

EÖTVÖS LORÁND UNIVERSITY
FACULTY OF SCIENCE

DÁNIEL HEGEDŰS, ÁRON JÁNOSIK, JÓZSEF OSZTÉNYI
ELTE Institute of Mathematics

Extremal spectral graph theory

FiFöMa OTDK thesis

Supervisor: PÉTER CSIKVÁRI
ELTE Institute of Mathematics, Department of Computer Science



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1 Introduction

Eigenvalues are no doubt one of the most important tools in linear algebra, also used in Computer Science, Physics and Chemistry [1] [2] [3], while graph theory is widely used for problems in Combinatorics and Discrete Mathematics. Spectral graph theory is the branch of Mathematics, which examines the eigenvalues of the adjacency matrix of graphs. It is often applied for example in Chemistry [4].

In our research, we only worked with undirected graphs without loops and multiple edges. For a graph $G = (V, E)$ with n vertices and m edges, its adjacency matrix A_G (or sometimes denoted shorter by A) is defined as follows:

$$(A_G)_{i,j} = \begin{cases} 1 & \text{if } (i, j) \in E, \\ 0 & \text{if } (i, j) \notin E. \end{cases}$$

We say that λ is an eigenvalue of a matrix A with eigenvector $v \neq 0$, if $Av = \lambda v$. For graphs, it can be interpreted as writing numbers on the vertices, and for each vertex the sum of its neighbours' numbers is λ times the number on the vertex. Notice that in our case the adjacency matrix is always symmetric, for which it is well-known from the Spectral theorem that all of its eigenvalues are real. By this, we can suppose that the eigenvalues are in the form of $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$.

Through our paper, we will use many well-known facts for graph eigenvalues. These include that $\sum_{i=1}^n \lambda_i = 0$ and $\sum_{i=1}^n \lambda_i^k$ counts the closed walks of length k . Furthermore, for connected graphs, λ_1 has multiplicity 1 and it is the only eigenvalue with an eigenvector that has only positive coordinates. Moreover, it is true that $\frac{2m}{n} \leq \lambda_1 \leq \Delta$ (where Δ denotes the maximum degree), with equality in each case if and only if the graph is Δ -regular. For a complete list of tools and their proofs, see [5]. A large list of unsolved problems can be found in [6]. We will use the notations $s^+(G)$ and $s^-(G)$ for the sum of squares of positive and negative eigenvalues, respectively. One of the main conjectures is the following.

Conjecture 1.1 (Elphick, Farber, Goldberg, Wocjan [7]). For every connected graph G on n vertices we have

$$\min(s^+(G), s^-(G)) \geq n - 1.$$

In our research, we mainly focused on two problems: bounding λ_k and calculating or bounding $s^+(G)$ and $s^-(G)$. The proofs and theorems taken from others are always cited, everything else is our original work and ideas.

2 Third largest eigenvalue

A famous conjecture investigated by Nikiforov in [8] states that $\lambda_k \leq \frac{n}{k} - 1$ for all graphs. Unfortunately it is not true for $k \geq 4$, but it is true for $k = 2$ and it is an unsolved question for $k = 3$. New results for $\lambda_k \geq \frac{n}{k} - 1$ can be found in [9].

Lemma 2.1. *The following three statements are equivalent:*

1. $\lambda_k \leq \frac{n}{k} - 1$ holds for all graphs,
2. $\lambda_k \leq \lfloor \frac{n}{k} \rfloor$ holds for all graphs,
3. $\lambda_k \leq \frac{n}{k}$ holds for all graphs.

Proof. The implications $1 \Rightarrow 2$ and $2 \Rightarrow 3$ are obvious, so it is enough to prove $3 \Rightarrow 1$. Take an arbitrary graph G with k -th largest eigenvalue λ_k . We can suppose that $\lambda_k > 0$, otherwise we are done. The statement holds for all of its closed blow-ups $G^{[t]}$ (described in [8]), that have k -th largest eigenvalue $\lambda_k^{[t]} = t\lambda_k + t - 1$ (from $\lambda_k > 0$, $t\lambda_k + t - 1 > 0$ so $\lambda_k^{[t]}$ cannot be (-1)). Using this, we have $t\lambda_k + t - 1 \leq \frac{tn}{k}$, so $\lambda_k \leq \frac{n}{k} - 1 + \frac{1}{t}$ for all $t > 0$. Taking $t \rightarrow \infty$ we get the statement for the original G . $\square$

Now we propose some new examples for which the equality case $\lambda_3 = \frac{n}{3} - 1$ holds. Let $3|n$ and $0 < k < \frac{n}{3}$ arbitrary. The graph contains the union of six disjoint complete graphs, three on k vertices and three on $\frac{n}{3} - k$ vertices, alternating around a circle, and the adjacent complete graphs have all the edges between their vertices.

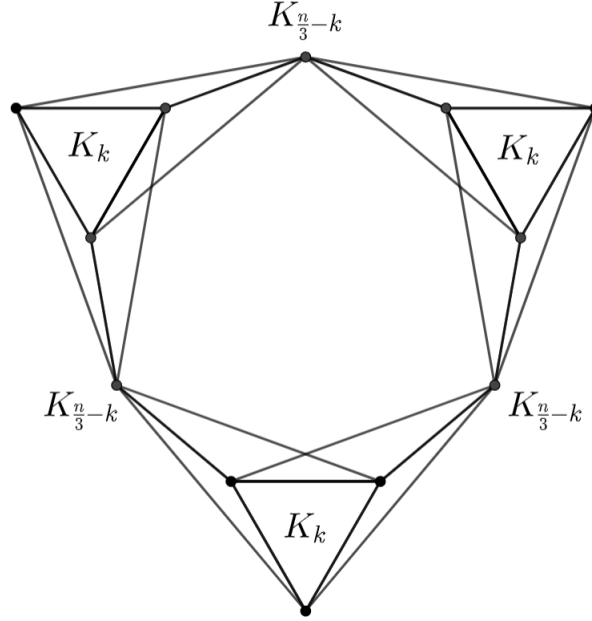


Figure 1. An example for the construction with parameters $n = 12$ and $k = 3$.

This graph has the following eigenvalues. It has (-1) with multiplicity $n - 4$. That is because $n - 6$ of them come from the eigenvalues of the complete graph parts: we choose an eigenvector corresponding to (-1) of a complete graph and 0 on all other vertices. While the other two (-1) -s come from the eigenvectors when we write 1 and (-1) on vertices of two adjacent complete graphs and (-1) and 1 on vertices of the two complete graphs opposite to the previously used ones, respectively, and 0 on all other vertices.

When we write 1 on all vertices of two adjacent complete graphs, (-1) on all vertices of the complete graphs opposite to them and 0 on all other vertices, we get an eigenvector for the eigenvalue $\frac{n}{3} - 1$ with multiplicity 2.

The last two eigenvalues come from the eigenvectors when we write 1 on all vertices from the complete graphs of size $\frac{n}{3} - k$ and x on all other vertices. Then the 2 equations are: $(k - 1)x + 2(\frac{n}{3} - k) = \lambda x$ and $\frac{n}{3} - k - 1 + 2kx = \lambda$. This gives the result

$$\lambda = \frac{\frac{n}{3} - 2 \pm \sqrt{(\frac{n}{3} - 2k)^2 + 16k(\frac{n}{3} - k)}}{2}.$$

This expression gives a positive eigenvalue that is greater than $\frac{n}{3} - 1$ (in the case of $k \leq \frac{n}{3}$), and a negative eigenvalue.

So we get $\lambda_3 = \frac{n}{3} - 1$, the case of equality.

Remark 2.2. This graph class is closed under the closed blow-up operation.

3 Third largest eigenvalue of a graph and its complement

In this section, we show that for every graph G , either the third eigenvalue of G or the third eigenvalue of G^c must be small, where G^c denotes the complement graph of G .

Let us denote the eigenvalues of the complement graph by $\lambda'_1 \geq \dots \geq \lambda'_n$. By Weyl's inequality, we have $\lambda_1 + 1 + \lambda'_n \geq 0$, $\lambda_2 + 1 + \lambda'_n \leq 0$, $\lambda_2 + 1 + \lambda'_{n-1} \geq 0$ and $\lambda_3 + 1 + \lambda'_{n-1} \leq 0$.

We can assume $\lambda_{n-1} \leq 0$ (otherwise $\lambda_3 < -1$), and $\lambda_3 + 1 \geq 0$. Then we have

$$(\lambda_1 + 1)^2 \geq \lambda'^2_n \geq (\lambda_2 + 1)^2 \geq \lambda'^2_{n-1} \geq (\lambda_3 + 1)^2.$$

By symmetry (with $\lambda_{n-1} \leq -1$, $\lambda'_3 \geq 0$) we have

$$\lambda'^2_1 \geq (\lambda_n + 1)^2 \geq \lambda'^2_2 \geq (\lambda_{n-1} + 1)^2 \geq \lambda'^2_3.$$

We know that

$$\sum_{i=1}^n ((\lambda_i + 1)^2 + \lambda_i'^2) = n^2,$$

which gives

$$n^2 \geq (\lambda_1 + 1)^2 + \lambda_n'^2 + (\lambda_2 + 1)^2 + \lambda_{n-1}'^2 + (\lambda_3 + 1)^2 + \lambda_1'^2 + (\lambda_n + 1)^2 + \lambda_2'^2 + (\lambda_{n-1} + 1)^2 + \lambda_3'^2 \geq 5((\lambda_3 + 1)^2 + \lambda_3'^2).$$

This means that $\lambda_3 \leq \frac{n}{\sqrt{10}} - 1$ or $\lambda_3' \leq \frac{n}{\sqrt{10}}$. The same proof can be told for the complement of G , giving $\lambda_3 \leq \frac{n}{\sqrt{10}}$ or $\lambda_3' \leq \frac{n}{\sqrt{10}} - 1$.

Notice that the above argument also works for λ_k : we have $\lambda_k \leq \frac{n}{\sqrt{4k-2}} - 1$ or $\lambda_k' \leq \frac{n}{\sqrt{4k-2}}$ and similarly $\lambda_k \leq \frac{n}{\sqrt{4k-2}}$ or $\lambda_k' \leq \frac{n}{\sqrt{4k-2}} - 1$.

4 Bounding the second largest eigenvalue

In this section, we will give a new, simple proof for the fact that $\lambda_2 \leq \frac{n}{2} - 1$ for all (not necessarily connected) graphs.

First, let us suppose that our graph is connected. Let v be an eigenvector for λ_2 . We can suppose that at most half of the coordinates of v is positive (as otherwise we can take $-v$). Let v_1 be a largest positive coordinate and let the other coordinates be v_i for $i \in \{2, 3, \dots, n\}$. Let V_+ be the set of vertices with positive coordinate and V_- be the set of vertices with negative coordinate. Then

$$\lambda_2 v_1 = \sum_{v_i \in N_G(v_1)} v_i \leq \sum_{v_i > 0} v_i - v_1 \leq (|V_+| - 1) v_1 \leq \left(\frac{n}{2} - 1\right) v_1.$$

Dividing by $v_1 \neq 0$ gives the desired statement (for connected graphs). We state that equality cannot hold in the connected case. That is because in the last inequality we have equality only if $|V_+| = \frac{n}{2}$, while in the middle one only if all $v_i > 0$ are equal to v_1 . In the first inequality we have equality only if the vertex of v_1 is adjacent to all vertices in V_+ . But this means that the vertex of v_1 , which is the maximal coordinate, is adjacent to all the other maximal coordinates, meaning that V_+ forms a complete graph. No edge can go out from V_+ , as we could suppose that there are no 0 coordinates, as both V_+ and V_- have size $\frac{n}{2}$. But because of the connectivity, this means that $V = V_+$, which contradicts the fact that only λ_1 has an eigenvector with only positive coordinates.

For the disconnected case, we will use that the spectrum of disjoint union of graphs is the union of the spectra, and that $\lambda_1 \leq n - 1$ with equality if and only if the graph is a K_n .

If λ_1 and λ_2 belong to the same component, then we are done, as the proof above works for this component as a connected graph, with fewer vertices.

