaba and Gregory [4, Lemma 3.3] showed that

$$x_{1,\max} \geq \frac{1}{\sqrt{n-1+\frac{\delta(G)}{\Delta(G)}}}, \tag{7}$$

with a stronger bound if G is not regular

$$x_{1,\max} > \frac{1}{\sqrt{n - \frac{1}{\Delta(G)}}} \geq \frac{1}{\sqrt{n - \frac{1}{n-1}}}. \tag{8}$$

Combining (6), $x_{1,\min} \leq \frac{1}{\sqrt{n}}$ and (7), we directly obtain (4). If G is not regular, then combining $x_{1,\min} \leq \frac{1}{\sqrt{n}}$ and (8) yields

$$x_{1,\max} - x_{1,\min} \geq \frac{1}{\sqrt{n-\frac{1}{n-1}}} - \frac{1}{\sqrt{n}} = \frac{1}{\sqrt{n(n^2-n-1)}\left(\sqrt{n^2-n}+\sqrt{n^2-n-1}\right)}$$
$$\geq \frac{1}{\sqrt{n\cdot n^2}\left(\sqrt{n^2}+\sqrt{n^2}\right)} = \frac{1}{2n^2\sqrt{n}}\,,$$

which in combination with (6) yields (5). ∎

Now we can disprove Conjecture 2 for all sufficiently large n.

Theorem 6. *There exists $n_0 \in \mathbb{N}$ such that $\Upsilon(P_n) < \Upsilon(S_n)$ for all $n \geq n_0$.*

Proof. The eigenvalues of P_n are equal to $2\cos\frac{\pi j}{n+1}$ for $j = 1, \ldots, n$, so that $\lambda_1(P_n) < 2$ and the upper bound (3) gives

$$\Upsilon(P_n) \leq \frac{n(n-1)\sqrt{2n}}{2}e.$$

On the other hand, the largest eigenvalue of S_n is $\sqrt{n-1}$ and the lower bound (5), since S_n is not regular for $n \geq 3$, yields

$$\Upsilon(S_n) \geq \frac{1}{2n^2\sqrt{n}}e^{\frac{\sqrt{n-1}}{2}}.$$

Since

$$\lim_{n\to\infty} \frac{\frac{1}{2n^2\sqrt{n}}e^{\frac{\sqrt{n-1}}{2}}}{\frac{n(n-1)\sqrt{2n}}{2}e} = \lim_{n\to\infty} \frac{e^{\frac{\sqrt{n-1}}{2}-1}}{n^4(n-1)\sqrt{2}} = \infty,$$

there exists n_0 such that $\Upsilon(S_n) > \Upsilon(P_n)$ for all $n \geq n_0$. ∎

Numerical results show that the smallest n for which $\Upsilon(P_n) < \Upsilon(S_n)$ is $n = 43$. However, the path ceases to have the largest value of Υ among trees on a much smaller number of vertices. The *double broom* graph $DB_{r,s,t}$ is obtained by identifying one endvertex of P_r with the center of the star S_{s+1} and the other endvertex of P_r with the center of the star S_{t+1}, so that $DB_{r,s,t}$ has $r+s+t$ vertices. Then the three largest Υ values among trees on 15 vertices are

$$\Upsilon(P_{15}) \approx 199.60736, \quad \Upsilon(B_{13,2}) \approx 199.62532, \quad \Upsilon(DB_{11,2,2}) \approx 199.64285.$$

As both paths and stars are special instances of brooms, our opinion is that it may be worthwhile to study further the behaviour of $\Upsilon(B_{r,s})$ and $\Upsilon(DB_{r,s,t})$, although that could not do much to save Conjecture 2 anyway.

On the other hand, we could not find any counterexample for Conjectures 1 and 3. Conjecture 1 makes sense, as K_n is a regular graph with the all-one vector as the principal eigenvector, so that the summand corresponding to e^{n-1} vanishes from (3), leaving only the summands corresponding to e^{-1} which make the value of $\Upsilon(K_n)$ smaller than Υ for many graphs whose eigenvalues are not bounded by a constant. The appearance of $L_{n-2,2}$ as the extremal graph in Conjecture 3 is somewhat unusual, despite a reasonable explanation provided by Estrada in [13]. As K_n is a special case of a lollipop as well, it would be worthwhile to study the behaviour of $\Upsilon(L_{r,s})$ to confirm Conjectures 1 and 3 among lollipops at least.

3. Nikiforov's Problem on Numbers of Walks and Spectral Radius

Let $w_k(G)$ denote the number of walks containing k vertices, and consequently having length $k-1$, in a graph G. The fact that w_k is the sum of entries of A^{k-1} relates it to the eigenvalues of G, and there are many results connecting numbers of walks and the spectral radius λ_1, with a thorough overview provided by Täubig in [34]. Nikiforov proved in [25] that the inequality

$$\lambda_1^r \geq \frac{w_{s+r}}{w_s}$$

holds for all odd $s > 0$ and all $r > 0$. Using complete bipartite graphs as the example, he showed that λ_1^r can be smaller than w_{s+r}/w_s for even s and odd r and then posed the following problem.

Problem 7 [25]**.** Let G be a connected bipartite graph. Is it true that

$$\lambda_1^r \geq \frac{w_{s+r}}{w_s}$$

for every even $s \geq 2$ and even $r \geq 2$?

Nikiforov mentioned without a proof that the complete tripartite graph $K_{2t,2t,t}$ satisfies $\lambda_1^2 < w_4/w_2$ and thus provides a counterexample for $s = r = 2$. Elphick and Réti [12] produced another infinite family of counterexamples for $s = r = 2$ and further showed that the path P_4 serves as a counterexample for arbitrary even r. Thanks to the proposition put forward by one of the reviewers, it will be shown here that any connected graph with two main eigenvalues, one of which is negative and not equal in absolute value to the spectral radius, serves as a counterexample for all even $s \geq 2$ and $r \geq 2$.

The spectral decomposition $A = Q\Lambda Q^T$ yields $A^{k-1} = Q\Lambda^{k-1}Q^T$ (recall that that the columns of Q are the orthonormal eigenvectors of A), so that

$$w_k = \sum_{i=1}^{n} \lambda_i^{k-1} \left(\sum_{j=1}^{n} x_{i,j} \right)^2. \tag{9}$$

Evidently, only those eigenvalues for which the corresponding sum $\sum_{j=1}^{n} x_{i,j}$ is not zero affect the value of w_k. Such eigenvalues are called the *main eigenvalues*. The spectral radius λ_1 of a connected graph is always a main eigenvalue, due to its strictly positive eigenvector x_1. Regular graphs, for which x_1 is proportional to the all-one vector $\mathbf{j}$, have exactly one main eigenvalue, as all their other eigenvectors are orthogonal to $\mathbf{j}$. The *main angle* β_λ corresponding to the main eigenvalue λ is defined as the cosine of the angle between $\mathbf{j}$ and the eigenspace of λ. Thus, if the repetitions of λ in the spectrum are $\lambda_p, \ldots, \lambda_{p+q-1}$ for some p and q, then

$$\beta_\lambda^2 = \frac{1}{n} \sum_{i=p}^{p+q-1} \left(\sum_{j=1}^{n} x_{i,j} \right)^2,$$

so that

$$w_k = n \sum_{i=1}^{n'} \mu_i^{k-1} \beta_{\mu_i}^2, \tag{10}$$

where $\mu_1, \ldots, \mu_{n'}$ are all distinct main eigenvalues of G.

