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Graph Polynomials and Graph Transformations in Algebraic Graph Theory

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To the memory of Gács András

Contents

Chapter 1

Introduction

In the center of this thesis graph polynomials and graph transformations stand, their role in algebraic and extremal graph theory. In the first half of this thesis we give a survey about the use of two special graph transformations on algebraically defined graph parameters and its consequences in extremal algebraic graph theoretic problems. In the second half of this thesis we study a purely extremal graph theoretic problem which turned out to be connected to algebraic graph theory in many ways, even its by-product provided an elegant solution to a longstanding open problem in algebraic graph theory.

The use of graph transformations in extremal graph theory has a long history. The application of Zykov's symmetrisation provided a very simple proof not only to Turán's theorem, but to several other problems. The situation is a bit different if one considers algebraic graph theoretic problems. The use of graph transformations is not as widespread due to the fact that it is not always easy to handle the change of the algebraic parameter at graph transformations. In this thesis I survey two graph transformations which turned out to be extremely powerful in several extremal algebraic graph theoretic problem.

The first transformation was defined by Alexander Kelmans and we will call it Kelmans transformation. Kelmans used it in his research on network reliability. Only very recently it turned out that this transformation can be applied to a wide range of problems. The Kelmans transformation increases the spectral radius of the adjacency matrix and this was a key observation to attain a breakthrough in Eva Nosal's problem of estimating

$$\mu(G) + \mu(\overline{G}),$$

where $\mu(G)$ and $\mu(\overline{G})$ denote the spectral radius of a graph G and its complement. The success of the Kelmans transformation in this problem was the motivation to study systematically this transformation.

The second transformation is the generalized tree shift. Strongly motivated by the Kelmans transformation I defined it to attack a problem of Vladimir Nikiforov on the number of closed walks of trees. Nikiforov conjectured that for any fixed ℓ the star has the maximum number, the path has the minimum number, of closed walks of length ℓ among the trees on fixed number of vertices. While the Kelmans transformation was applicable to prove the extremality of the star, it failed to attack the extremality of the path. The generalized tree shift was defined so as to overcome the weakness of the Kelmans transformation. The generalized tree shift did it so successfully that it became much more powerful than I expected originally. The generalized tree shift increases not only the number of closed walks of length ℓ, but the spectral radius of the adjacency matrix and the Laplacian matrix, the coefficients of several graph polynomials including the characteristic polynomial of the adjacency matrix and Laplacian matrix and the independence polynomial.

In the second half of the thesis we study an extremal graph theoretic problem, the so-called "density Turán problem". The problem asks for the critical edge density which ensures that a graph appears as a subgraph in its blown-up graph. At first sight the problem has no connection with algebraic graph theory. Only when one starts to study the case of trees, it turns out that the critical edge density can be expressed in terms of the spectral radius of the adjacency matrix of the tree. For a general graph G, this connection is more involved, the critical edge density is related to the spectral radius of the so-called monotone-path tree of the graph G. This relationship lead to the construction of integral trees, trees whose spectrum of the adjacency matrix entirely consists of integers. More precisely, it turned out that among the monotone-path trees of complete bipartite graphs one can easily find integral trees of arbitrarily large diameters. The existence of such trees was a longstanding open problem in algebraic graph theory.

Notation and basic definitions

We will follow the usual notation: G is a simple graph, $V(G)$ is the set of its vertices, $E(G)$ is the set of its edges. In general, $|V(G)| = n$ and $|E(G)| = e(G) = m$. We will use the notation $N(x)$ for the set of the neighbors of the vertex x, $|N(v_i)| = \deg(v_i) = d_i$ denote the degree of the vertex v_i. We will also use the notation $N[v]$ for the closed neighborhood $N(v) \cup \{v\}$. The complement of the graph G will be denoted by $\overline{G}$.

Special graphs. K_n will denote the complete graph on n vertices, meanwhile $K_{n,m}$ denotes the complete bipartite graph with color classes of size n and m. Let P_n and S_n denote the path and the star on n vertices, respectively. We also use the notation xPy for the path with endvertices x and y. C_n denotes the cycle on n vertices.