Now we can suppose that λ_1 belongs to the component G_1 with n_1 vertices and λ_2 belongs to the component G_2 with n_2 vertices. If $n_2 \leq n_1$, then $\lambda_2 \leq n_2 - 1 \leq \frac{n_1 + n_2}{2} - 1 \leq \frac{n}{2} - 1$, which is enough. Otherwise if $n_2 \geq n_1$, then $\lambda_2 \leq \lambda_1 \leq n_1 - 1 \leq \frac{n_1 + n_2}{2} - 1 \leq \frac{n}{2} - 1$, which finishes the other case.

Now we will look at the case of equality. We cannot have more than two components, as it would mean $n_1 + n_2 \neq n$. If we have exactly two components, then $n_1 = \frac{n_1 + n_2}{2}$ or $n_2 = \frac{n_1 + n_2}{2}$ must hold, meaning that $n_1 = n_2$. But this means that $\lambda_2 = n_1 - 1$, meaning that both G_1 and G_2 are complete graphs of the same size. In this case $\lambda_2 = \frac{n}{2} - 1$ really holds. This finishes the proof.

If we take a look back at connected graphs, we saw that $\lambda_2 = \frac{n}{2} - 1$ cannot hold. But in the next section, we will prove that the graphs, which are two cliques connected by an edge, have the property that as their sizes converge to infinity, $(\frac{n}{2} - 1) - \lambda_2$ converges to 0.

5 Relations between λ_1 and other eigenvalues

In this section we will investigate the distance of λ_1 to the other eigenvalues of graphs.

Theorem 5.1. *For any fixed $k > 1$, the difference $0 \leq \lambda_1 - \lambda_k$ can be arbitrarily close to 0, even for connected graphs.*

Proof. Let us fix $k > 1$ and define $G_{n,k}$ as follows: take k disjoint K_n graphs and take an arbitrary vertex v . Draw exactly one edge from v to every other K_n (with which we add $k - 1$ edges). We state that these graphs are sufficient.

We will calculate the eigenvalues of $G_{n,k}$. First of all, $G_{n,k}$ has kn vertices. It has eigenvalue -1 with multiplicity $k(n - 2) + k - 2$: let us write 0 on v , and fix the coordinates of its neighbours from other cliques, with sum of 0 ($k - 2$ comes from this). Now for each clique, the other $n - 1$ coordinates should be chosen such that the sum of the coordinates on a clique is 0. It has eigenvalue $n - 1$ with multiplicity $k - 2$ as we can take the vectors, for which we write 1 on all vertices of a clique not containing v and -1 on all vertices of another clique not containing v . Only four eigenvalues are left, they are not as easy as the previous ones.

We state that there are four eigenvectors in the form of having coordinate 1 on all the vertices, which are not in the same clique as v and not adjacent to v and having coordinate $\pm\sqrt{k - 1}$ on the vertices which are in the same clique as v but not the same as v . Let us write $\pm\sqrt{k - 1}a$ on v and a to the remaining $k - 1$ vertices. This yields the following equations:

$$\begin{aligned}\lambda \cdot 1 &= n - 2 + a \\ \lambda \cdot (\pm\sqrt{k - 1}) &= (n - 2)(\pm\sqrt{k - 1}) \pm \sqrt{k - 1}a \\ \lambda \cdot a &= n - 1 \pm \sqrt{k - 1}a \\ \lambda \cdot (\pm\sqrt{k - 1})a &= (n - 1)(\pm\sqrt{k - 1}) + (k - 1)a.\end{aligned}$$

This system of equations has exactly four solutions: precisely they are in the form of

$$\lambda = \frac{\pm_1 \sqrt{n^2 + k - 1} \mp_2 2n\sqrt{k - 1} \pm_2 4\sqrt{k - 1} \pm_2 \sqrt{k - 1} + n - 2}{2}$$

Now we calculate the limes of the λ -s as n converges to ∞ . If we take $-$ and $-$, the limes is $-1 - \sqrt{k - 1}$, which is negative, so less than $n - 1$. If we take $-$ and $+$, the limes is $-1 + \sqrt{k - 1}$, which is less than $n - 1$, for large enough n . On the other hand, for the other two cases, the distance of λ and $n - 1$ converges to 0. This means, that no matter which eigenvalue is λ_1 and which is λ_k , as we already have $n - 1$ as an eigenvalue with multiplicity $k - 2$, the difference of λ_1 and λ_k converges to 0. $\square$

Remark 5.2. The fact that $\frac{\lambda_1}{\lambda_k}$ can converge to 1 is an immediate corollary of Theorem 5.1.

Notice that we fixed the index of the eigenvalue which was investigated. A really different problem is to look at $\lambda_1 - \lambda_{f(n)}$, where the index is growing with n .

Theorem 5.3. *The difference $\lambda_1 - \lambda_{\frac{n}{2}}$ cannot be arbitrarily close to 0 for connected graphs.*

Proof. Take an $\varepsilon > 0$ and suppose that $\lambda_{\frac{n}{2}} \geq (1 - \varepsilon)\lambda_1$. By this, we have

$$\frac{n}{2}(1 - \varepsilon)\lambda_1 \leq \sum_{i=1}^{\frac{n}{2}} \lambda_i = - \sum_{i=\frac{n}{2}+1}^n \lambda_i \leq \sum_{i=\frac{n}{2}+1}^n |\lambda_i|.$$

Using the inequality between the arithmetic mean and quadratic mean gives $\frac{n}{2}(1 - \varepsilon)^2 \lambda_1^2 \leq \sum_{i=\frac{n}{2}+1}^n |\lambda_i|^2$. Now calculating the sum of squares of the eigenvalues gives

$$n(1 - \varepsilon)^2 \lambda_1^2 \leq \frac{n}{2}(1 - \varepsilon)^2 \lambda_1^2 + \sum_{i=\frac{n}{2}+1}^n |\lambda_i|^2 \leq \sum_{i=1}^n \lambda_i^2 = 2m.$$

Using $\lambda_1 \geq \frac{2m}{n}$ gives

$$2m(1 - \varepsilon)^2 \leq n.$$

The inequality $n - 1 \leq m$ is true for every connected graph, so

$$2(n - 1)\varepsilon^2 - 4(n - 1)\varepsilon + n - 2 \leq 0.$$

This gives $1 - \sqrt{\frac{n}{2(n - 1)}} \leq \varepsilon \leq 1 + \sqrt{\frac{n}{2(n - 1)}}$. So if $n \geq 3$ and $\varepsilon < 1 - \sqrt{\frac{n}{2(n - 1)}} (\rightarrow 1 - \frac{\sqrt{2}}{2})$, then no such graph exists. $\square$

6 Ratio of negative and positive square energy

Computer calculation and the difference between proving bounds suggests that $s^+(G)$ is usually larger than $s^-(G)$. On the other hand, $\frac{s^-(G)}{s^+(G)}$ can be arbitrarily large: in this section we show a set of graphs proving this. Let G be a strongly regular graph with parameters

$$((q^2 + 1)(q^5 + 1), q^5 + q^2, q^2 - 1, q^3 + 1).$$

This graph exists for any prime power q , as was proved in [10].

For a strongly regular graph, it is easy to compute the eigenvalues: it has only 3 of them and their multiplicities can also be calculated from their parameters. In many books you can find the calculation of eigenvalues and their multiplicities, as in [5], from which

$$\lambda_1 = d, m_1 = 1, \lambda_{\pm} = \frac{a - b \pm \sqrt{(a - b)^2 + 4(d - b)}}{2}, m_{\pm} = \frac{1}{2} \left(n - 1 \mp \frac{2d + (n - 1)(a - b)}{\sqrt{(a - b)^2 + 4(d - b)}} \right),$$

where (n, d, a, b) are the parameters of a strongly regular graph and m is multiplicity of the eigenvalue. From here it can be calculated that its eigenvalues are $q^5 + q^2$ with multiplicity 1, $q^2 - 1$ with multiplicity $q^3(q^2 + 1)(q^2 - q + 1)$ and $-(q^3 + 1)$ with multiplicity $q^2(q^4 - q^3 + q^2 - q + 1)$. Further calculations show that

$$\frac{s^-(G)}{s^+(G)} = \frac{q^2(q^4 - q^3 + q^2 - q + 1)(q^3 + 1)^2}{(q^5 + q^2)^2 + q^3(q^2 + 1)(q^2 - q + 1)(q^2 - 1)^2} = \frac{q^2 - q + 1}{q}.$$

As q and the number of vertices converge to infinity, the ratio above converges to infinity too, which finishes the proof.

7 Relation between positive and negative square energy of Kneser-graphs

The Kneser(n, k) graphs have vertices each corresponding to a k -element subset of an n -element set. A vertex is adjacent to another if and only if their subsets are disjoint. The Kneser(n, k) graph has eigenvalues $(-1)^i \binom{n-k-i}{k-i}$ with multiplicity $\binom{n}{i} - \binom{n}{i-1}$ for $i = 0, \dots, k$, as was proved in [11]. Computer computation suggested the following theorem:

Theorem 7.1. *For the Kneser(n, k) graphs, if we have $k \leq \frac{n}{4}$, then $s^-(G) < s^+(G)$. Furthermore, if $k > \frac{n}{4}$, then if n is even, we have $s^-(G) = s^+(G)$, while if $n \equiv 1 \pmod{4}$, then $s^-(G) > s^+(G)$ and if $n \equiv 3 \pmod{4}$, then $s^-(G) < s^+(G)$.*

Proof. By the definition of s^+ and s^- in $s^+ - s^-$, the task is to calculate the sign of

$$\sum_{i=0}^k (-1)^i \binom{n-k-i}{k-i}^2 \left(\binom{n}{i} - \binom{n}{i-1} \right).$$

First notice, that $\binom{n}{i} - \binom{n}{i-1} = \frac{n!}{i!(n-i)!} - \frac{n!}{(i-1)!(n-i+1)!} = \binom{n}{i} \frac{n-2i+1}{n-i+1}$. So the desired sum is actually in the form of

$$\sum_{i=0}^k (-1)^i \binom{n-k-i}{k-i}^2 \binom{n}{i} \frac{n-2i+1}{n-i+1}.$$

Dividing by $0 < s^-(G) + s^+(G) = m = \binom{n}{k} \binom{n-k}{k} = \frac{n!}{(k!)^2(n-2k)!}$ keeps the sign. Rewriting the binomials using the $\binom{p}{q} = \frac{p!}{q!(p-q)!}$ formula implies, that it is enough to calculate the sign of

$$\sum_{i=0}^k (-1)^i \frac{\binom{n-k-i}{k-i} \binom{k}{i}}{\binom{n-i}{k}} \frac{n-2i+1}{n-i+1}.$$

We state, that the above equals to

$$\frac{\Gamma(-\frac{n}{2})\Gamma(2k - \frac{n}{2})}{\Gamma(k - \frac{n}{2})^2}$$

at every point where they are defined. Use the notation $c_i = (-1)^i \frac{\binom{n-k-i}{k-i} \binom{k}{i}}{\binom{n-i}{k}} \cdot \frac{n-2i+1}{n-i+1}$. Then

$$\frac{c_{i+1}}{c_i} = \frac{(-1)^{i+1}(i-k)^2(-2i+n-1)(-i+n+1)}{(-1)^i(i+1)(-2i+n+1)(i+k-n)^2} = \frac{(-1)(i-k)^2(-i+\frac{n-1}{2})(-i+n+1)}{(i+1)(-i+\frac{n+1}{2})(i+k-n)^2}.$$

Also, $c_0 = \frac{\binom{n-k}{k}}{\binom{n}{k}}$. Then

$$c_i = c_0 \prod_{j=0}^{i-1} \frac{c_{j+1}}{c_j} = \frac{\binom{n-k}{k}}{\binom{n}{k}} \prod_{j=0}^{i-1} \frac{(-1)(j-k)^2(-j+\frac{n-1}{2})(-j+n+1)}{(j+1)(-j+\frac{n+1}{2})(j+k-n)^2} = \frac{\binom{n-k}{k}}{\binom{n}{k}} \cdot \frac{((-k)^{(i)})^2 (\frac{1-n}{2})^{(i)} (-1-n)^{(i)}}{i! (-\frac{1-n}{2})^{(i)} ((k-n)^{(i)})^2},$$

where $x^{(j)}$ denotes the rising factorial (or Pochhammer function), so $x^{(j)} = x(x+1)\dots(x+j-1)$.