One of the reviewers suggested the following proposition.

Proposition 8. *Let G be a connected graph with two main eigenvalues μ_1 and μ_2, such that $\mu_1 > 0 > \mu_2 > -\mu_1$. If $s \geq 2$ and $r \geq 2$ are even, then*

$$\mu_1^r < \frac{w_{s+r}}{w_s}.$$

Proof. Let $n = |V(G)|$ and $m = |E(G)|$, and let β_1 and β_2 be the main angles corresponding to μ_1 and μ_2, respectively. We have

$$w_k = n(\mu_1^{k-1} \beta_1^2 + \mu_2^{k-1} \beta_2^2) \tag{11}$$

by (10) (see also [10, Theorem 1.3.5]). From $w_1 = n$ we have $\beta_1^2 + \beta_2^2 = 1$, while from $w_2 = 2m$ we get, by eliminating one of the main angles in turn from (11),

$$\beta_1^2 = \frac{2m - n\mu_2}{n(\mu_1 - \mu_2)} \quad \text{and} \quad \beta_2^2 = -\frac{2m - n\mu_1}{n(\mu_1 - \mu_2)}.$$

Hence

$$w_k = \frac{2m(\mu_1^{k-1} - \mu_2^{k-1}) - n\mu_1\mu_2(\mu_1^{k-2} - \mu_2^{k-2})}{\mu_1 - \mu_2}, \tag{12}$$

so that $\mu_1^r < w_{s+r}/w_s$ if and only if

$$\frac{(2m - n\mu_1)\mu_2^{s-1}(\mu_1^r - \mu_2^r)}{\mu_1 - \mu_2} > 0.$$

The last inequality is satisfied as the expression on the left-hand side is a product of two positive and two negative factors: G is not regular, as it has two main eigenvalues, so that $\mu_1 > \frac{2m}{n}$ (see [10, Theorem 3.2.1]) and $2m - n\mu_1$ is negative; μ_2^{s-1} is negative as $\mu_2 < 0$ and $s-1$ is odd; while $\mu_1^r - \mu_2^r$ and $\frac{1}{\mu_1-\mu_2}$ are positive, as $\mu_1 > |\mu_2|$. ∎

Although Cvetković [5] proposed the problem of characterizing graphs with k main eigenvalues already in 1978, results on graphs with two main eigenvalues started to appear only after a seminal paper by Hagos in 2002 [16]. Hagos showed that a graph has exactly k main eigenvalues if and only if k is the maximum number such that $\mathbf{j}$, $A\mathbf{j}, \dots, A^{k-1}\mathbf{j}$ are linearly independent. For $k = 2$ this means that there exists α and β such that

$$A^2\mathbf{j} = \alpha A\mathbf{j} + \beta\mathbf{j}, \tag{13}$$

and that G is not regular. Graph G satisfying (13) is called a 2*-walk* (α, β)*-linear graph* and its main eigenvalues are [16, Corollary 2.5]

$$\mu_1, \mu_2 = \frac{\alpha \pm \sqrt{\alpha^2 + 4\beta}}{2}. \tag{14}$$

Rowlinson [27] observed that both cone over a regular graph and a strongly regular graph with one vertex deleted have two main eigenvalues. Hayat *et al.* [17] provided a general construction of equitable biregular graphs with two main eigenvalues, while further constructions were provided by Chen and Huang [3] for two main eigenvalues and by Huang *et al.* [22] for arbitrary fixed number of main eigenvalues. Unicyclic, bicyclic and tricyclic graphs with two main eigenvalues are characterized in a series of papers [14, 19–21, 29], while integral graphs with spectral radius 3 and two main eigenvalues are characterized in [33].

Graphs satisfying the requirements of Proposition 8 can be found in most of these papers, and the counterexample we initially found is a particular instance of a general construction described by Hayat *et al.* [17]. Our counterexample, denoted by $G_{p,q}$, consists of the complete bipartite graph $K_{p,p}$ with q pendant vertices attached to each of the $2p$ vertices of $K_{p,p}$, so that the resulting graph has $n = 2p(1+q)$ vertices. It is a 2-walk (p, q)-linear graph, so that its main eigenvalues are $\mu_1, \mu_2 = (p \pm \sqrt{p^2 + 4q})/2$ by (14), which satisfy requirements of Proposition 8. As a matter of fact, if one resorts to combinatorial instead of analytical counting of walks in $G_{p,q}$, then an even stronger inequality can be obtained in a simple way for $q = p^4$,

$$\lim_{p\to\infty} \frac{w_{s+r}(G_{p,p^4})}{\lambda_1^r(G_{p,p^4}) w_s(G_{p,p^4})} = \frac{s+r-2}{s-2}.$$

Details are given in the Appendix.

4. Smallest Integral Graph with a Given Diameter

After these counterexamples, we can now move on to a few interesting examples. DS met Simone Severini at a workshop in Aveiro back in 2006, and he asked then a few questions stemming from his studies of state transfer in quantum spin networks. One question, translated to the usual terminology of spectral graph theory, reduced to the following.

What is the smallest integral graph with a given diameter?

Let us recall that a graph is integral if all its eigenvalues are integers. Circulant integral graphs, whose study became popular after Wasin So's characterization of them appeared about that time in [30], were not good candidates as examples had shown that their expected diameter is too low. Instead, natural candidates are the graphs that generalize paths in the sense that each vertex v of the path P_k is replaced by a set B_v of independent vertices with two new vertices $a \in B_u$ and $b \in B_v$ adjacent in the new, expanded graph if u and v are adjacent in P_k. We will call such expanded graphs the *superpaths* and denote by $SP(a_1, \ldots, a_n)$ the superpath obtained by replacing the vertices of the path P_n with independent sets having, respectively, $a_1, \ldots, a_n$ vertices. Figure 1 shows, for example, the superpath $SP(4, 1, 3, 2, 2, 3, 1, 4)$.

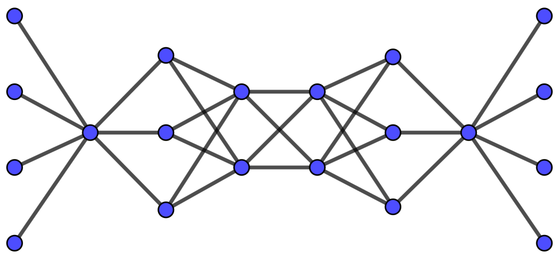

Figure 1. The superpath $SP(4, 1, 3, 2, 2, 3, 1, 4)$ is integral, with spectrum consisting of simple eigenvalues $\pm 4, \pm 3, \pm 2, \pm 1$ and eigenvalue 0 with multiplicity 12.