Special sets. $\mathcal{I}$ denotes the set of independent sets. $\mathcal{M}$ denotes the set of matchings (independent edges), $\mathcal{M}_r$ denotes the set of matchings of size r. Let $\mathcal{P}(S)$ denote the set of partitions of the set S, $\mathcal{P}_k(S)$ denotes the set of partitions of the set S into exactly k sets. If the set S is clear from the context then we simply write $\mathcal{P}_k$.

Special graph transformations. For $S \subset V(G)$ the graph $G - S$ denotes the subgraph of G induced by the vertex set $V(G)\backslash S$. If $S = \{v\}$ then we will use the notation $G - v$ and $G - \{v\}$ as well. If $e \in E(G)$ then $G - e$ denotes the graph with vertex set $V(G)$ and edge set $E(G)\backslash\{e\}$. We also use the notation G/e for the graph obtained from G by contracting the edge e; clearly, the resulting graph is a multigraph.

Let M_1 and M_2 be two graphs with distinguished vertices u_1, u_2 of M_1 and M_2, respectively. Let $M_1 : M_2$ be the graph obtained from M_1, M_2 by identifying the vertices of u_1 and u_2. So $|V(M_1 : M_2)| = |V(M_1)| + |V(M_2)| - 1$ and $E(M_1 : M_2) = E(M_1) \cup E(M_2)$. Note that this operation depends on the vertices u_1, u_2, but in general, we do not indicate it in the notation. Sometimes to avoid confusion we use the notation $(M_1|u_1) : (M_2|u_2)$.

Matrices and polynomials of graphs. The matrix $A(G)$ will denote the adjacency matrix of the graph G, i.e., $A(G)_{ij}$ is the number of edges going between the vertices v_i and v_j. Since $A(G)$ is symmetric, its eigenvalues are real and we will denote them by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$. We will also use the notation $\mu(G)$ for the largest eigenvalue and we will call it the spectral radius of the graph G. The characteristic polynomial of the adjacency matrix will be denoted by

$$\phi(G, x) = \det(xI - A(G)) = \prod_{i=1}^{n}(x - \mu_i).$$

We will simply call it the adjacency polynomial.

The Laplacian matrix of G is $L(G) = D(G) - A(G)$ where $D(G)$ is the diagonal matrix for which $D(G)_{ii} = d_i$, the degree of the vertex v_i. The matrix $L(G)$ is symmetric, positive semidefinite, so its eigenvalues are real and non-negative, the smallest one is 0; we will denote them by $\lambda_1 \geq \lambda_2 \geq \dots \lambda_{n-1} \geq \lambda_n = 0$. We will also use the notation $\lambda_{n-1}(G) = a(G)$ for the so-called algebraic connectivity of the graph G. We introduce the notation $\theta(G)$ for the Laplacian spectral radius $\lambda_1(G)$. The characteristic polynomial of the Laplacian matrix will be denoted by

$$L(G, x) = \det(xI - L(G)) = \prod_{i=1}^{n}(x - \lambda_i).$$

We will simply call it the Laplacian polynomial.

We mention here that $\tau(G)$ will denote the number of spanning trees of the graph G.

Let $m_r(G)$ denote the number of set of independent edges of size r (i.e., the r-matchings) in the graph G. We define the matching polynomial of G as

$$M(G, x) = \sum_{r=0}(-1)^r m_r(G) x^{n-2r}.$$

The roots of this polynomial are real, and we will denote the largest root by $t(G)$.

Let $i_k(G)$ denotes the number of independent sets of size k. The independence polynomial of the graph G is defined as

$$I(G, x) = \sum_{k=0}^{n}(-1)^k i_k(G) x^k.$$

Let $\beta(G)$ denote the smallest real root of $I(G,x)$; it exists and it is positive because of the alternating sign of the coefficients of the polynomial.

Let $ch(G,\lambda)$ be the chromatic polynomial of G; so for a positive integer λ the value $ch(G,\lambda)$ is the number of ways that G can be well-colored with λ colors. It is indeed a polynomial in λ and it can be written in the form

$$ch(G,x)=\sum_{k=1}^{n}(-1)^{n-k}c_k(G)x^k,$$

where $c_k(G)\geq 0$.