So the original sum is

$$\begin{aligned} \sum_{i=0}^k c_i &= \frac{\binom{n-k}{k}}{\binom{n}{k}} \cdot \sum_{i=0}^k \frac{((-k)^{(i)})^2 (\frac{1-n}{2})^{(i)} (-1-n)^{(i)}}{i! (-\frac{1-n}{2})^{(i)} ((k-n)^{(i)})^2} = \\ &= \frac{\binom{n-k}{k}}{\binom{n}{k}} \cdot {}_4F_3 \left(-k, -k, \frac{1-n}{2}, -1-n; \frac{-1-n}{2}, k-n, k-n; 1 \right), \end{aligned}$$

where ${}_4F_3$ is the generalized hypergeometric function. By a formula in [12] for this special case of ${}_4F_3$, when $k > \frac{n}{4}$, we have

$${}_4F_3 \left(-k, -k, \frac{1-n}{2}, -1-n; \frac{-1-n}{2}, k-n, k-n; 1 \right) = \frac{\Gamma(-\frac{n}{2})\Gamma(2k - \frac{n}{2})\Gamma(k-n)^2}{\Gamma(k - \frac{n}{2})^2\Gamma(-n)\Gamma(2k-n)}.$$

And $c_0 = \frac{\binom{n-k}{k}}{\binom{n}{k}} = \frac{\Gamma(n-k+1)^2}{\Gamma(n-2k+1)\Gamma(n+1)}$. By the identity for the gamma function, $\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin(\pi z)}$, we know that for integer k (and non-integer n), we have

$$\begin{aligned} \Gamma(k-n)^2\Gamma(1+n-k)^2 &= \left(\frac{\pi}{\sin(\pi(k-n))} \right)^2 = \frac{\pi}{\sin(\pi(-n))} \cdot \frac{\pi}{\sin(\pi(2k-n))} \\ &= \Gamma(1+n)\Gamma(-n)\Gamma(2k-n)\Gamma(1+n-2k). \end{aligned}$$

Using this, we get

$$\begin{aligned} \sum_{i=0}^k c_i &= \frac{\binom{n-k}{k}}{\binom{n}{k}} \cdot {}_4F_3 \left(-k, -k, \frac{1-n}{2}, -1-n; \frac{-1-n}{2}, k-n, k-n; 1 \right) = \\ &= \frac{\Gamma(n-k+1)^2}{\Gamma(n-2k+1)\Gamma(n+1)} \cdot \frac{\Gamma(-\frac{n}{2})\Gamma(2k - \frac{n}{2})\Gamma(k-n)^2}{\Gamma(k - \frac{n}{2})^2\Gamma(-n)\Gamma(2k-n)} = \frac{\Gamma(-\frac{n}{2})\Gamma(2k - \frac{n}{2})}{\Gamma(k - \frac{n}{2})^2} \end{aligned}$$

So we got that in the points where they are defined, we have

$$\sum_{i=0}^k (-1)^i \frac{\binom{x-k-i}{k-i} \binom{k}{i}}{\binom{x-i}{k}} \cdot \frac{x-2i+1}{x-i+1} = \frac{\Gamma(-\frac{x}{2})\Gamma(2k - \frac{x}{2})}{\Gamma(k - \frac{x}{2})^2}$$

Now look at the sign of the right-hand side. As the denominator is a square, its sign is positive. It is well-known, that the first part of the numerator is positive if and only if $n < x < n+2$ for some integer n , for which $n \equiv 0 \pmod{4}$. If $2k > \frac{x}{2}$, then the second part of the numerator is positive, otherwise its sign is

equal to the sign of the first part. So the right-hand side is positive, if $2k > \frac{x}{2}$, otherwise positive if and only if $n < x < n + 2$ for some integer n , for which $n \equiv 0 \pmod{4}$.

Luckily, the Γ function is undefined only on the non-positive integers. Also luckily, the sum-formula is a rational function of x , so continuous in every point where the denominator is nonzero. But it is nowhere zero, because in the case of Kneser-graphs we can suppose $k \leq \frac{x}{2}$. So we got the value of this rational function at almost every x , meaning that the desired values at integers must be the limit of the values around that integer. But we saw that the limit of the right-hand side for even x -es is 0, as one of the left limit and right limit is non-negative and one of them is non-positive. In the case of odd x -es, we got that if $x \equiv 1 \pmod{4}$, then the function is positive in a neighbourhood, while if $x \equiv 3 \pmod{4}$, then the function is negative in a neighbourhood. We also use the fact that between integers, the formula with the Γ function is monotone, so the limit cannot be 0 at the odd integers. (Here we should also mention, that the ${}_4F_3$ -formula can only be used for sufficient pairs of n, k . But this is enough because if we know the degree of a rational function and its value at infinitely many points, then it is the only such rational function.) $\square$

8 Sum of squares of positive and negative eigenvalues of cycles of odd length

Take a cycle of length n , where n is odd. We will show that $\min(s^+(G), s^-(G)) \geq n - 1$ by calculating their exact values using trigonometric identities.

It is well-known that the eigenvalues of a cycle are $2 \cos\left(\frac{2k\pi}{n}\right)$, where $0 \leq k \leq n - 1$. From these, the sum of the positive ones can be written in the form of

$$\sum_{k=-\lfloor n/4 \rfloor}^{\lfloor n/4 \rfloor} \left(2 \cos\left(\frac{2k\pi}{n}\right) \right)^2.$$

If $n = 4\ell + 1$, where ℓ is an integer, then it is enough to have

$$\sum_{k=-\ell}^{\ell} \left(2 \cos\left(\frac{2k\pi}{n}\right) \right)^2 \geq 4\ell.$$

Using the double cosine identity gives, that the previous is equivalent to

$$\sum_{k=-\ell}^{\ell} 2 \left(1 + \cos\left(\frac{4k\pi}{4\ell + 1}\right) \right) \geq 4\ell,$$

which is equivalent to

$$\sum_{k=-\ell}^{\ell} \cos\left(\frac{4k\pi}{4\ell + 1}\right) \geq -1.$$

But the left-hand side is exactly $-\frac{1}{2} \sec\left(\frac{\pi}{4\ell+1}\right)$, so it is enough to have $\cos\left(\frac{\pi}{4\ell+1}\right) \geq \frac{1}{2}$, which is true as $\ell \geq 1$.

Actually the previous proof gives that $s^+(G) = n + 1 - \sec\left(\frac{\pi}{n}\right)$. Also, as the sum of the square of all eigenvalues is $2e(G) = 2n$, we have that $s^-(G) = n - 1 + \sec\left(\frac{\pi}{n}\right)$, which is also greater than $n - 1$.

In the case of $n = 4\ell + 3$, the previous proof gives that $s^+(G) = n - 1 + \sec\left(\frac{\pi}{n}\right)$ and $s^-(G) = n + 1 - \sec\left(\frac{\pi}{n}\right)$ finishing the calculation.

9 Weighted matching polynomial and adjacency matrix

In this section we study the weighted matching polynomial and its connection with the weighted adjacency matrix in the case of weighted trees.

Definition 9.1. Let G be a graph with a weight function $w : E \rightarrow \mathbb{R}_{\geq 0}$. Then the weighted adjacency matrix $A_{G,\underline{w}}$ as follows.

$$(A_{G,\underline{w}})_{u,v} = \begin{cases} \sqrt{w_e} & \text{if } e = (u,v) \in E, \\ 0 & \text{otherwise.} \end{cases}$$

Let $\varphi_{\underline{w}}(G, x) = \det(xI - A_{G,\underline{w}})$ denote the characteristic polynomial of $A_{G,\underline{w}}$.

We also need the concept of weighted matching polynomials.

Definition 9.2. Let G be a graph on n vertices with a weight function $w : E \rightarrow \mathbb{R}_{\geq 0}$. Then the weighted matching polynomial is defined as

$$\mu_{\underline{w}}(G, x) = \sum_{M \in \mathcal{M}(G)} (-1)^{|M|} \left(\prod_{e \in M} w_e \right) x^{n-2|M|},$$

where $\mathcal{M}(G)$ is the set of matchings of G including the empty one.

The main theorem about the matching polynomial is proved by Heilmann and Lieb in [13]:

Theorem 9.3. Let G be a graph with a weight function $w : E \rightarrow \mathbb{R}_{\geq 0}$. Then the weighted matching polynomial $\mu_{\underline{w}}(G, x)$ has only real zeros.

We will use several other recursions and lemmas about the matching polynomial.

Lemma 9.4. For arbitrary $u \in V(G)$ we have

$$\mu_{\underline{w}}(G, x) = x\mu_{\underline{w}}(G - u, x) - \sum_{v \in N_G(u)} w_{u,v} \mu_{\underline{w}}(G - \{u, v\}, x).$$

Furthermore, for arbitrary edge $e = (u, v) \in E(G)$ we have

$$\mu_{\underline{w}}(G, x) = \mu_{\underline{w}}(G - e, x) - w_e \mu_{\underline{w}}(G - \{u, v\}, x).$$

Proof. Expanding the left-hand side gives

$$\begin{aligned} \mu_{\underline{w}}(G, x) &= \sum_{M \in \mathcal{M}(G)} (-1)^{|M|} \left(\prod_{e \in M} w_e \right) x^{n-2|M|} \\ &= \sum_{\substack{M \in \mathcal{M}(G) \\ u \notin M}} (-1)^{|M|} \left(\prod_{e \in M} w_e \right) x^{n-2|M|} + \sum_{\substack{M \in \mathcal{M}(G) \\ u \in M}} (-1)^{|M|} \left(\prod_{e \in M} w_e \right) x^{n-2|M|}. \end{aligned}$$

Sorting the first term

$$\sum_{\substack{M \in \mathcal{M}(G) \\ u \notin M}} (-1)^{|M|} \left(\prod_{e \in M} w_e \right) x^{n-2|M|} = x \sum_{M \in \mathcal{M}(G-u)} (-1)^{|M|} \left(\prod_{e \in M} w_e \right) x^{n-2|M|-1} = x\mu_{\underline{w}}(G - u, x),$$

and the second

$$\begin{aligned} \sum_{\substack{M \in \mathcal{M}(G) \\ u \in M}} (-1)^{|M|} \left(\prod_{e \in M} w_e \right) x^{n-2|M|} &= \sum_{v \in N_G(u)} (-1)w_{u,v} \left(\sum_{M \in \mathcal{M}(G-u,v)} (-1)^{|M|} \left(\prod_{e \in M} w_e \right) x^{n-2|M|-2} \right) \\ &= - \sum_{v \in N_G(u)} w_{u,v} \mu_{\underline{w}}(G - \{u, v\}, x). \end{aligned}$$

□

Lemma 9.5. For arbitrary graph $G = (V, E)$ and weight function $w : E \rightarrow \mathbb{R}_{\geq 0}$ we have

$$\mu'_{\underline{w}}(G, x) = \sum_{u \in V} \mu_{\underline{w}}(G - u, x).$$

Proof. Expanding the left-hand side gives

$$\begin{aligned} \mu'_{\underline{w}}(G, x) &= \sum_{M \in \mathcal{M}(G)} (-1)^{|M|} \left(\prod_{e \in M} w_e \right) (n - 2|M|) x^{n-2|M|-1} = \sum_{u \in V} \left(\sum_{\substack{M \in \mathcal{M}(G) \\ u \notin M}} (-1)^{|M|} \left(\prod_{e \in M} w_e \right) x^{n-2|M|-1} \right) \\ &= \sum_{u \in V} \mu_{\underline{w}}(G - u, x). \end{aligned}$$

□

Lemma 9.6. For arbitrary graph $G = (V, E)$ and weight function $w : E \rightarrow \mathbb{R}_{\geq 0}$ we have

$$\mu_{\underline{w}}(G - u, x) \mu_{\underline{w}}(G - v, x) - \mu_{\underline{w}}(G, x) \mu_{\underline{w}}(G - \{u, v\}, x) = \sum_{P \in \mathcal{P}_{u,v}} \left(\prod_{e \in P} w_e \right) \mu_{\underline{w}}(G - P, x)^2,$$

where $\mathcal{P}_{u,v}$ is the set of paths with end vertices u and v . Furthermore,

$$\mu_{\underline{w}}(G - u, x) \mu'_{\underline{w}}(G, x) - \mu_{\underline{w}}(G, x) \mu'_{\underline{w}}(G - u, x) = \sum_{P \in \mathcal{P}_u} \left(\prod_{e \in P} w_e \right) \mu_{\underline{w}}(G - P, x)^2,$$

where $\mathcal{P}_u$ is the set of paths starting at vertex u .