A few quick experiments with Octave suggested that integral superpaths should be those whose cardinalities of independent sets either form a sequence

$$n, 1, n-1, 2, \ldots, 2, n-1, 1, n,$$

or represent multiples of this sequence. We will prove here this observation.

Theorem 9. *The superpath $SP(n, 1, n-1, 2, \ldots, 2, n-1, 1, n)$ is integral for each natural number n. Its spectrum consists of the simple eigenvalues $\pm n, \pm(n-1)$, $\ldots, \pm 1$ and the eigenvalue 0 with multiplicity $n(n-1)$.*

Proof. Let us first deal with the eigenvalue 0. Denote by $B_1, \dots, B_{2n}$ the constituent independent sets of the superpath $SP(n, 1, n-1, 2, \dots, 2, n-1, 1, n)$. It is easy to see that a vector x is an eigenvector corresponding to 0 if and only if the components of x in each set B_i sum to 0, $i = 1, \dots, 2n$. Thus, the dimension of this eigenspace is equal to $n(n-1)$.

Next, we show that $SP(n, 1, n-1, 2, \dots, 2, n-1, 1, n)$ has $2n$ more distinct nonzero eigenvalues, which consequently must all be simple. So, suppose that λ is an eigenvalue of $SP(n, 1, n-1, 2, \dots, 2, n-1, 1, n)$ having an eigenvector x whose components are equal within each set B_i, $i = 1, \dots, 2n$. Let x_i be the component of x corresponding to the vertices within set B_i. The eigenvalue equations for the vertices of this superpath then become

$$\begin{aligned}
\lambda x_1 &= x_2, \\
\lambda x_2 &= n x_1 + (n-1) x_3, \\
&\dots \\
\lambda x_{2i} &= (n-i+1) x_{2i-1} + (n-i) x_{2i+1}, \\
\lambda x_{2i+1} &= i x_{2i} + (i+1) x_{2i+2}, \\
&\dots \\
\lambda x_{2n-1} &= (n-1) x_{2n-2} + n x_{2n}, \\
\lambda x_{2n} &= x_{2n-1}.
\end{aligned}$$

The determinant of this linear system is

$$D_N(\lambda) = \begin{vmatrix}
\lambda & -1 & & & & & & & & \\
-n & \lambda & -n+1 & & & & & & & \\
 & -1 & \lambda & -2 & & & & & & \\
 & & -n+1 & \lambda & -n+2 & & & & & \\
 & & & -2 & \lambda & -3 & & & & \\
 & & & & -n+2 & \lambda & \dots & & & \\
 & & & & & -3 & \dots & & & \\
 & & & & & & \dots & & & \\
 & & & & & & \dots & -1 & & \\
 & & & & & & \dots & \lambda & -n \\
 & & & & & & & -1 & \lambda
\end{vmatrix}.$$

It is easy to see that the precise arrangement of the terms on the subdiagonals is not important. To be precise, one can change entries along the subdiagonals as long as the product of pairs (A, B) of entries located like

$$\begin{matrix} \lambda & A \\ B & \lambda \end{matrix}$$

remains invariant. In particular,

$$D_N(\lambda) = \begin{vmatrix} \lambda & 1 & & & & & & & & \\ n & \lambda & 1 & & & & & & & \\ & n-1 & \lambda & 2 & & & & & & \\ & & n-1 & \lambda & 2 & & & & & \\ & & & n-2 & \lambda & 3 & & & & \\ & & & & n-2 & \lambda & \dots & & & \\ & & & & & n-3 & \dots & & & \\ & & & & & & \dots & & & \\ & & & & & & \dots & n-1 & & \\ & & & & & & \dots & \lambda & n & \\ & & & & & & & 1 & \lambda & \end{vmatrix}.$$

For the next step, we apply first the row transformations

$\mathrm{row}_1 + \mathrm{row}_3 + \mathrm{row}_5 + \dots$
$\mathrm{row}_2 + \mathrm{row}_4 + \mathrm{row}_6 + \dots$
$\mathrm{row}_3 + \mathrm{row}_5 + \mathrm{row}_7 + \dots$
$\dots \quad \dots \quad \dots$

and then the column transformations

$\mathrm{col}_{2n} - \mathrm{col}_{2n-2}$
$\mathrm{col}_{2n-1} - \mathrm{col}_{2n-3}$
$\mathrm{col}_{2n-2} - \mathrm{col}_{2n-4}$
$\dots \quad \dots \quad .$

After the row transformations, we get

$$D_N(\lambda) = \begin{vmatrix} \lambda & n & \lambda & n & \lambda & n & \dots & \lambda & n \\ n & \lambda & n & \lambda & n & \lambda & \dots & n & \lambda \\ & n-1 & \lambda & n & \lambda & n & \dots & \lambda & n \\ & & n-1 & \lambda & n & \lambda & \dots & n & \lambda \\ & & & n-2 & \lambda & n & \dots & \lambda & n \\ & & & & n-2 & \lambda & \dots & n & \lambda \\ & & & & & n-3 & \dots & \lambda & n \\ & & & & & & \dots & & \\ & & & & & & \dots & n & \lambda \\ & & & & & & \dots & \lambda & n \\ & & & & & & & 1 & \lambda \end{vmatrix},$$

while after the column transformations, we get

$$D_N(\lambda) = \begin{vmatrix} \lambda & n & & & & & & & \\ n & \lambda & & & & & & & \\ & n-1 & \lambda & 1 & & & & & \\ & & n-1 & \lambda & 1 & & & & \\ & & & n-2 & \lambda & 2 & & & \\ & & & & n-2 & \lambda & \dots & & \\ & & & & & n-3 & \dots & & \\ & & & & & & \dots & & \\ & & & & & & \dots & n-2 & \\ & & & & & & \dots & \lambda & n-1 \\ & & & & & & & 1 & \lambda \end{vmatrix}.$$

From here, it follows that

$$\begin{aligned} D_N(\lambda) &= \begin{vmatrix} \lambda & n \\ n & \lambda \end{vmatrix} \cdot \begin{vmatrix} \lambda & 1 & & & & & & \\ n-1 & \lambda & 1 & & & & & \\ & n-2 & \lambda & 2 & & & & \\ & & n-2 & \lambda & \dots & & & \\ & & & n-3 & \dots & & & \\ & & & & \dots & & & \\ & & & & \dots & n-2 & \\ & & & & \dots & \lambda & n-1 \\ & & & & & 1 & \lambda \end{vmatrix} \\ &= \left(\lambda^2 - n^2\right) D_{n-1}(\lambda). \end{aligned}$$

From this reccurence formula and $D_1(\lambda) = (\lambda - 1)(\lambda + 1)$ we easily get that

$$D_n(\lambda) = \prod_{j=1}^{n} \left(\lambda^2 - j^2\right).$$

Thus, the nonzero eigenvalues of the superpath $SP(n, 1, n-1, 2, \dots, 2, n-1, 1, n)$ are $n, \dots, 2, 1, -1, -2, \dots, -n$. ■

Remark 10. The transformation described above is essentially the same as the one used in Mazza's proof of evaluation of the Sylvester's determinant found in the historical treatise [23, p. 442]. We are grateful to Prof. Christian Krattenthaler for pointing us to Mazza's proof. More recent articles on Sylvester-type determinants are [1, 18].