If the polynomial $P(G,x)$ has the form

$$P(G,x)=\sum_{k=0}^{n}(-1)^{n-k}s_k(G)x^k,$$

where $s_k(G)\geq 0$, then $\widehat{P}(G,x)$ denote the polynomial

$$\widehat{P}(G,x)=(-1)^n P(G,-x)=\sum_{k=0}^{n}s_k(G)x^k.$$

For polynomials P_1 and P_2 we will write $P_1(x)\gg P_2(x)$ if they have the same degree and the absolute value of the coefficient of x^k in $P_1(x)$ is at least as large as the absolute value of the coefficient of x^k in $P_2(x)$ for all $0\leq k\leq n$.

How to read this thesis?

In this section I would like to call attention to the Appendix which can be found at the end of this thesis. It contains the required background. I propose to take a look at the statements of the Appendix without reading the proofs before one starts to read this thesis. Whenever I invoke a result from the Appendix, I copy the required statement into the text (sometimes with a slight modification in order to make it more clear how we wish to use it in the present situation). I hope this way one can read this thesis more easily.

Acknowledgment

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I am certainly aware that I owe a lot to many peoples not listed here. I ask them to accept my gratitude and also my apology for my laziness at the same time.

Chapter 2

Applications of the Kelmans transformation

In [43] Kelmans studied the following problem. Let $R_q^k(G)$ be the probability that if we remove the edges of the graph G with probability q, independently of each other, then the obtained random graph has at most k components. He obtained many results on extremal values of the parameter $R_q^k(.)$ and on comparing graphs according to this parameter. One of his results was that a certain transformation increases this probability for every q. The study of this transformation (or more precisely its inverse), which we will call Kelmans transformation, will be the main topic of this chapter.

Definition 2.0.1. Let u, v be two vertices of the graph G, we obtain the Kelmans transformation of G as follows: we erase all edges between v and $N(v)\backslash(N(u)\cup\{u\})$ and add all edges between u and $N(v)\backslash(N(u)\cup\{u\})$. Let us call u and v the *beneficiary* and the *co-beneficiary* of the transformation, respectively. The obtained graph has the same number of edges as G; in general we will denote it by G' without referring to the vertices u and v.

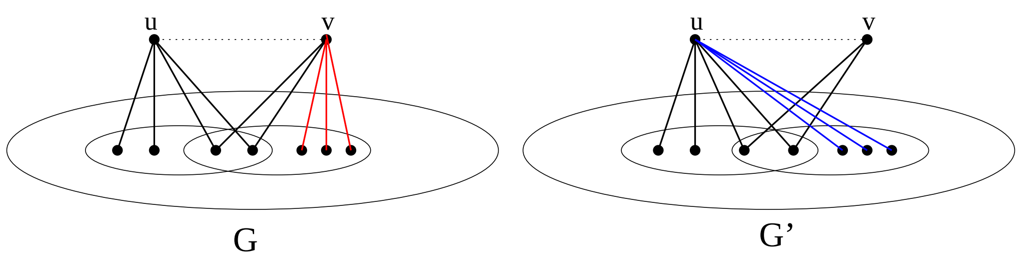

Figure 2.1: The Kelmans transformation.

The original application of the Kelmans transformation was the following (see Theorem 3.2 of [43]). We note that we use our notation.

Theorem 2.0.2. [43] *Let G be a graph and G' be a graph obtained from G by a Kelmans transformation. Then $R_q^k(G) \geq R_q^k(G')$ for every $q \in (0,1)$.*

Satyanarayana, Schoppmann and Suffel [59] rediscovered Theorem 2.0.2, they called the inverse of the Kelmans transformation "swing surgery". They also proved the following theorem which we will also use and prove.

Theorem 2.7.3. [59] *Let G be a graph and G' be a graph obtained from G by a Kelmans transformation. Let $\tau(G)$ and $\tau(G')$ be the number of spanning trees of the graph G and G', respectively. Then $\tau(G') \leq \tau(G)$.*

Brown, Colbourn and Devitt [10] studied the Kelmans transformation further in the context of network reliability. They also extended it to multigraphs. We will primarily concern with simple graphs, but we show that the Kelmans transformation can be applied efficiently in a much wider range of problems.

⋆ ⋆ ⋆

We end this introductory part by some simple observations which are crucial in many applications.