Proof. We will prove by induction on the number of vertices. The statement is true for $n = 2$. Suppose that we know that the statement is true for some n and let us take a graph with $n + 1$ vertices. By induction on the graph $G - u$ and substituting in $u' \in N_G(u)$ and the original v we have

$$\mu_{\underline{w}}(G - \{u, u'\}, x) \mu_{\underline{w}}(G - \{u, v\}, x) - \mu_{\underline{w}}(G - u, x) \mu_{\underline{w}}(G - \{u, u', v\}, x) = \sum_{P \in \mathcal{P}_{u',v}} \left(\prod_{e \in P} w_e \right) \mu_{\underline{w}}(G - \{u, P\}, x)^2.$$

Expanding the original right-hand side, we have

$$\begin{aligned} \sum_{P \in \mathcal{P}_{u,v}} \left(\prod_{e \in P} w_e \right) \mu_{\underline{w}}(G - P, x)^2 &= \sum_{u' \in N_G(u)} w_{u,u'} \left(\sum_{P \in \mathcal{P}_{u',v}} \left(\prod_{e \in P} w_e \right) \mu_{\underline{w}}(G - \{u, P\}, x)^2 \right) = \\ &= \sum_{u' \in N_G(u)} w_{u,u'} \cdot (\mu_{\underline{w}}(G - \{u, u'\}, x) \mu_{\underline{w}}(G - \{u, v\}, x) - \mu_{\underline{w}}(G - u, x) \mu_{\underline{w}}(G - \{u, u', v\}, x)). \end{aligned}$$

By Lemma 9.4 we get

$$\begin{aligned} \sum_{P \in \mathcal{P}_{u,v}} \left(\prod_{e \in P} w_e \right) \mu_{\underline{w}}(G - P, x)^2 &= \\ &= (x \mu_{\underline{w}}(G - u, x) - \mu_{\underline{w}}(G, x)) \cdot \mu_{\underline{w}}(G - \{u, v\}, x) - (x \mu_{\underline{w}}(G - \{u, v\}, x) - \mu_{\underline{w}}(G - v, x)) \cdot \mu_{\underline{w}}(G - u, x) = \\ &= \mu_{\underline{w}}(G - u, x) \mu_{\underline{w}}(G - v, x) - \mu_{\underline{w}}(G, x) \mu_{\underline{w}}(G - \{u, v\}, x). \end{aligned}$$

The second statement comes from summing up the first equation for all v and using Lemma 9.5. From the left-hand side sum we have

$$\sum_{v \in V(G)} (\mu_{\underline{w}}(G - u, x) \mu_{\underline{w}}(G - v, x) - \mu_{\underline{w}}(G, x) \mu_{\underline{w}}(G - \{u, v\}, x)) =$$

$$\begin{aligned}
&= \mu_{\underline{w}}(G - u, x) \cdot \sum_{v \in V(G)} \mu_{\underline{w}}(G - v, x) - \mu_{\underline{w}}(G, x) \cdot \sum_{v \in V(G)} \mu_{\underline{w}}(G - \{u, v\}, x) = \\
&= \mu_{\underline{w}}(G - u, x) \mu'_{\underline{w}}(G, x) - \mu_{\underline{w}}(G, x) \mu'_{\underline{w}}(G - u, x)
\end{aligned}$$

From the right-hand side sum we have

$$\sum_{v \in V(G)} \left(\sum_{P \in \mathcal{P}_{u,v}} \left(\prod_{e \in P} w_e \right) \mu_{\underline{w}}(G - P, x)^2 \right) = \sum_{P \in \mathcal{P}_u} \left(\prod_{e \in P} w_e \right) \mu_{\underline{w}}(G - P, x)^2,$$

which finishes the proof. $\square$

Lemma 9.7. *Let T be a tree. Then*

$$\varphi_{\underline{w}}(T, x) = \mu_{\underline{w}}(T, x).$$

Proof. Let $A_{T, \underline{w}}$ be the weighted adjacency matrix. Expanding the left-hand side gives

$$\varphi_{\underline{w}}(T, x) = \det(xI - A_{T, \underline{w}}) = \sum_{\pi \in S_n} \text{sgn}(\pi) x^{|\{a: \pi(a)=a\}|} \prod_{a: \pi(a) \neq a} (-(A_{T, \underline{w}})_{a, \pi(a)}).$$

Notice, that only those permutations contributes to the sum, in which $\pi(\pi(a)) = a$ holds for every a . That is, because otherwise the permutation π would have a cycle of length at least 3, but in a tree T there are no such cycles. On the other hand, these $(a, \pi(a))$ pairs (where $a \neq \pi(a)$) are exactly the matchings of the graph. In both case x is on the same power: in one case, the number of vertices which are not in the matching, while in the other one it is the number of those, for which $\pi(a) = a$. $\square$

Definition 9.8. For a graph $G = (V, E)$ let us call a function $w : E \rightarrow \mathbb{R}_{\geq 0}$ generic if all non-zero roots of $\mu_{\underline{w}}(G, x)$ has multiplicity 1.

Lemma 9.9. *The generic weight functions are dense in $\mathbb{R}_{\geq 0}^E$.*

Proof. By induction on the number of edges, we can suppose that the generic weight functions are dense in $\mathbb{R}_{\geq 0}^{E(G-e)}$. Let

$$p(x) = \mu_{\underline{w}}(G - e, x) \mu'_{\underline{w}}(G - \{u, v\}) - \mu'_{\underline{w}}(G - e, x) \mu_{\underline{w}}(G - \{u, v\}, x).$$

Proposition 9.10. $p(x) \not\equiv 0$.

Proof. Let us suppose, that $p(x) \equiv 0$. This means that

$$\frac{\mu'_{\underline{w}}(G - \{u, v\}, x)}{\mu_{\underline{w}}(G - \{u, v\}, x)} = \frac{\mu'_{\underline{w}}(G - e, x)}{\mu_{\underline{w}}(G - e, x)}.$$

Denoting the roots of the denominators by α_i and β_i ($\alpha_i = \alpha_j$ and $\beta_i = \beta_j$ might happen for some $i \neq j$), this is in the form of

$$\sum_{i=1}^{n-2} \frac{m_i}{x - \alpha_i} = \sum_{i=1}^n \frac{n_i}{x - \beta_i}.$$

But this is a contradiction, as the two sides have a different amount of summands. $\square$

So we got that $p(x)$ have finitely many roots, let them be $\lambda_1, \lambda_2, \dots, \lambda_n$. If $\lambda \neq \lambda_i$, then for all $w_e \in \mathbb{R}$, we have that

$$\begin{aligned}
\mu_{\underline{w}}(G - e, \lambda) - w_e \mu_{\underline{w}}(G - \{u, v\}, \lambda) &= 0 \\
\mu'_{\underline{w}}(G - e, \lambda) - w_e \mu'_{\underline{w}}(G - \{u, v\}, \lambda) &= 0
\end{aligned}$$

But this means that for the matrix

$$\begin{pmatrix} \mu_{\underline{w}}(G - e, \lambda) & \mu_{\underline{w}}(G - \{u, v\}, \lambda) \\ \mu'_{\underline{w}}(G - e, \lambda) & \mu'_{\underline{w}}(G - \{u, v\}, \lambda) \end{pmatrix},$$

the vector $(1, -w_e)^T$ is an eigenvector with eigenvalue 0. But the determinant is the product of the eigenvalues, so the determinant would be 0. Notice that the determinant is exactly $p(\lambda)$, which contradicts Proposition 9.10. If $\lambda = \lambda_i$, then there must be only finitely many solutions in w_e , because that would mean

$$\begin{pmatrix} \mu_{\underline{w}}(G - \{u, v\}, \lambda) \\ \mu'_{\underline{w}}(G - \{u, v\}, \lambda) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

which implies

$$\begin{pmatrix} \mu_{\underline{w}}(G - e, \lambda) \\ \mu'_{\underline{w}}(G - e, \lambda) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

which cannot hold because of the induction. So we conclude that there are only finitely many bad cases, finishing the proof of the density. $\square$

Lemma 9.11. *Assume that given a graph $G = (V, E)$, a weight function $w : E \rightarrow \mathbb{R}_{\geq 0}$ and $\lambda \in \mathbb{R}$. If $\mu'(G, \lambda) \neq 0$, then there exists an $o \in V$ such that $\mu_{\underline{w}}(G - o, \lambda) \neq 0$.*

Proof. By Lemma 9.5 we have $\mu'_{\underline{w}}(G, \lambda) = \sum_{v \in V} \mu_{\underline{w}}(G - v, \lambda)$ and so there is a vertex o such that $\mu_{\underline{w}}(G - o, \lambda) \neq 0$. $\square$

Lemma 9.12. *Let $T = (V, E)$ be a tree with a root vertex o . Let $w : E \rightarrow \mathbb{R}_{\geq 0}$ be a generic weight function. Let λ be a non-zero eigenvalue of $A_{T, \underline{w}}$. Assume that $\mu_{\underline{w}}(T - o, \lambda) \neq 0$. Consider the vector $\underline{x}^{(o)} \in \mathbb{R}^V$ for which*

$$x_u^{(o)} = \left(\prod_{e \in P_{o, u}} x_e \right)^{1/2} \mu_{\underline{w}}(T - P_{o, u}, \lambda).$$

Then $\underline{x}^{(o)}$ is an eigenvector of $A_{T, \underline{w}}$ corresponding to eigenvalue λ . We have

$$\|\underline{x}^{(o)}\|^2 = \mu_{\underline{w}}(T - o, \lambda) \mu'_{\underline{w}}(T, \lambda),$$

which is non-zero.

Proof. First let us check the eigenvalue equation for vertex o :

$$0 = \varphi_{\underline{w}}(T, \lambda) = \mu_{\underline{w}}(T, \lambda) = \lambda \mu_{\underline{w}}(T - o, \lambda) - \sum_{v \in N_T(o)} w_{o, v} \mu_{\underline{w}}(T - \{o, v\}, \lambda) = \lambda x_o^{(o)} - \sum_{v \in N_T(o)} \sqrt{w_{o, v}} x_v^{(o)},$$

that is, $\lambda x_o^{(o)} = \sum_{v \in N_T(o)} \sqrt{w_{o, v}} x_v^{(o)}$. Now let $u \neq o$ be another vertex. Assume that $N_T(u) = \{v_0, v_1, \dots, v_k\}$, where v_0 is the parent of u , and $v_1, \dots, v_k$ are its children. Then

$$\mu_{\underline{w}}(T - P_{o, v_0}, \lambda) = \mu_{\underline{w}}(T - P_{o, v_0} - u, \lambda) - \sum_{v_i \in N_{T - v_0}(u)} w_{u, v_i} \mu_{\underline{w}}(T - P_{o, v_0} - \{u, v_i\}, \lambda),$$

that is,

$$\mu_{\underline{w}}(T - P_{o, v_0}, \lambda) = \mu_{\underline{w}}(T - P_{o, u}, \lambda) - \sum_{i=1}^k w_{u, v_i} \mu_{\underline{w}}(T - P_{o, v_i}, \lambda).$$

After multiplying both sides by $\left(\prod_{e \in P_{o, u}} w_e \right)^{1/2}$ we get that

$$\sqrt{w_{u, v_0}} x_{v_0}^{(o)} = \lambda x_u^{(o)} - \sum_{i=1}^k \sqrt{w_{u, v_i}} x_{v_i}^{(o)}.$$

In other words, $\lambda x_u^{(o)} = \sum_{v \in N_T(u)} \sqrt{w_{u, v}} x_v^{(o)}$. This proves that $A_{T, \underline{w}} \underline{x}^{(o)} = \lambda \underline{x}^{(o)}$.