The superpath $SP(n, 1, n-1, 2, \dots, 2, n-1, 1, n)$ is thus integral with diameter $D = 2n - 1$ and $n^2 + n = (D+1)(D+3)/4$ vertices. Now we can rephrase our original question as the following problem.

Problem 11. Does there exist an integral graph of diameter D with fewer than $(D+1)(D+3)/4$ vertices?

5. Maximum Wiener Index of Trees with Given Radius

While the large majority of research publications of Professor Slobodan Simić belong to spectral graph theory, he has also published several results on graph equations (mostly prior to 1983), some papers on graph algorithms and even one paper on Szeged index [28], that officially belongs to mathematical chemistry. So, the next interesting example could be considered to belong to Professor Simić's interests as well.

The Wiener index of a graph is the sum of distances between all pairs of its vertices. A particular type of extremal problem on the Wiener index, that does not allow an easy approach, is to characterize graphs or trees with given diameter or radius. According to Das and Nadjafi-Arani [11], such problems were first studied by Plesnik [26] back in 1984 and to this day there are only a few results: Das and Nadjafi-Arani gave upper bounds on the Wiener index for graphs and trees with given radius, and also for graphs and trees with given radius and given maximum vertex degrees, but these bounds are sharp in very special cases only, not allowing one to get a sense of the structure of extremal graphs or trees. Mukwembi and Vetrík [24], on the other hand, obtained upper bounds on the Wiener index of trees with diameters at most six that are sharp in many more cases and either characterize (for smaller diameters) or suggest (for larger diameters) the structure of extremal trees.

A variant of this problem that we were interested in is to characterize trees with maximum Wiener index among trees with a given number of vertices and radius. Early computer experiments, with Java programs that would later become part of the *graph6java* framework [15], suggested that such extremal trees should have an easily characterizable structure. Define the *broom-fan* $BF_{n,r,k}$ to be a tree on n vertices with radius r having a vertex u of degree k such that each subtree obtained after removing u is either a broom $B_{r,\lfloor\frac{n-1}{k}\rfloor-r}$ or a broom $B_{r,\lceil\frac{n-1}{k}\rceil-r}$. For all radii of trees with up to 23 vertices, a broom-fan is always a tree with the maximum Wiener index for a given radius. However, we have a surprising change in structure of extremal trees on 24 vertices, which are shown in Figures 2–13. As can be seen from this figures, extremal trees are still broom-fans except for radius seven! In this particular case, the extremal tree in Figure 8 has Wiener index 1836, while Wiener index of the broom-fan $BF_{24,7,2}$ is 1835. This example suggests that there may be similar surprises awaiting at even higher numbers of vertices and that, despite the fact that the extremal tree for radius seven is still formed by joining three brooms, a simple characterization of the structure of extremal trees will probably be out of our reach in some foreseeable future.

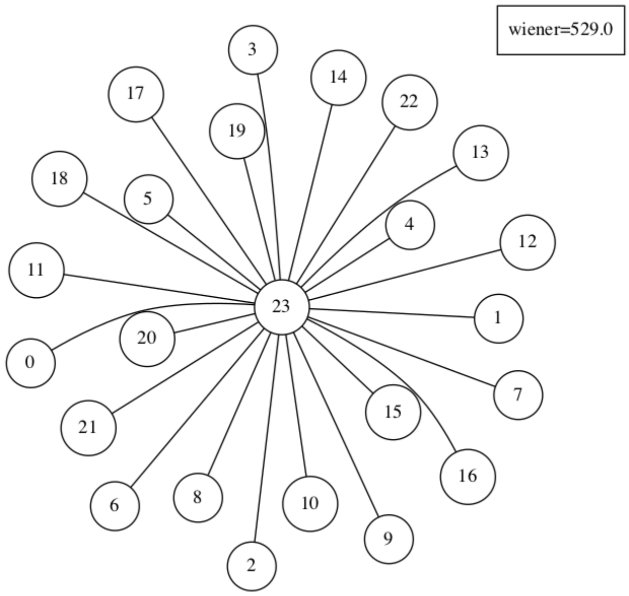

Figure 2. Tree on 24 vertices with the maximum Wiener index and radius 1.

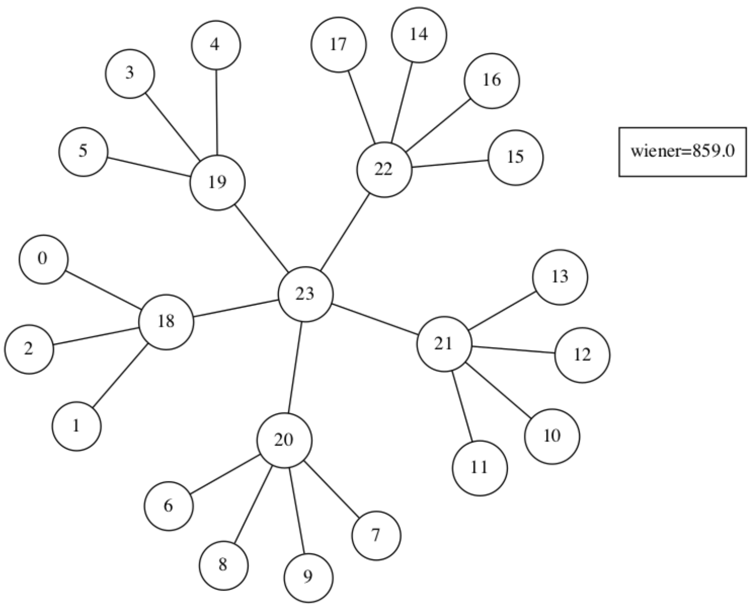

Figure 3. Tree on 24 vertices with the maximum Wiener index and radius 2.

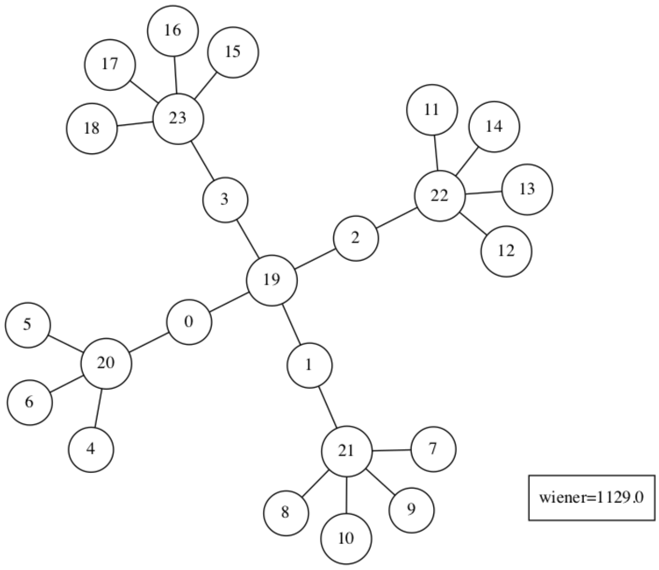

Figure 4. Tree on 24 vertices with the maximum Wiener index and radius 3.