Remark 2.0.3. *The $\{u, v\}$-independence and the Nordhaus-Gaddum property of the Kelmans transformation.* The key observation is that up to isomorphism G' is independent of u or v being the beneficiary or the co-beneficiary if we apply the transformation to u and v. Indeed, in G' one of u or v will be adjacent to $N_G(u) \cup N_G(v)$, the other will be adjacent to $N_G(u) \cap N_G(v)$ (and if the two vertices are adjacent in G then they will remain adjacent, too). This observation also implies that the Kelmans transformation is also a Kelmans transformation to the complement of the graph G with the change of the role of u and v.

This means that whenever we prove that the Kelmans transformation increases some parameter $p(G)$, i.e., $p(G') \geq p(G)$ then we immediately obtain that $p(\overline{G'}) \geq p(\overline{G})$ as well. This observation will be particularly fruitful in those problems where one considers a graph and its complement together like in Nosal's problem.

2.1 Threshold graphs of the Kelmans transformation

Now we determine the threshold graphs of this transformation. Let us say that u dominates v if $N(v)\backslash\{u\} \subseteq N(u)\backslash\{v\}$. Clearly, if we apply the Kelmans transformation to a graph G and u and v such that u is the beneficiary then u will dominate v in G'. If neither u dominates v, nor v dominates u we say that u and v are incomparable; in this case we call the Kelmans transformation applied to u and v proper.

Theorem 2.1.1. *(a) By the application of a sequence of Kelmans transformation one can always transform an arbitrary graph G to a graph G_{tr} in which the vertices can be ordered so that whenever $i < j$ then v_i dominates v_j.*

(b) Furthermore, one can assume that G_{tr} has exactly the same number of components as G. (Note that all but one component of a threshold graph G_{tr} are isolated vertices.)

Proof. (a) Let $d_1(G) \geq d_2(G) \geq \cdots \geq d_n(G)$ be the degree sequence of the graph G. One can define a lexicographic ordering: let us say that $G_1 \succ G_2$ if for some k we have $d_k(G_1) > d_k(G_2)$ and $d_i(G_1) = d_i(G_2)$ for $1 \leq i \leq k-1$. Those graphs which have the same degree sequence cannot be distinguished by this ordering, but this will not be a problem for us.

Now let us choose the graph G^* which can be obtained by some application of Kelmans transformation from G and in the lexicographic ordering is one of the best among these graphs. We show that this graph has the desired property. Indeed, if $\deg_{G^*}(v_i) \geq \deg_{G^*}(v_j)$, but v_i does not dominate v_j then one can apply a Kelmans transformation to G^* and v_i and v_j, where v_i is the beneficiary; then in the obtained graph the degree of v_i is strictly greater than $\deg(v_i)$, thus the obtained graph is better in the lexicographic ordering than G^* contradicting the choice of G^*.

(b) Let $H_1, H_2, \dots, H_k$ be the connected components of G and let us choose vertices $u_i \in V(H_i)$. Now let us apply a Kelmans transformation to u_1 and u_i $(2 \leq i \leq k)$ such that u_1 is the beneficiary in each case. Then the resulting graph has one giant component and $k-1$ isolated vertices, namely $u_2, \dots u_k$. Thus it is enough to prove the statement if G is connected. We will slightly modify the proof of part (a).

First of all, let us observe that if we obtained G' by a Kelmans transformation applied to the connected graph G and vertices u and v such that u was the beneficiary, then $G' - \{v\}$ is necessarily connected; indeed, if there was a walk between $x_1, x_2 \in V(G) - \{v\}$ in G then replacing v by u everywhere in the walk (or simply erasing v if u was one of its neighbors in the walk) then we would get a proper walk of G' between x_1 and x_2 in $G' - \{v\}$. Hence the only possible way that G' is not connected is that v is an isolated vertex of G'. This situation occurs if and only if u and v were not adjacent and their neighborhoods were disjoint in G.

Let us choose two incomparable elements of G closest to each other among incomparable pairs of vertices. We claim that the distance between these two vertices is at most two. Indeed, if u and v are two vertices of G and $u_0 u_1 \dots u_k$ $(u = u_0,\ v = u_k)$ is the shortest path between them and $k \geq 3$, then u_1 and u_2 are incomparable: u_2 cannot be adjacent to u_0 and u_1 cannot be adjacent to u_3 because otherwise we obtain a shorter path between u and v. So the distance of the closest pair of incomparable vertices is at most two, i.e., they are adjacent or they have a common neighbor. Applying the Kelmans transformation to these elements will result in a connected graph.