By Lemma 9.6 we have

$$\begin{aligned}\|\underline{x}^{(o)}\|^2 &= \sum_{P \in \mathcal{P}_o} \left(\prod_{e \in P} w_e \right) \mu_{\underline{w}}(T - P, \lambda)^2 \\ &= \mu_{\underline{w}}(T - o, \lambda) \mu'_{\underline{w}}(T, \lambda) - \mu_{\underline{w}}(T, \lambda) \mu'_{\underline{w}}(T - o, \lambda) \\ &= \mu_{\underline{w}}(T - o, \lambda) \mu'_{\underline{w}}(T, \lambda).\end{aligned}$$

Since $w : E \rightarrow \mathbb{R}$ was generic and $\lambda \neq 0$, we get that $\mu'_{\underline{w}}(T, \lambda) \neq 0$. This proves that $\|\underline{x}^{(o)}\|^2 \neq 0$, and so this is a proper eigenvector. $\square$

Remark 9.13. The assumption $\mu_{\underline{w}}(T - o, \lambda) \neq 0$ is crucial to have a non-zero $\underline{x}^{(o)}$. If $T = P_5$, the path on 5 vertices with the constant 1 weight function, then choosing o to be the middle vertex of P_5 , and $\lambda = 1$ we get that $\underline{x}^{(o)} = \underline{0}$.

Lemma 9.14. Let $T = (V, E)$ be a tree with a generic weight function $w : E \rightarrow \mathbb{R}_{\geq 0}$. For $u, v \in V(T)$ we have

$$(A_{T, \underline{w}}^+)_{u, v} = \left(\prod_{e \in P_{u, v}} w_e \right) \cdot \sum_{\lambda > 0} \lambda \frac{\mu_{\underline{w}}(T - P_{u, v}, \lambda)}{\mu'_{\underline{w}}(T, \lambda)},$$

where the sum is for the positive eigenvalues of $A_{T, \underline{w}}$.

Proof. We know that $A_{T, \underline{w}}^+ = \sum_{\lambda > 0} \lambda E_\lambda$, where λ is an eigenvalue of $A_{T, \underline{w}}$ and E_λ is the corresponding idempotent. Since w is generic, the multiplicity of any positive eigenvalue λ is 1, and so $E_\lambda = \underline{x}_\lambda \underline{x}_\lambda^T$, where $\underline{x}_\lambda$ is an eigenvector with norm 1 corresponding to the eigenvalue λ . For a fixed $\lambda > 0$ if u is such a vertex that $\mu_{\underline{w}}(T - u, \lambda) \neq 0$, then we can use the previous lemma with $o = u$ and

$$\underline{x}_\lambda = \frac{1}{\sqrt{\mu_{\underline{w}}(T - u, \lambda) \mu'_{\underline{w}}(T, \lambda)}} \underline{x}^{(u)},$$

and we get that

$$(E_\lambda)_{u, v} = \left(\prod_{e \in P_{u, v}} w_e \right) \cdot \frac{\mu_{\underline{w}}(T - u, \lambda) \mu_{\underline{w}}(T - P_{u, v}, \lambda)}{\mu_{\underline{w}}(T - u, \lambda) \mu'_{\underline{w}}(T, \lambda)} = \left(\prod_{e \in P_{u, v}} w_e \right) \cdot \frac{\mu_{\underline{w}}(T - P_{u, v}, \lambda)}{\mu'_{\underline{w}}(T, \lambda)}.$$

If $\mu_{\underline{w}}(T - u, \lambda) = 0$, then for all $v \in V$ we have $\mu_{\underline{w}}(T - P_{u, v}, \lambda) = 0$ since $\underline{x}^{(u)} = \underline{0}$. In this case if we consider a vertex o for which $\mu_{\underline{w}}(T - o, \lambda) \neq 0$, then $\underline{x}^{(o)} = \left(\prod_{e \in P_{o, u}} w_e \right)^{1/2} \cdot \mu_{\underline{w}}(T - P_{o, u}, \lambda) = 0$. Whence $(E_\lambda)_{u, v} = c \left(\underline{x}_u^{(o)} \right) \left(\underline{x}_v^{(o)} \right) = 0$, where c is some normalizing constant. Since $\left(\prod_{e \in P_{u, v}} w_e \right) \cdot \frac{\mu_{\underline{w}}(T - P_{u, v}, \lambda)}{\mu'_{\underline{w}}(T, \lambda)} = 0$ too, we get that

$$(E_\lambda)_{u, v} = \left(\prod_{e \in P_{u, v}} w_e \right) \cdot \frac{\mu_{\underline{w}}(T - P_{u, v}, \lambda)}{\mu'_{\underline{w}}(T, \lambda)}$$

in both cases. This finishes the proof. $\square$

10 Polynomials with real zeros

Proposition 10.1. Let $f(x) = \sum_{k=0}^n a_k x^k$ be a polynomial of degree n with distinct real zeros. Let $R(f)$ denote the set of its zeros. Then

$$\sum_{\lambda \in R(f)} \frac{\lambda^j}{f'(\lambda)} = \begin{cases} 0 & \text{if } 0 \leq j \leq n-2, \\ \frac{1}{a_n} & \text{if } j = n-1. \end{cases}$$

Proof. It can be found in [14], Problem 67. □

Proposition 10.2. Let $b_1, \dots, b_n \in \mathbb{R}$ and $a_1, \dots, a_n \in \mathbb{R}_{>0}$. Then the function

$$f(z) = \sum_{k=1}^n b_k a_k^z$$

has at most $n - 1$ real zeros.

Proof. It can be found in [15], Problem 75. □

Proposition 10.3. Let $q(x) = x^{n-2t} \prod_{j=1}^t (x^2 - \lambda_j^2)$, where $0 < \lambda_1 < \dots < \lambda_t$. Then

$$g(r) = \sum_{i=1}^t \frac{\lambda_i^r}{q'(\lambda_i)}$$

is zero if $r = n - 2t + 1 + 2k$ for $k = 0, 1, \dots, t - 2$, it is positive if $r > n - 3$, and changes sign at every zero. In particular, for $r = (n - 2t + 1) + 2k + 1$ it has sign $(-1)^{k-t}$ for $k = -1, 0, 1, \dots, t - 2$.

Proof. We have

$$q'(\lambda_i) = 2\lambda_i^{n-2t+1} \prod_{j \neq i} (\lambda_i^2 - \lambda_j^2).$$

Whence

$$\sum_{i=1}^t \frac{\lambda_i^r}{q'(\lambda_i)} = \sum_{i=1}^t \frac{\lambda_i^{r-(n-2t+1)}}{\prod_{j \neq i} (\lambda_i^2 - \lambda_j^2)}.$$

By introducing $a_i = \lambda_i^2$, we get that

$$\sum_{i=1}^t \frac{\lambda_i^r}{q'(\lambda_i)} = \sum_{i=1}^t \frac{a_i^{(r-(n-2t+1))/2}}{\prod_{j \neq i} (a_i - a_j)}.$$

We have seen that if $\frac{r-(n-2t+1)}{2} = 0, 1, \dots, t - 2$, then it is 0. By introducing the notation $b_i = \frac{1}{\prod_{j \neq i} (a_i - a_j)}$, and $z = \frac{r-(n-2t+1)}{2}$ we can rewrite it as $\sum_{i=1}^t b_i a_i^z$. This has at most $t - 1$ zeros and we already found $t - 1$ zeros. If $z \rightarrow \infty$, then the term $b_t a_t^z$ will dominate. This gives that if $\frac{r-(n-2t+1)}{2} > t - 2$, then the expression is positive. At every zero the function will change sign, otherwise the derivative would have t zeros. □

11 Elements of A_T^+ for a tree T

The adjacency matrix A_T is decomposed as $A_T^+ - A_T^-$, the difference of two positive semidefinite matrices such that their product is 0. As T is a tree, it is a bipartite graph: the vertices can be partitioned into classes X and Y . If the biadjacency matrix of that bipartite graph is $2K$, then A_T^+ is formed as below.

	X	Y
X	$(KK^T)^{\frac{1}{2}}$	K
Y	K^T	$(K^T K)^{\frac{1}{2}}$

Using the notation $\text{diag}(x_1, x_2, \dots, x_n)$ for the diagonal matrix with elements x_i , we can suppose that

$$KK^T = U^T \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)U$$

for an orthogonal matrix U . Let us denote $(U)_{i,j}$ by $u_{i,j}$.

Lemma 11.1.

$$\left((KK^T)^{1/2}\right)_{i,j} = \sum_{l=1}^n \sqrt{\lambda_l} u_{l,i} u_{l,j}.$$

Proof. Using the above $KK^T = U^T \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)U$ gives

$$(KK^T)^{1/2} = U^T \text{diag}(\sqrt{\lambda_1}, \sqrt{\lambda_2}, \dots, \sqrt{\lambda_n})U,$$

meaning that

$$\left((KK^T)^{1/2}\right)_{i,j} = \sum_{l=1}^n \sqrt{\lambda_l} u_{l,i} u_{l,j}.$$

□

Theorem 11.2. *Let $T = (V, E)$ be a tree with a generic weight function $w : E \rightarrow \mathbb{R}_{\geq 0}$. Let u, v be two vertices of V being in the same part of the bipartition of T . Then*

$$\left(A_{T, \underline{w}}^+\right)_{u,v} \begin{cases} < 0 & \text{if } 4 \mid d(u, v) \text{ and } d(u, v) \neq 0, \\ > 0 & \text{if } 4 \nmid d(u, v) \text{ or } d(u, v) = 0. \end{cases}$$

Proof. If $d(u, v) = 0$, then $u = v$, so $\left(A_{T, \underline{w}}^+\right)_{u,u} = \sum_{l=1}^n \sqrt{\lambda_l} u_{l,i}^2 > 0$.

If $d(u, v) \neq 0$, then they represent different vertices. Let us apply Lemma 9.14, which gives that

$$\left(A_{T, \underline{w}}^+\right)_{u,v} = \left(\prod_{e \in P_{u,v}} w_e\right)^{1/2} \sum_{\lambda > 0} \lambda \frac{\mu_{\underline{w}}(T - P_{u,v}, \lambda)}{\mu'_{\underline{w}}(T, \lambda)}.$$

As all w_e is positive and we only want to know the sign of this formula, we can leave out the first part. This leaves us to calculate

$$\text{sgn} \left(\sum_{\lambda > 0} \lambda \frac{\mu_{\underline{w}}(T - P_{u,v}, \lambda)}{\mu'_{\underline{w}}(T, \lambda)} \right).$$

Now let $p(x) = x \mu_{\underline{w}}(T - P_{u,v}, x)$, its degree n_1 and let $q(x) = \mu_{\underline{w}}(T, x)$. Clearly, $n_1 = n - d(u, v)$. Observe that by Theorem 9.3 the polynomial $p(x)$ has only real zeros, and it is an even or odd polynomial, so it is in the form of $\sum_{j=0}^s (-1)^j a_{n_1-2j} x^{n_1-2j}$, where s is the size of the largest matching in $T - P_{u,v}$. Let us apply Lemma 10.3 and let t be the size of the largest matching in T . Observe that $n_1 - 2s \geq n - 2t$, otherwise the number of uncovered vertices by the largest matching would be smaller than $n - 2t$ as in $P_{u,v}$ there is a matching that covers all but at most one vertex. Since $u \neq v$ and they are in the same parts in the bipartition, we get that $n_1 \leq n - 2$. This means that all terms in the sum

$$\sum_{j=0}^s (-1)^j a_{n_1-2j} \sum_{\lambda > 0} \frac{\lambda^{n_1-2j}}{q'(\lambda)}$$

have the same sign, and this sign is $(-1)^{(n-n_1+2)/2} = (-1)^{d(u,v)/2-1}$ which is exactly the statement of the theorem.

□

Corollary 11.3. *Let $T = (V, E)$ be a tree. Let u, v be two vertices of V being in the same part of the bipartition of T . Then*

$$\left(A_T^+\right)_{u,v} \begin{cases} \leq 0 & \text{if } 4 \mid d(u, v) \text{ and } d(u, v) \neq 0, \\ \geq 0 & \text{if } 4 \nmid d(u, v) \text{ or } d(u, v) = 0. \end{cases}$$

Proof. This immediately follows from Theorem 11.2 and Lemma 9.9. Note that now we only have $\geq$ and $\leq$ in the statement. $\square$

Remark 11.4. We believe that the inequality is strict in Corollary 11.3.