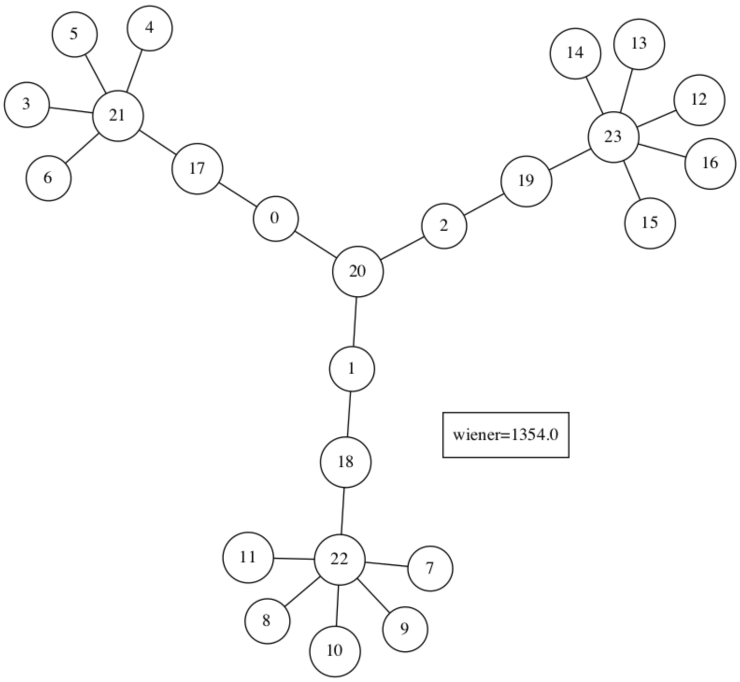

Figure 5. Tree on 24 vertices with the maximum Wiener index and radius 4.

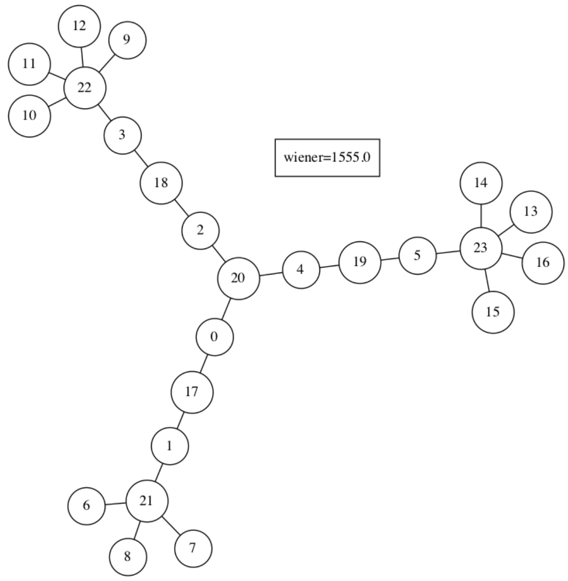

Figure 6. Tree on 24 vertices with the maximum Wiener index and radius 5.

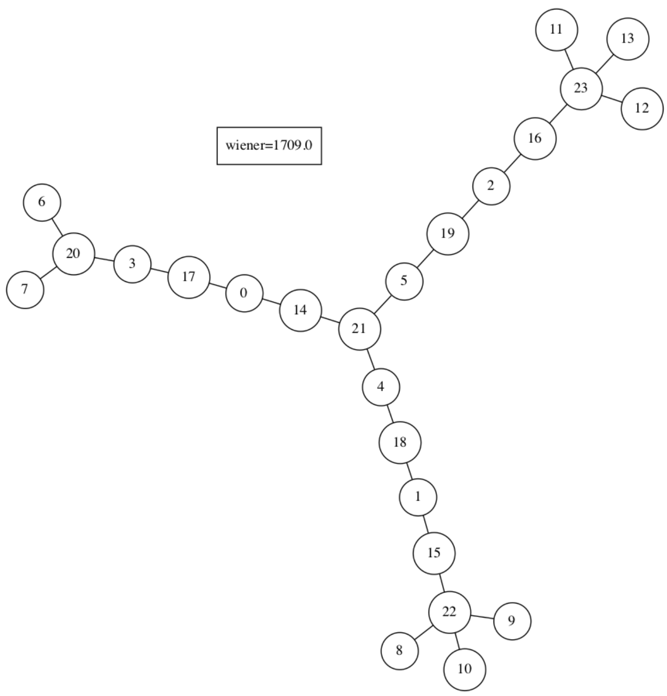

Figure 7. Tree on 24 vertices with the maximum Wiener index and radius 6.

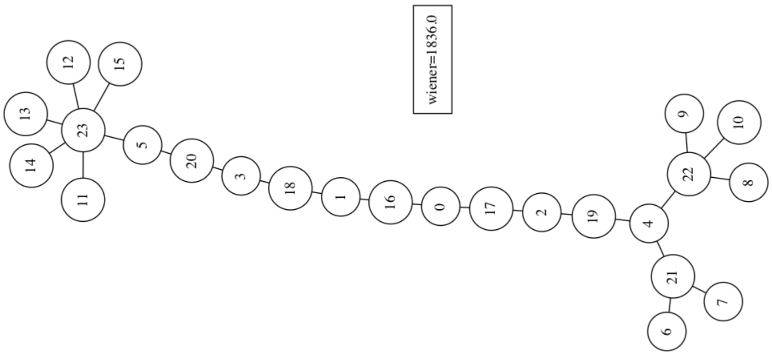

Figure 8. Tree on 24 vertices with the maximum Wiener index and radius 7.

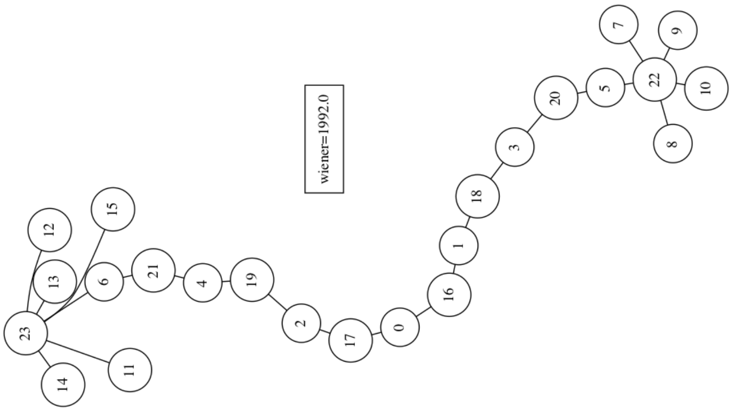

Figure 9. Tree on 24 vertices with the maximum Wiener index and radius 8.