Now we can proceed as in the proof of part (a). We apply Kelmans transformations always to the closest pairs of incomparable vertices and let G^* be the maximal graph with respect to the lexicographic ordering among the graphs which can be obtained this way. Then G^* must have the desired structure. □

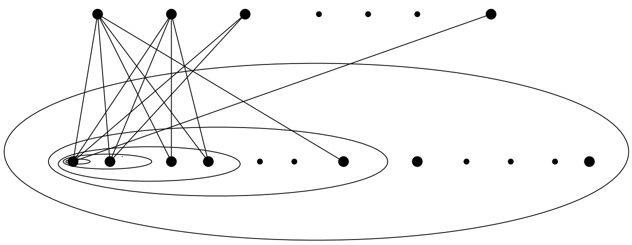

Figure 2.2: A threshold graph of the Kelmans transformation.

Theorem 2.1.2. *A graph G is the threshold graph of the Kelmans transformation if and only if it can be obtained from the empty graph by the following steps: adding some isolated vertices to the graph or complementing the graph.*

Proof. We prove the statement by induction on the number of vertices. Let G be a threshold graph of G on n vertices. If $n = 1$ or 2 the claim is trivial. If v_n is an isolated vertex then by induction we can build up the graph $G - v_n$ since it is a threshold graph; then we take v_n to obtain G. If v_n is not an isolated vertex then v_1 must be adjacent to each vertex of G. Let us consider $\overline{G}$, this is also a threshold graph of the Kelmans transformation with the reversed order of the vertices and in $\overline{G}$ the vertex v_1 is an isolated vertex. Hence by induction we can build up $\overline{G}$ and so the graph G.

The other direction of the statement is even more trivial. If we take an isolated vertex to the graph we put it to the end of the order of the vertices. If we take the complement of the graph we reverse the order of the vertices. □

Remark 2.1.3. Note that the graphs described in the previous theorem are called "threshold graphs" in the literature. Hence the threshold graphs of the Kelmans transformation are exactly the threshold graphs. (It seems to me that this statement is nontrivial in the sense that the threshold graphs are called threshold graphs not because of the Kelmans transformation.) From now on we simply refer to these graphs as threshold graphs.

Remark 2.1.4. These graphs, or more precisely their adjacency matrices also appear in the article of Brualdi and Hoffman [11]. Rowlinson called these matrices stepwise matrices [58].

2.2 Spectral radius

Theorem 2.2.1. *Let G be a graph and let G' be a graph obtained from G by some Kelmans transformation. Then*

$$\mu(G') \geq \mu(G).$$

Proof. Let $\underline{x}$ be the non-negative eigenvector of unit length belonging to $\mu(G)$ and let A_G and $A_{G'}$ be the corresponding adjacency matrices. Assume that $x_u \geq x_v$ and choose u to be the beneficiary of the Kelmans transformation. Since the exact role of u and v is not important in the Kelmans transformation, this choice does not affect the resulting graph G'.

Then

$$\mu(A_{G'}) = \max_{||\underline{y}||=1} \underline{y}^T A_{G'} \underline{y} \geq \underline{x}^T A_{G'} \underline{x} =$$

$$= \underline{x}^T A_G \underline{x} + 2(x_u - x_v) \sum_{w \in N(u) \setminus (N(v) \cup \{v\})} x_w \geq \mu(A_G)$$

Hence $\mu(G') \geq \mu(G)$. □

2.3 The matching polynomial

In this section we study the matching polynomials of graphs. For fundamental results on matching polynomials see [30, 31, 41].

Recall that we define the matching polynomial as follows. Let $m_r(G)$ denote the number of r independent edges (i.e., r-matchings) in the graph G. Then the matching polynomial of G is

$$M(G, x) = \sum_{r=0} (-1)^r m_r(G) x^{n-2r}.$$

The main theorem of this section is the following.

Theorem 2.3.1. *Assume that G' is a graph obtained from G by some Kelmans transformation, then*

$$M(G, x) \gg M(G', x).$$

In other words, this means that $m_r(G) \geq m_r(G')$ for $1 \leq r \leq n/2$. In particular, the Kelmans transformation decreases the maximum number of independent edges.

Remark 2.3.2. I invite the reader to prove this theorem on their own; although I give this proof of the theorem here, it takes much longer to read it than to prove it by himself or herself.