We end this section with some applications.

Theorem 11.5. *Let G be a graph on n vertices. Suppose that it has a spanning tree T such that every edge of G not in T closes a cycle with T of length not divisible by 4. Then $s^+(G) \geq n - 1$. In particular, this holds if T has diameter at most 3.*

If it has a spanning tree T such that every edge of G not in the tree closes a cycle of length not in the form of $4k + 2$, then $s^-(G) \geq n - 1$.

Proof. We have

$$s^-(G) = \|A_G^-\|_F^2 = \|A_G - A_G^+\|_F^2 \leq \|A_G - A_T^+\|_F^2 = (A - A_T^+, A - A_T^+) = 2m + (n-1) - 2(A, A_T^+) \leq 2m - (n-1).$$

$$\text{Hence } s^+(G) = 2m - s^-(G) \geq n - 1.$$

The other inequality works the same way:

$$s^+(G) = \|A_G^+\|_F^2 = \|A + A_G^-\|_F^2 \leq \|A + A_T^-\|_F^2 = (A + A_T^-, A + A_T^-) = 2m + (n-1) + 2(A, A_T^-) \leq 2m - (n-1).$$

$$\text{Hence } s^-(G) = 2m - s^+(G) \geq n - 1.$$

$\square$

Theorem 11.6. *Let G be a graph without isolated vertices. Then $s^+(G) \geq \frac{n}{2}$.*

Proof. Let R be the subgraph of G with maximum number of edges that is a disjoint union of stars. Suppose that it has k edges. If G has no isolated vertices, then $k \geq \frac{n}{2}$ because we can choose R in such a way that it covers every vertex. Indeed, if v is not covered and $u \in N_G(v)$, then adding the edge (u, v) to R and if u was a leaf in a star with at least 2 edges, then by deleting the other incident to u from R we can achieve that the number of uncovered vertices in R is decreased by 1 without decreasing the number of edges in R . If R covers all vertices, then the number of its edges is at least $\frac{n}{2}$. Then

$$s^-(G) = \|A_G^-\|_F^2 = \|A_G - A_G^+\|_F^2 \leq \|A_G - A_R^+\|_F^2 = (A - A_R^+, A - A_R^+) = 2m + k - 2(A, A_R^+) \leq 2m - k.$$

$$\text{Hence } s^+(G) = 2m - s^-(G) \geq k \geq \frac{n}{2}.$$

$\square$

Remark 11.7. Clearly, we could have considered a forest R with all of its components having diameter at most 3, giving a better lower bound for $s^+(G)$ for general graphs.

12 Further results on square energy

Theorem 12.1. *Let G be a graph on n vertices. Then*

$$s^+(G) \leq s^+(K_n) = (n-1)^2.$$

Proof. Using the notation n_- for the number of negative eigenvalues, we have

$$s^+(G) = \sum_{\lambda > 0} \lambda^2 \leq \left(\sum_{\lambda > 0} \lambda \right)^2 = \left(\sum_{\lambda < 0} \lambda \right)^2 \leq n_- \left(\sum_{\lambda < 0} \lambda^2 \right) = n_- s^-(G) = n_- (2m - s^+(G)).$$

Whence

$$s^+(G) \leq \frac{n_-}{n_- + 1} 2m \leq \frac{n-1}{n} 2 \binom{n}{2} = (n-1)^2.$$

$\square$

Remark 12.2. The inequality $s^-(G) \leq \frac{n^2}{4}$ was proved in [7], similar to what follows. Suppose that $s^-(G) \geq \frac{n^2}{4}$, then

$$2m = s^+(G) + s^-(G) \geq \lambda_1^2 + s^-(G) \geq \frac{4m^2}{n^2} + s^-(G) \geq \frac{4m^2}{n^2} + \frac{n^2}{4}$$

Then we have $0 \geq (\frac{2m}{n} - \frac{n}{2})^2$. We add the following part, characterizing the graphs on n vertices for even n , which maximize $s^-(G)$.

Theorem 12.3. *We have*

$$s^-(G) \leq \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil,$$

with equality if and only if G is a triangle or G is isomorphic to the complete graph $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.

The above-mentioned proof from [7] implies, that the indirect $s^-(G) \geq \frac{n^2}{4}$ can hold only if there is equality, which implies that there is equality in all inequalities. This means, that $m = \frac{n^2}{4}$ and also that $\lambda_1 = \frac{2m}{n}$, the average degree. This implies that G is a regular graph with degree $\frac{n}{2}$. But $s^+(G) = \lambda_1^2 = m$ means that the only positive eigenvalue is λ_1 and $\lambda_1^2 = \sum_{\lambda_i < 0} \lambda_i^2$ holds. But together with $\lambda_1 = -\sum_{\lambda_i < 0} \lambda_i$, it implies that there exists only one summand, meaning that $\lambda_n = -\lambda_1$. As $\sum_{i=1}^n \lambda_i^k$ is the number of closed walks of length k and this is 0 for all odd k , it means that there are no odd cycles of odd length. The only regular bipartite graph with degree $\frac{n}{2}$ is the complete bipartite graph. This means, that for even n , exactly $K_{n,n}$ are the graphs, for which $s^-(G)$ is maximal.

When n is odd, it is much harder to prove which graphs have maximal $s^-(G)$ for a fixed number of vertices. Notice that for the graphs $K_{\frac{n+1}{2}, \frac{n-1}{2}}$ and for K_3 , we have $s^-(G) = \frac{n^2-1}{4}$. We state that $s^-(G)$ is maximal for exactly these graphs.

Proof. We have the chain

$$s^-(G) = \sum_{\lambda < 0} \lambda^2 \leq 2m - \lambda_1^2 \leq 2m - \frac{1}{n} \sum_{i=1}^n d_i^2 = \sum_{i=1}^n d_i - \frac{1}{n} \sum_{i=1}^n d_i^2 = \frac{1}{n} \sum_{i=1}^n d_i(n - d_i) \leq \frac{1}{n} \sum_{i=1}^n \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil = \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil.$$

We used the well-known inequality $\lambda_1^2 \geq \frac{1}{n} \sum_{i=1}^n d_i^2$, which can be proved by noticing that $\lambda_1^2 = \max_{x \neq 0} \frac{x^T A^2 x}{\|x\|^2} \geq \frac{1^T A^2 1}{\|1\|^2} = \frac{1}{n} \sum_{i=1}^n d_i^2$.

Equality implies that $\lambda_2 \leq 0$ and all degrees are either $\lfloor \frac{n}{2} \rfloor$ or $\lceil \frac{n}{2} \rceil$. Since $\lambda_2 \leq 0$, the graph has to be a complete multipartite graph. If there are t parts, where $t > 2$, then the largest degree is at least $\frac{t-1}{t}n \geq \frac{2}{3}n$. This is at most $\lceil \frac{n}{2} \rceil$ only if $n \leq 3$. If $t = 2$, then the degree condition implies that G is isomorphic to the complete graph $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$. The case $t = 1$ implies the case of K_n , in which only $n = 3$ has equality. $\square$

Corollary 12.4. *The complete bipartite graph has the following property: for fixed n , it has the most edges between graphs with $s^+ = s^-$ and only it has $m = \frac{n^2}{4}$. In other words, complete bipartite graphs maximize the number of edges between the graphs with $s^+ = s^-$.*

Proof. We know that $s^+ + s^- = 2m$, so $s^- = m$, which means that it is enough to maximize s^- . By Theorem 12.3, we know the maximum possible value of s^- is $\frac{n^2}{4}$, acquired only in the case of $K_{n,n}$, in which luckily $s^+ = s^-$ actually holds. $\square$

Remark 12.5. One could come up with the idea that the complete bipartite graph maximizes the product $s^+ s^-$ too, but it is actually not true. Two strongly regular counterexamples are $(10, 6, 3, 4)$ and $(16, 9, 4, 6)$. We do not have a formula for the maximum of $s^+ s^-$.

Theorem 12.6. *Let G be a graph on n vertices. Then $s^+(G) \gtrsim \frac{2m}{\sqrt{n}}$.*

Proof. We have

$$s^-(G) = 2m - s^+(G) = \|A^-\|_F^2 = \|A - A^+\|_F^2 \leq \|A - P\|_F^2,$$

where $P = \alpha(A + |\lambda_n| I)$ and I denotes the identity matrix. If $\alpha \geq 0$, then P is a positive semi-definite matrix. For $\alpha = \frac{2m}{2m + n|\lambda_n|}$, the formula $\|A - P\|_F^2$ reaches its minimum value, because $\|A - P\|_F^2 = n(\alpha|\lambda_n|)^2 + 2m(1 - \alpha)^2$.

This gives the minimum value

$$2m - s^+(G) \leq n \left(\frac{2m|\lambda_n|}{2m + n|\lambda_n|^2} \right)^2 + 2m \left(\frac{n|\lambda_n|}{2m + n|\lambda_n|^2} \right)^2 = \frac{2mn|\lambda_n|^2 (2m + n|\lambda_n|^2)}{(2m + n|\lambda_n|^2)^2} = \frac{2mn|\lambda|^2}{2m + n|\lambda_n|^2}.$$

Using this inequality $s^+(G) \geq \lambda_1^2 \geq |\lambda_n|^2$, we claim that $s^+(G) \geq \max \left(\lambda_n^2, \frac{4m^2}{2m + n|\lambda_n|^2} \right)$. The right-hand side reaches its minimum value as a function of $|\lambda_n|^2$ if the two values equal. Solving the quadratic polynomial gives $\lambda_n^2 = \frac{-2m + \sqrt{4m^2 + 16m^2n}}{2n}$, meaning $s^+(G) \gtrsim \frac{2m}{\sqrt{n}}$. $\square$

Theorem 12.7. *Let G be an arbitrary graph on n vertices. If G has $\frac{n}{3}$ vertex-disjoint triangles, then $s^+(G) \geq \frac{4}{3}n$.*

Proof. Let K_s be the complete graph on s vertices. Then $A_{K_s}^+ = \frac{s-1}{s}J$, where J denotes the matrix with all elements equal to 1. Now we calculate some scalar products which will be useful later in the proof. We know that $(A, A_{K_s}^+) = 2e(G \cap K_s) \frac{s-1}{s}$ and $(A_{K_s}^+, A_{K_s}^+) = (s-1)^2$. Also, let H be a disjoint union of t cliques with sizes s_i . Then $(A, A_H^+) = \sum_{i=1}^t 2e(G \cap K_{s_i}) \frac{s_i-1}{s_i}$. Using these, one gets the inequality chain

$$\begin{aligned} 2m - s^+(G) &= s^+(G) = \|A - A_G^+\|_F^2 \leq \|A - A_H^+\|_F^2 = (A, A) - 2(A, A_H) + (A_H^+, A_H^+) \\ &= 2m - \left(\sum_{i=1}^t 4e(G \cap K_{s_i}) \frac{s_i-1}{s_i} - \sum_{i=1}^t (s_i-1)^2 \right). \end{aligned}$$

This gives that $s^+(G) \geq \sum_{i=1}^t \left(4e(G \cap K_{s_i}) \frac{s_i-1}{s_i} - (s_i-1)^2 \right)$. If H is a subgraph of G , then this gives that $s^+(G) \geq \sum_{i=1}^t (s_i-1)^2$. In particular, if $s = 3$ and $t = \frac{n}{3}$, then $s^+(G) \geq \frac{4}{3}n$ and if $s = 2$ and $t = \frac{n}{2}$ (meaning if G has a perfect matching), then $s^+(G) \geq \frac{1}{2}n$. $\square$

Remark 12.8. If G has a perfect matching, then $\min(s^+(G), s^-(G)) \geq \frac{n}{2}$.