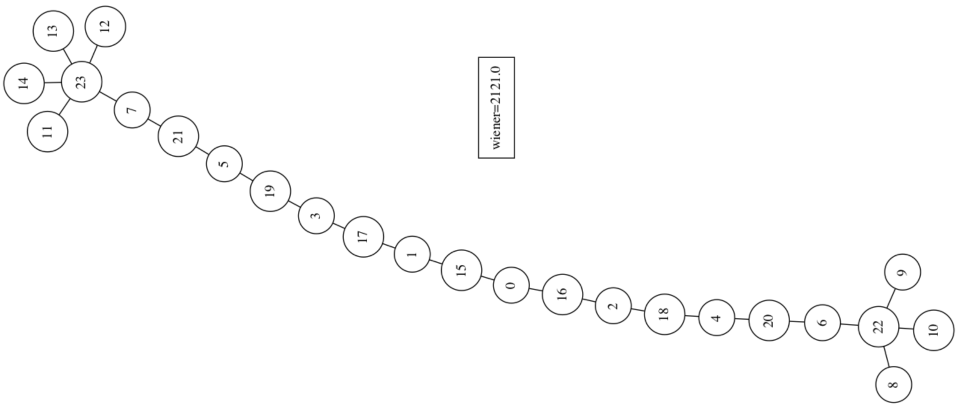

Figure 10. Tree on 24 vertices with the maximum Wiener index and radius 9.

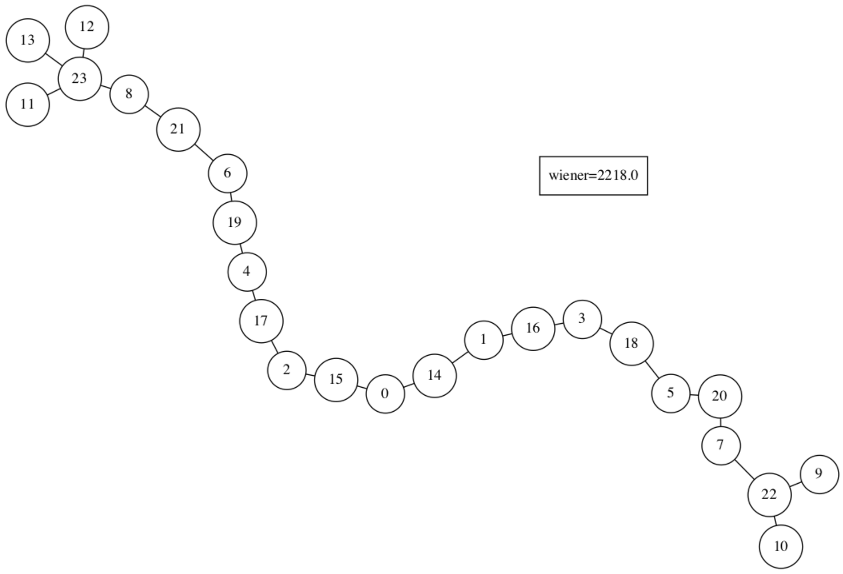

Figure 11. Tree on 24 vertices with the maximum Wiener index and radius 10.

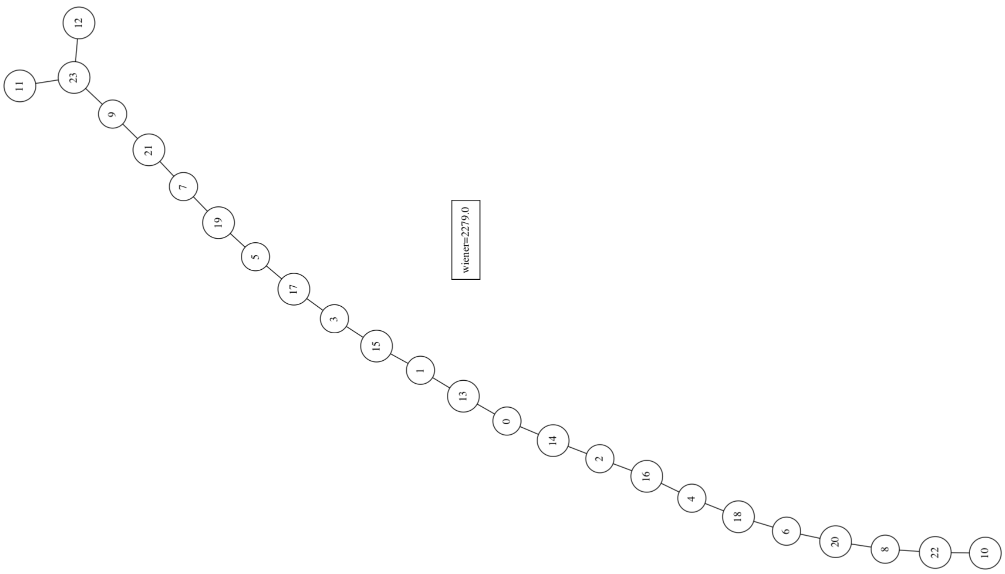

Figure 12. Tree on 24 vertices with the maximum Wiener index and radius 11.

6. Bounds on the Laplacian Spectral Radius of Graphs

We now shift our focus to conjectures that, in our opinion, deserve more attention. Let $\mu(G)$ denote the spectral radius of the Laplacian matrix of G, and for $v \in$

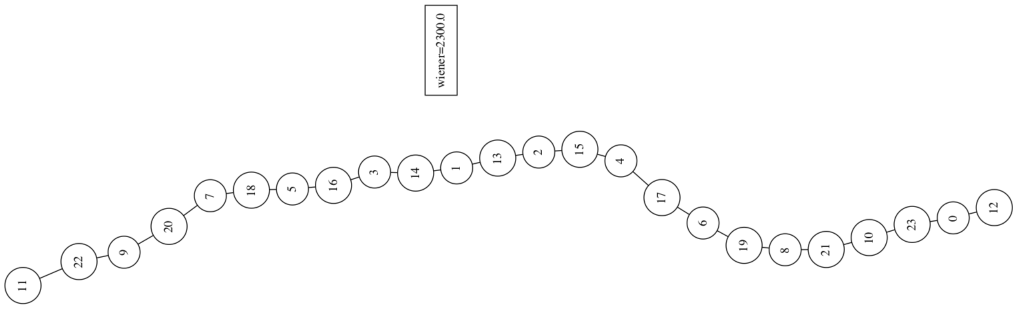

Figure 13. Tree on 24 vertices with the maximum Wiener index and radius 12.

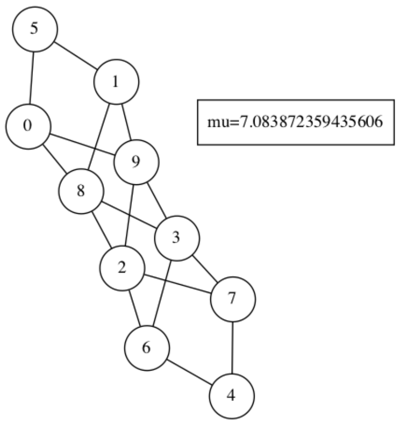

Figure 14. A counterexample for the conjectured bound $\mu \leq \max_v m_v \sqrt{1 + \frac{3m_v}{d_v}}$.