Proof. The inequality was proven for $s^+(G)$ earlier. For $s^-(G)$, we will use, that $A_H^- = A_H^+ - A_H$. This means that if H is a perfect matching, then

$$(A, A_H^-) = (A, A_H^+ - A_H) = (A, A_H^+) - (A, A_H) = \sum_{i=1}^t 2e(G \cap K_{s_i}) \frac{s_i-1}{s_i} - n = \frac{n}{2} - n = -\frac{n}{2}$$

Also

$$(A_H^-, A_H^-) = (A_H^+ - A_H, A_H^+ - A_H) = (A_H^+, A_H^+) - 2(A_H^+, A_H) + (A_H, A_H) = \frac{n}{2} - 2\frac{n}{2} + n = \frac{n}{2}$$

With these, we get

$$2m - s^-(G) = s^+(G) = \|A + A_G^-\|_F^2 \leq \|A + A_H^-\|_F^2 = (A, A) + 2(A, A_H^-) + (A_H^-, A_H^-) = 2m - 2\frac{n}{2} + \frac{n}{2} = 2m - \frac{n}{2}$$

This gives the desired $s^-(G) \geq \frac{n}{2}$. $\square$

Conjecture 12.9. Let G be a graph and H be a bipartite subgraph of G . Then $s^+(G) \geq s^+(H)$.

Remark 12.10. Conjecture 12.9 does not hold for s^- , as in Theorem 12.3 we saw that s^- is maximal for fixed n , only in the case of K_3 and $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.

Definition 12.11. A complex matrix A is Hermitian (or self-adjoint), if it is the conjugate transpose of itself, meaning that $A^* = A$. Let G be a graph with complex-valued edge weights. Let its adjacency matrix be

$$(A_G)_{i,j} = \begin{cases} w_e & \text{if } i < j \text{ and } (i,j) \in E, \\ \overline{w_e} & \text{if } i > j \text{ and } (i,j) \in E, \\ 0 & \text{if } (i,j) \notin E. \end{cases}$$

It is well-known not only for symmetric, but for Hermitian matrices too, that they have real eigenvalues. This means that the above-mentioned definitions can be extended for the complex-weighted case.

Conjecture 12.12. For every connected graph G on n vertices with unit-length complex edge-weights, we have

$$\min(s^+(G), s^-(G)) \geq n - 1.$$

Notice that Conjecture 12.12 is a generalization of Conjecture 1.1.

Theorem 12.13. For every complete graph G on n vertices with unit-length complex edge-weights, we have

$$\min(s^+(G), s^-(G)) \geq n - 1.$$

Proof. We know that $s^+(G) + s^-(G) = 2m = n(n-1)$, so it is enough to prove that $\max(s^+(G), s^-(G)) \leq (n-1)^2$. As we multiply A_G by -1 , the eigenvalues are also multiplied by -1 , so it is enough to prove that $s^+(G) \leq (n-1)^2$. Now we can tell the exact same proof as in Theorem 12.1. We have

$$s^+(G) = \sum_{\lambda > 0} \lambda^2 \leq \left(\sum_{\lambda > 0} \lambda \right)^2 = \left(\sum_{\lambda < 0} \lambda \right)^2 \leq n_- \left(\sum_{\lambda < 0} \lambda^2 \right) = n_- s^-(G) = n_- (2m - s^+(G)).$$

Whence

$$s^+(G) \leq \frac{n_-}{n_- + 1} 2m \leq \frac{n-1}{n} 2 \binom{n}{2} = (n-1)^2.$$

□

Remark 12.14. The equality case is not as simple as it was in Theorem 12.1. It is still immediate that we must have the eigenvalue $n-1$ with multiplicity 1 and the eigenvalue -1 with multiplicity $n-1$. Let an eigenvector corresponding to $n-1$ be v . Let v_1 be the coordinate with the largest absolute value. From $(n-1)v = Av$ we have $(n-1)v_1 = A_{11}v_1 + A_{12}v_2 + \dots + A_{1n}v_n$, and since $A_{11} = 0$ and $|A_{1j}| = 1$ for $2 \leq j \leq n$, by the triangle inequality we get $(n-1)|v_1| \leq |A_{12}| \cdot |v_2| + \dots + |A_{1n}| \cdot |v_n| = |v_2| + \dots + |v_n| \leq (n-1)|v_1|$ which implies that there is equality everywhere. This means that the length of each coordinate of v must be the same, let it be 1. From the equality case of the triangle-inequality, we have for all $j \neq k$ that $v_j = v_k A_{jk}$ and similarly $v_k = v_j A_{kj}$, so $A_{jk} A_{kj} = 1$. As $A_{jk} = \overline{A_{kj}}$, this implies that A_{jk} must be ± 1 or $\pm i$. So if we fix $v_1 = 1$, then the other coordinates can only be ± 1 or $\pm i$. Notice that for each vector v of this type, there is exactly one matrix of the above type, with v being the eigenvector of the eigenvalue $n-1$. From this and the $v_j = v_k A_{jk}$ type equations, we get that $s^+(G) = (n-1)^2$ if and only if the rows/columns of A_G are ± 1 or $\pm i$ multiples of each other (excluding the 0 elements on the diagonal).

Remark 12.15. One should notice that in the above characterization, for a diagonal matrix D , the matrices A and DAD^{-1} have the same eigenvalues. This is the same as multiplying rows of the matrices by ± 1 or $\pm i$, which is the same as multiplying the edge-weights on graph-cuts by ± 1 or $\pm i$. This relation between the matrices (or graphs) is of course an equivalence-relation.

13 Every tree is a subgraph of a tree, which has eigenvalues only with multiplicity 1

Theorem 13.1. Let T be a tree graph, with strictly positive weight-function $\underline{w}$. Then there is a tree T' such that T is a subgraph of T' and all the eigenvalues of T' have multiplicity 1.

Proof. Let the weights of the edges in T be w_i , where $w_i = w_j$ might hold for some $i \neq j$. Order the weights such that for all k , the union of the edges represented by the first k weights is a connected graph. We will present a sufficient T' graph with 2^n vertices recursively. At first, take a simple edge with weight w_1 . Now for every existing vertex (2 at the moment), append an edge with weight w_2 . Now for every existing vertex (4 at the moment), append an edge with weight w_3 , and so on. In the i -th step, for all the 2^{i-1} vertices, we append an edge with weight w_i . Call these steps *appending steps*.

We can see that T is indeed a subgraph of T' , as for all i , we can choose (recursively) a proper edge with weight w_i , such that the union of these i edges is a connected subgraph of T .

Now we will prove that all the eigenvalues of T' have multiplicity 1 and also neither of the eigenvalues, nor any of the coordinates of eigenvectors are 0. We prove this by induction on the number of steps: for $i = 1, 2$, the statement is true. Now suppose that the statement is true for k -th steps and we want to prove for the $k+1$ -th step. Let G_i be the graph after i steps. As all tree graphs are bipartite graphs, we can suppose that the eigenvalues of G_k are $\pm\lambda_i$ for $i = 1, 2, \dots, 2^{k-1}$, where $\lambda_i > 0$. Now we calculate the exact eigenvalues of G_{k+1} , if the appended edges have weight w_{k+1} . Actually we state that the eigenvectors for G_{k+1} will be the same restricted to G_k as the eigenvectors of G_k themselves. Let the value of an eigenvector on a new vertex be u' , the value of its neighbour u , let μ be an eigenvalue of G_{k+1} and λ be a $\pm\lambda_i$. Then we know for the new vertex that

$$\mu u' = w_{k+1}u,$$

while for the old vertex we have

$$\mu u = \lambda u + w_{k+1}u'.$$

Since μ cannot be zero as $\lambda \neq 0$, we get from the first equation that $u' = \frac{w_{k+1}u}{\mu}$. Substituting this into the second equation gives $\mu u = \lambda u + w_{k+1} \frac{w_{k+1}u}{\mu}$. Multiplying both sides by the nonzero μ gives $\mu^2 u = \lambda \mu u + w_{k+1}^2 u$. Subtracting the right-hand side and dividing by the nonzero u gives $\mu^2 - \lambda \mu - w_{k+1}^2 = 0$. Solving this quadratic equation gives

$$\mu_{1,2} = \frac{\lambda \pm \sqrt{\lambda^2 + 4w_{k+1}^2}}{2}$$

Now it is sufficient to prove that for a pair of positive λ_1 and λ_2 , we cannot have

$$\frac{\pm\lambda_1 \pm \sqrt{\lambda_1^2 + 4w_{k+1}^2}}{2} = \frac{\pm\lambda_2 \pm \sqrt{\lambda_2^2 + 4w_{k+1}^2}}{2}$$

in any of the cases. If the signs are the same in both options, then it is enough to have that the derivative

$$\left(\frac{\pm\lambda \pm \sqrt{\lambda^2 + 4w_{k+1}^2}}{2} \right)' = \frac{1}{2} \left(\pm 1 \pm \frac{\lambda}{\sqrt{\lambda^2 + 4w_{k+1}^2}} \right)$$

is never 0. But it could be equal to 0 only if $4w_{k+1}^2 = 0$, which cannot happen. Also from this, we know that $\lambda < \sqrt{\lambda^2 + 4w_{k+1}^2}$ is always true, meaning that the only possibility left is

$$\frac{+\lambda_1 + \sqrt{\lambda_1^2 + 4w_{k+1}^2}}{2} = \frac{-\lambda_2 + \sqrt{\lambda_2^2 + 4w_{k+1}^2}}{2}$$

(or its reversed or negated version). But this also cannot happen, as the only solution would be $\lambda_1 = -\lambda_2$, but we supposed that they are positive. So the desired condition holds for every case, meaning that we finished the proof. $\square$

Corollary 13.2. *Let n be fixed, and let $w_1, w_2, \dots, w_{n-1}$ be fixed edge-weights. Then there exists a tree T' , which has eigenvalues only with multiplicity 1 and all the trees which has n vertices and edge-weights $w_1, w_2, \dots, w_{n-1}$, are subgraphs of T' .*

Proof. Take the shortest sequence S of elements w_i , such that it contains all possible permutations as a subsequence. In [16], it is proved that S has length at most $n^2 - 2n + 4$. We do the recursion above, for this sequence of length (at most) $n^2 - 2n + 4$. The eigenvalues of the graph have multiplicity 1, as the construction is the same. The only difference is that now we do the appending step more than only $n - 1$ times. Also this graph has all n -vertex, w_i weighted trees as a subgraph, because for every tree, its connected weight order is also represented in the graph, as every permutation is a subsequence of S . $\square$

Corollary 13.3. *Let T be a tree graph, with edge-weights only 1. It is true that there is a tree T' such that T is a subgraph of T' , every edge weight of T' is 1, and all the eigenvalues of T' have multiplicity 1.*

Proof. In the construction above, we only used edge-weights which are also present in T . In this case, for T' we only use weights equal to 1. $\square$

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¹Page of the REU 2023 Program: <https://coge.elte.hu/reu23.html>

Extremal spectral graph theory

Own results

Dániel Hegedűs
hegedani1226@gmail.com

Áron Jánosik
aron@janosik.hu

József Oszténi
osztényi2003@gmail.com

Supervisor: Péter Csikvári
peter.csikvari@gmail.com

Below, we list the lemmas and theorems which are our results, as well as our conjectures. It should be noted that we participated together in the REU program, so it would be meaningless to partition the results into different parts for the different participants.

- We found a new set of graphs for which the conjecture $\lambda_3 \leq \frac{n}{3} - 1$ has equality.
- We proved that $\min(\lambda_k, \lambda'_k) \leq \frac{n}{\sqrt{4k-2}}$, where λ'_k denotes the k -th largest eigenvalue of G^c .
- We gave a new, simple proof for the statement $\lambda_2 \leq \frac{n}{2} - 1$ and characterized the graphs with equality.
- We proved for all k that $\lambda_1 - \lambda_k$ can be arbitrarily close to 0 (when n is not fixed) and also proved that this does not hold for $\lambda_1 - \lambda_{\frac{n}{2}}$.
- We proved that the ratio $\frac{s^-}{s^+}$ can be arbitrarily large (for not fixed n).
- We determined the sign of $s^+ - s^-$ in the case of Kneser(n, k) graphs as a function of n, k .
- We collected various properties with (partially original) proofs of the matching polynomial, which we used as a tool.
- We determined the sign of elements in A_T^+ for tree graphs T .
- We determined the maximal possible values of s^+ and s^- for fixed n and characterized the graphs with equality.
- We proved that if a graph has a spanning tree T such that every edge of G not in T closes a cycle with T of length not divisible by 4, then $s^+(G) \geq n - 1$. In particular, it is true if T has diameter at most 3.
- We proved that $s^+ \geq \frac{n}{2}$ for graphs without isolated vertices and also for graphs with a perfect matching.
- We proved that $s^+ \geq \frac{4}{3}n$ for graphs with $\frac{n}{3}$ vertex-disjoint triangles.
- We proved the asymptotic inequality $s^+(G) \gtrsim \frac{2m}{\sqrt{n}}$.
- We conjectured that the generalization of $\min(s^+, s^-)$ is true in the case of complex-weighted graphs. We proved it for complete graphs, and also characterized the complete graphs which have equality.
- We conjectured that if H is a bipartite subgraph of G , then $s^+(H) \leq s^+(G)$.
- We proved that every tree is a subgraph of a tree, which has eigenvalues only with multiplicity 1.

Extremális spektrál-gráfelmélet

Összefoglalás

Hegedűs Dániel
hegedani1226@gmail.com

Jánosik Áron
aron@janosik.hu

Osztenyi József
osztényi2003@gmail.com

Témavezető: Csikvári Péter
peter.csikvari@gmail.com

Bevezetés

A sajátértékek vizsgálata a lineáris algebra egyik legfontosabb eszköze, amelyet a számítástudományban, fizikában és kémiában is széleskörűen alkalmaznak. A spektrál-gráfelmélet a gráfok szomszédsági mátrixainak sajátértékeit vizsgálja. Kutatásunk során irányítatlan, hurokél és többszörös él nélküli gráfokkal foglalkoztunk.

Egy $G = (V, E)$ gráf A_G szomszédsági mátrixa az az $n \times n$ -es mátrix, ahol n a gráf csúcsainak száma, amire

$$(A_G)_{i,j} = \begin{cases} 1 & , \text{ ha } (i, j) \in E, \\ 0 & , \text{ ha } (i, j) \notin E. \end{cases}$$

Azt mondjuk, hogy a λ komplex szám az A mátrix sajátértéke a hozzá tartozó $v \neq 0$ sajátvektorral, ha $Av = \lambda v$. A főtengety-tétel miatt tudjuk, hogy a szimmetrikus valós mátrixok sajátértékei valós számok, emiatt a továbbiakban a sajátértékeket a következő módon jelölhetjük: $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$.

A pozitív, illetve a negatív sajátértékek négyzetösszegére rendre az $s^+(G)$ és $s^-(G)$ jelölést és a pozitív és negatív négyzetes energia elnevezést használjuk. Az egyik fő sejtés a következő:

Sejtés (Elphick, Farber, Goldberg, Wocjan). Minden összefüggő n csúcsú G gráfra

$$\min(s^+(G), s^-(G)) \geq n - 1.$$

Kutatásunk során főként két problémára összpontosítottunk: λ_k értékének becslése, valamint $s^+(G)$ és $s^-(G)$ kiszámítása és becslése.

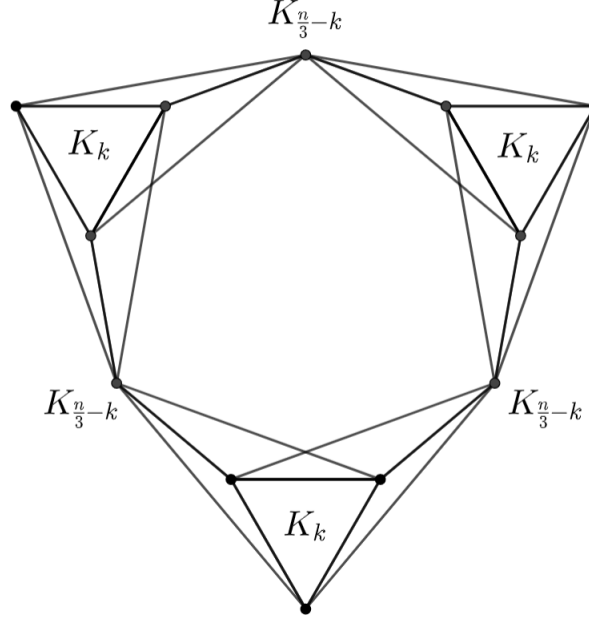
A második és a harmadik legnagyobb sajátérték

Egy híres sejtés szerint $\lambda_k \leq \frac{n}{k} - 1$ minden gráf esetén teljesül. Sajnos ez $k \geq 4$ esetén nem igaz, de $k = 2$ -re igen, és a $k = 3$ esetben pedig megoldatlan. Az alábbi lemma kimond λ_k -ra vonatkozó ekvivalens állításokat:

Lemma. A következő három állítás ekvivalens:

- $\lambda_k \leq \frac{n}{k} - 1$ minden gráfra teljesül,
- $\lambda_k \leq \lfloor \frac{n}{k} \rfloor$ minden gráfra teljesül,
- $\lambda_k \leq \frac{n}{k}$ minden gráfra teljesül.

Ezen kívül kutatásunk során találtunk egy új gráfosztályt, amelyben a harmadik legnagyobb sajátértékre a sejtésben egyenlőség áll fenn, azaz $\lambda_3 = \frac{n}{3} - 1$. Legyen $3|n$ és $0 < k < \frac{n}{3}$ tetszőleges. A gráf hat csúcsdiszjunkt teljes gráf unióját tartalmazza, három k csúcsú és három $\frac{n}{3} - k$ csúcsú teljes gráfot, amelyek egy kör mentén felváltva helyezkednek el, és a szomszédos teljes gráfok között minden él be van húzva.



1. Ábra. Egy példa a konstrukcióra $n = 12$ és $k = 3$ paraméterekkel.

Ezek mellett megmutattuk, hogy minden gráfra a gráfnak vagy a komplementerének harmadik legnagyobb sajátértéke legfeljebb $\frac{n}{\sqrt{10}}$.

A $\lambda_2 \leq \frac{n}{2} - 1$ állítás már ismert volt, de mi adtunk egy új, az eddiginél egyszerűbb bizonyítást (nem feltétlenül összefüggő gráfokra). A bizonyításból az egyenlőség esetét is levezettük.

Kapcsolat λ_1 és a többi sajátérték között

Vizsgáltuk λ_1 és a gráf többi sajátértéke közötti távolságot. Beláttuk az alábbi tételt:

Tétel. Bármely fix $k > 1$ esetén a $0 \leq \lambda_1 - \lambda_k$ különbség tetszőlegesen közel lehet 0-hoz, még összefüggő gráfok esetén is.

Ennek igazolásához a $G_{n,k}$ gráfsorozatot a következőképpen definiáltuk (fix k -ra): vegyünk k csúcsdiszjunkt K_n gráfot, és válasszunk ki egy tetszőleges csúcsot, v -t. Húzzunk be v -ből minden tőle diszjunkt K_n -hez egy-egy élt (ezzel $k - 1$ élt hozzáadva a gráfhoz). Ekkor ha n -nel tartunk a végtelenbe, akkor a $\lambda_1 - \lambda_k$ különbség 0-hoz tart. Beláttuk továbbá az alábbi tételt is arra az esetre, amikor az index függ n -től:

Tétel. A $\lambda_1 - \lambda_{\frac{n}{2}}$ különbség nem lehet tetszőlegesen közel 0-hoz összefüggő gráfok esetén.

Pozitív és negatív négyzetes energiák konkrét gráfokra

Számítógépes programmal tesztelve azt láttuk, hogy $s^+(G)$ általában nagyobb, mint $s^-(G)$. Ezzel szemben megmutattuk, hogy az $\frac{s^-(G)}{s^+(G)}$ arány tetszőlegesen nagy lehet. Erre a példánk a következő gráfcsoport volt: G_q legyen az az erősen reguláris gráf, aminek paraméterei $((q^2 + 1)(q^5 + 1), q^5 + q^2, q^2 - 1, q^3 + 1)$.

Emellett beláttuk a Kneser-gráfokra az alábbi tételt:

Tétel. A $Kneser(n, k)$ gráfra ha $k \leq \frac{n}{4}$, akkor $s^-(G) < s^+(G)$. Továbbá ha $k > \frac{n}{4}$, akkor ha n páros, akkor $s^-(G) = s^+(G)$, míg ha $n \equiv 1 \pmod{4}$, akkor $s^-(G) > s^+(G)$, míg ha $n \equiv 3 \pmod{4}$, akkor $s^-(G) < s^+(G)$.

További eredmények pozitív és negatív négyzetes energiákkal

Foglalkoztunk a súlyozott párosítási polinommal, ahol fontos kiemelni, hogy fagráf esetén a szomszédsági mátrix karakterisztikus polinomja megegyezik a párosítási polinommal. Ezt a szomszédsági mátrix $A = A^+ - A^-$ pozitív szemidefinit felbontásánál alkalmaztuk, azon belül is T fa esetén az A_T^+ elemeinek meghatározásában. Beláttuk az alábbi tételt:

Tétel. Legyen $T = (V, E)$ egy fa tetszőleges $w : E \rightarrow \mathbb{R}_{\geq 0}$ súlyfüggvénnyel. Legyen u és v a gráf két csúcsa, amelyek T ugyanazon osztályában vannak. Ekkor

$$\left(A_{T,w}^+\right)_{u,v} \begin{cases} \leq 0 & \text{ha } 4 \mid d(u,v) \text{ és } d(u,v) \neq 0, \\ \geq 0 & \text{ha } 4 \nmid d(u,v) \text{ vagy } d(u,v) = 0. \end{cases}$$

Ennek alkalmazásával bebizonyítottuk a fő sejtést a gráfoknak egy csoportjára:

Tétel. Legyen G egy n csúcsú gráf. Tegyük fel, hogy van egy olyan T feszítőfája, hogy minden G -beli, de nem T -beli él olyan kört zár be T -vel, aminek a hossza nem osztható 4-gyel. Ekkor $s^+(G) \geq n-1$. Speciálisan a fő sejtés s^+ -ra igaz, ha T átmérője legfeljebb 3. Továbbá ha olyan T feszítőfája van, hogy minden G -beli, de nem T -beli él olyan kört zár be T -vel, aminek a hossza nem $4k+2$ alakú, akkor $s^-(G) \geq n-1$.

Továbbá ennek alkalmazásával beláttuk az alábbi, nem csak összefüggő gráfokra vonatkozó tételt:

Tétel. Legyen G egy gráf izolált csúcsok nélkül. Ekkor $s^+(G) \geq \frac{n}{2}$.

Megvizsgáltuk fix n -re az s^+ és s^- legnagyobb lehetséges értékeit:

Tétel. Minden gráfra

$$s^+(G) \leq (n-1)^2,$$

ahol egyenlőség pontosan akkor áll fenn, ha G a K_n teljes gráf. Továbbá minden gráfra

$$s^-(G) \leq \left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil,$$

ahol egyenlőség pontosan akkor áll fenn, ha G háromszög vagy G a $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ teljes páros gráf.

Beláttunk egy, az élek számától függő becslést s^+ -ra, miszerint:

Tétel. Legyen G egy n csúcsú gráf. Ekkor $s^+(G) \gtrsim \frac{2m}{\sqrt{n}}$.

Diszjunkt klikkekkel való fedéssel beláttunk két másik, nem csak összefüggő gráfokra vonatkozó tételt is:

Tétel. Legyen G egy tetszőleges n csúcsú gráf. Ha G -ben van $\frac{n}{3}$ páronként csúcsdiszjunkt háromszög, akkor $s^+(G) \geq \frac{4}{3}n$.

Tétel. Ha G -ben van teljes párosítás, akkor $\min(s^+(G), s^-(G)) \geq \frac{n}{2}$.

Megfogalmaztuk a fő sejtés komplex általánosítását, ahogy a főtengety-tétel Hermit-mátrixokra is garantálja a sajátértékek valóságát:

Sejtés. Minden összefüggő n csúcsú G gráfra, aminek élei egység hosszú komplex számokkal vannak súlyozva, arra

$$\min(s^+(G), s^-(G)) \geq n-1.$$

Beláttuk a sejtést súlyozott teljes gráfokra és karakterizáltuk azokat a teljes gráfokat, amikre egyenlőség áll fenn.

Beláttuk, hogy minden fa az részfa egy olyan fában, aminek sajátértékei egyszeres multiplicitásúak.