$V(G)$, let m_v denote the average degree of the neighbors of v. Observing that a number of upper bounds on μ expressed in terms of d_v and m_v have a very similar structure of their expressions, Brankov, Hansen and Stevanović [2] suggested a few simple algebraic rules that can regenerate these expressions from scratch. When we applied these rules to generate further such expressions and tested them on connected graphs with up to nine vertices, we were surprised to find out that more than half of them (190 out of 361 generated expressions) represented valid upper bounds for the Laplacian spectral radius on this set of graphs. We had further selected a subset of the strongest of these expressions in the sense that for each connected graph on nine vertices at least one of the selected expressions yields the smallest upper bound among all considered expressions when evaluated for that graph. Except for Merris' well-known bound $\mu \leq \max_v d_v + m_v$, this selection contains conjectured upper bounds that, being selected by computer, do not always look intuitive,

$$\mu \le \max_v \frac{4m_v^2}{d_v+m_v} \qquad \mu \le \max_v \frac{d_v^2}{m_v}+\frac{m_v^3}{d_v^2}$$

$$\mu \le \max_v \sqrt{d_v(d_v+3m_v)} \qquad \mu \le \max_v \sqrt{\frac{d_v(3d_v+5m_v)}{2}}$$

$$\mu \le \max_v \frac{\sqrt{d_v(5d_v+11m_v)}}{2} \qquad \mu \le \max_v \frac{\sqrt{7d_v^2+9m_v^2}}{2}$$

$$\mu \le \max_v \sqrt{2d_v^2+\frac{2m_v^3}{d_v}} \qquad \mu \le \max_v \sqrt{3m_v^2+\frac{d_v^3}{m_v}}$$

$$\mu \le \max_v m_v\sqrt{1+\frac{3m_v}{d_v}} \qquad \mu \le \max_v \frac{\sqrt{m_v^3(m_v+3d_v)}}{d_v}$$

$$\mu \le \max_v \sqrt{2m_v\left(d_v+\frac{m_v^3}{d_v^2}\right)} \qquad \mu \le \max_v \sqrt[4]{5d_v^4+11m_v^4}$$

$$\mu \le \max_v \sqrt[4]{6d_v^4+10m_v^4} \qquad \mu \le \max_v \sqrt[4]{4d_v(d_v^3+3m_v^3)}$$

$$\mu \le \max_v \sqrt[4]{d_v^2(2d_v^2+14m_v^2)} \qquad \mu \le \max_v \sqrt[4]{d_v^2(3d_v^2+13m_v^2)}.$$

The proof techniques known at the time of writing [2] could not be used to prove any of the above conjectured bounds, and none of them appears to have been proved or disproved in the meantime. This time we have tested the above conjectured bounds on all connected graphs with ten vertices as well. As a result we have found a single graph, shown in Figure 14, for which $\mu > \max_v m_v\sqrt{1+\frac{3m_v}{d_v}}$, while the remaining conjectured bounds are satisfied for all connected graphs with ten vertices. This single counterexample on ten vertices suggests it is unlikely that connected graphs on 11 or 12 vertices would provide counterexamples for more than a few more of these conjectured bounds, and the largest benefit would definitely be obtained by devising new proof techniques for the Laplacian spectral radius that would be able to deal with upper bounds of the above form.

7. Almost Cospectrality of Components of NEPS

The non-complete extended p-sum (NEPS) of graphs is a very general graph operation, introduced by Cvetković and Lučić [9]. Let $\mathcal{B}$ be a set of nonzero binary n-tuples, i.e., $\mathcal{B} \subseteq \{0,1\}^n \setminus \{(0,\dots,0)\}$. The NEPS of graphs $G_1,\dots,G_n$ with the basis $\mathcal{B}$, denoted as NEPS$(G_1,\dots,G_n;\mathcal{B})$, is the graph with the vertex set $V(G_1)\times\cdots\times V(G_n)$ in which two vertices $(u_1,\dots,u_n)$ and $(v_1,\dots,v_n)$ are adjacent if and only if there exists $(\beta_1,\dots,\beta_n)\in\mathcal{B}$ such that u_i is adjacent to v_i in G_i whenever $\beta_i=1$, and $u_i=v_i$ whenever $\beta_i=0$. One of the most important properties of NEPS is that its eigenvalues can be represented via eigenvalues of its factors: namely, the spectrum of $\mathrm{NEPS}(G_1, \dots, G_n; \mathcal{B})$ consists of all possible values $\Lambda = \sum_{\beta \in \mathcal{B}} \lambda_1^{\beta_1} \cdots \lambda_n^{\beta_n}$, where λ_i is an eigenvalue of G_i for $i = 1, \dots, n$ (see, e.g., [8, Theorem 2.23]).

Two graphs are said to be *almost cospectral* if their nonzero eigenvalues, including multiplicities, coincide. Cvetković [6] conjectured in 1983 that the components of NEPS of connected bipartite graphs are almost cospectral, and proved it for the direct product of graphs in [6] and some further cases of NEPS in [7]. On the other hand, we disproved this conjecture in 2000 by exhibiting a small counterexample in [31] and then went on to determine for which bases of NEPS almost cospectrality of components holds. For $S \subsetneq \{1, \dots, n\}$ let

$$\mathrm{Ann}(\mathcal{B}, S) = \{\beta \in \mathcal{B} \colon (\forall i \in S)\beta_i = 0\}$$

and for a matrix M with n columns, let M^{-S} denote the matrix obtained from M by removing the columns whose indices belong to S. Further, let $\mathrm{rank}_2(M)$ denote the rank of a binary matrix M over the two element field GF_2. The following results, that rely heavily on binary linear algebra, give one necessary and one sufficient condition for almost cospectrality of the components of NEPS.

Theorem 12 [31]**.** *Let* $\mathcal{B} \subseteq \{0,1\}^n \setminus \{(0, \dots, 0)\}$*. If there exists* $S \subsetneq \{1, \dots, n\}$ *such that* $\mathrm{Ann}(\mathcal{B}, S) \neq \emptyset$ *and*

$$\mathrm{rank}_2(\mathrm{Ann}(\mathcal{B}, S)) > \mathrm{rank}_2(\mathcal{B}) - |S|, \tag{15}$$

then there exist infinitely many sets of connected bipartite graphs whose NEPS with the basis $\mathcal{B}$ *has components that are not almost cospectral.*

Theorem 13 [32]**.** *Let* $G = \mathrm{NEPS}(G_1, \dots, G_n; \mathcal{B})$*, where* $G_1, \dots, G_n$ *are connected bipartite graphs. If for each* $S \subsetneq \{1, \dots, n\}$ *such that* $\mathrm{Ann}(\mathcal{B}, S) \neq \emptyset$ *holds*

$$\mathrm{rank}_2(\mathcal{B}^{-S}) = \mathrm{rank}_2(\mathcal{B}) - |S|, \tag{16}$$

then the components of G *are almost cospectral.*

The sufficient condition (16) implies the necessary condition

$$\mathrm{rank}_2(\mathrm{Ann}(\mathcal{B}, S)) \leq \mathrm{rank}_2(\mathcal{B}) - |S|,$$

because the S-indexed columns of $\mathrm{Ann}(\mathcal{B}, S)$ are zero so that

$$\mathrm{rank}_2(\mathrm{Ann}(\mathcal{B}, S)) = \mathrm{rank}_2(\mathrm{Ann}^{-S}(\mathcal{B}, S)) \leq \mathrm{rank}_2(\mathcal{B}^{-S}),$$

as $\mathrm{Ann}^{-S}(\mathcal{B}, S)$ is a submatrix of $\mathcal{B}^{-S}$. Hence our next problem is as follows.

Problem 14. Find a necessary and sufficient condition for the basis $\mathcal{B}$ such that the components of NEPS of arbitrary connected bipartite graphs with the basis $\mathcal{B}$ are almost cospectral. In particular, is $\mathrm{rank}_2(\mathrm{Ann}(\mathcal{B}, S)) \leq \mathrm{rank}_2(\mathcal{B}) - |S|$ such a necessary and sufficient condition?

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Appendix

Number of Walks in $G_{p,q}$ and G_{p,p^4}

Let the vertices of $K_{p,p}$ be denoted as type A and the pendant vertices as type B vertices. From each type B vertex a walk can continue only to its unique neighbor of type A, while from each type A vertex a walk can continue to either one of its p type A neighbors or one of its q type B neighbors. Due to symmetry of vertices in $G_{p,q}$ we can classify the k-walks of $G_{p,q}$ according to the sequence of types of vertices appearing along each walk.

For a given k-sequence of letters A and B, the number of the corresponding k-walks can be determined by choosing the first vertex of a walk and then by considering pairs of successive letters:

- each pair AA yields p choices for the second A after the vertex corresponding to the first A is chosen;
- each pair AB yields q choices for B after the vertex for A is chosen;
- each pair BA yields a unique choice for A after the vertex for B is chosen.

For example, the sequence $BAABA$ encodes $(2pq)\cdot 1\cdot p\cdot q\cdot 1 = 2p^2q^2$ walks of length 5, while $AABAABA$ encodes $(2p)\cdot p\cdot q\cdot 1\cdot p\cdot q\cdot 1 = 2p^3q^2$ walks of length 7.

The fact that a feasible type sequence does not contain the pair BB means that each letter B may occupy either a single position between any two consecutive letters A, or a single position prior to the first A or after the last A. Since the number of walks of length k with a given type sequence is influenced by the first and the last type appearing in the sequence, we will count them separately, working out in detail the first possibility only.

Hence suppose that a given type sequence starts and ends with the letter A and that it contains l letters B (and consequently $k-l$ letters A). There are $k-l-1$ feasible positions for letters B between consecutive letters A, so that the number of such type sequences is $\binom{k-l-1}{l}$. The initial letter A yields $2p$ choices for the initial vertex of a k-walk. Each letter B appearing in the type sequence produces one pair AB and one pair BA, which together yield q choices for two corresponding vertices along a k-walk. This leaves a total of $k-1-2l$ pairs AA remaining in the type sequence, each of which yields p choices for the corresponding vertex in a k-walk. Hence each type sequence starting and ending with A corresponds to a total of $2p\cdot q^l\cdot p^{k-1-2l} = 2p^{k-2l}q^l$ walks of length k, and the number of k-walks corresponding to all such type sequences is equal to

$$\sum_{l\geq 0}\binom{k-l-1}{l}2p^{k-2l}q^l.$$

Following the similar argument, we can get that the number of k-walks corresponding to type sequences starting with A and ending with B is equal to

$$\sum_{l\geq 1}\binom{k-l-1}{l-1}2p^{k-2l+1}q^l,$$

which is also equal to the number of k-walks corresponding to type sequences starting with B and ending with A. Finally, the number of k-walks corresponding to type sequences starting and ending with B is equal to

$$\sum_{l\geq 2}\binom{k-l-1}{l-2}2p^{k-2l+2}q^l.$$

Summing up these four cases we see that the total number of k-walks in $G_{p,q}$ is

$$\begin{aligned} w_k(G_{p,q}) \; &= \sum_{l\geq 0}\binom{k-l-1}{l}2p^{k-2l}q^l + 2\sum_{l\geq 1}\binom{k-l-1}{l-1}2p^{k-2l+1}q^l \\ &+ \sum_{l\geq 2}\binom{k-l-1}{l-2}2p^{k-2l+2}q^l. \end{aligned}$$

Upper limits for the three sums above can be determined from the corresponding binomial coefficients:

- nonzero summands in the first sum are obtained for $k-l-1\geq l$, i.e., for $l\leq\left\lfloor\frac{k-1}{2}\right\rfloor$;
- nonzero summands in the second sum are obtained for $k-l-1\geq l-1$, i.e., for $l\leq\left\lfloor\frac{k}{2}\right\rfloor$;
- nonzero summands in the third sum are obtained for $k-l-1\geq l-2$, i.e., for $l\leq\left\lfloor\frac{k+1}{2}\right\rfloor$.

If we now set $q=p^4$, then

$$\begin{aligned} w_k(G_{p,p^4}) \; &= \sum_{l=0}^{\left\lfloor\frac{k-1}{2}\right\rfloor}\binom{k-l-1}{l}2p^{k+2l} + 2\sum_{l=1}^{\left\lfloor\frac{k}{2}\right\rfloor}\binom{k-l-1}{l-1}2p^{k+2l+1} \\ &+ \sum_{l=2}^{\left\lfloor\frac{k+1}{2}\right\rfloor}\binom{k-l-1}{l-2}2p^{k+2l+2}. \end{aligned}$$

Thus, $w_k(G_{p,p^4})$ is a polynomial in p, whose leading term is obtained by setting $l=\left\lfloor\frac{k+1}{2}\right\rfloor$ in the third sum and is equal to

$$\binom{k-\left\lfloor\frac{k+1}{2}\right\rfloor-1}{\left\lfloor\frac{k+1}{2}\right\rfloor-2}2p^{k+2\left\lfloor\frac{k+1}{2}\right\rfloor+2} = \begin{cases} 2p^{2k+3}, & \text{if } k \text{ is odd,}\\ (k-2)p^{2k+2}, & \text{if } k \text{ is even.}\end{cases}$$

Recalling from (14) that $\lambda_1(G_{p,p^4})=\frac{p+\sqrt{p^2+4p^4}}{2}=p^2\left(\sqrt{1+\frac{1}{4p^2}}+\frac{1}{2p}\right)$, we get that for every even $s\geq 2$ and even $r\geq 2$

$$\lim_{p\to\infty}\frac{w_{s+r}}{\lambda_1^r w_s} = \lim_{p\to\infty}\frac{w_{s+r}}{p^{2(s+r)+2}}\frac{p^{2r}}{\lambda_1^r}\frac{p^{2s+2}}{w_s} = \frac{s+r-2}{s-2}.$$