Proof. We need to prove that for every r the Kelmans transformation decreases the number of r-matchings. Assume that we applied the Kelmans transformation to G such that u was the beneficiary and v was the co-beneficiary. Furthermore, let $\mathcal{M}_r(G)$ and $\mathcal{M}_r(G')$ denote the set of r-matchings in G and G', respectively. We will give an injective map from $\mathcal{M}_r(G')$ to $\mathcal{M}_r(G)$.

In those cases where all edges of the r-matching of G' are also edges in G we simply take the identity map.

Next consider those cases where v is not covered by the matching, but for some $w \in N_G(v)\backslash N_G(u)$ we have uw in the r-matching. Map this r-matching to the r-matching obtained by exchanging uw to vw in the r-matching, but otherwise we do not change the other edges of the matching. Clearly, the image will be an r-matching of G and since $vw \notin E(G')$ this is not in the image of the previous case.

Finally, consider those cases where both u and v are covered in the r-matching of G' and the r-matching does not belong to the first case. In this case there exist a $w_1 \in N_G(v)\backslash N_G(u)$ and a $w_2 \in N_G(v) \cap N_G(u)$ such that uw_1 and vw_2 are in the r-matching of G'. Let the image of this r-matching be defined as follows. We exchange uw_1 and vw_2 to uw_2 and vw_1 in G, but otherwise we leave the other $r-2$ edges of the r-matching. Clearly we get an r-matching of G and the image of this r-matching is not in the image of the previous cases, because both u and v are covered (not as in the second case) and $vw_1 \in E(G)$ is in the r-matching (not as in the first case).

Hence we have given an injective map from $\mathcal{M}_r(G')$ to $\mathcal{M}_r(G)$ proving that $m_r(G') \leq m_r(G)$. $\square$

We mentioned that the Kelmans transformation is also a Kelmans transformation of the complement of the graph. As an example one can prove the following (very easy) result on maximal matchings. We leave the details to the Reader.

Corollary 2.3.3. *Let G be a graph on n vertices. Then G or $\overline{G}$ contains $\lfloor \frac{n}{3} \rfloor$ independent edges.*

Remark 2.3.4. The statement is best possible as it is shown by the clique of size $\frac{2n}{3}$ and additional $\frac{n}{3}$ isolated vertices. Corollary 2.3.3 is well-known, in fact, it is a motivating result of several colored matching problem, see e.g. [22].

2.3.1 The largest root of the matching polynomial

It is a well-known theorem of Heilmann and Lieb [41] that all the roots of the matching polynomial are real; so it is meaningful to speak about its largest root. In this section we will show that the Kelmans transformation increases the largest root of the matching polynomial (see Theorem 2.3.5). To do this we need some preparation; this is done in the Appendix, here we quote the relevant definition and results for the convenience.

Definition A.1.16. Let $t(G)$ be the largest root of the matching polynomial $M(G,x)$. Furthermore, let $G_1 \succ G_2$ if for all $x \geq t(G_1)$ we have $M(G_2,x) \geq M(G_1,x)$.

Statement A.1.17. *The relation $\succ$ is transitive and if $G_1 \succ G_2$ then $t(G_1) \geq t(G_2)$.*

We will use the following two facts about the matching polynomial. The first one is the well-known recursion formula for the matching polynomials. The second fact is a result of D. Fisher and J. Ryan [28], it was a corollary of their theorem on the dependence polynomials; a simple proof can be found in the Appendix.

Fact 1. (Statement A.1.18, [30, 31, 41]) Let $e = uv \in E(G)$. Then we have the following recursion formula for matching polynomials

$$M(G, x) = M(G - e, x) - M(G\backslash\{u, v\}, x).$$

Fact 2. (Statement A.1.15, [28]) If G_2 is a subgraph of G_1 then $t(G_1) \geq t(G_2)$.

We note that we will use the following slight extension of Fact 2 when the subgraph G_2 has the same vertex set as the graph G_1.

Statement A.1.19. *If G_2 is a spanning subgraph of G_1 then $G_1 \succ G_2$.*

Theorem 2.3.5. *Assume that G' is a graph obtained from G by some Kelmans transformation, then $G' \succ G$. In particular, $t(G') \geq t(G)$.*

Proof. Let u, v be the two vertices of the graph G for which we apply the Kelmans transformation such that u is the beneficiary. We will prove that $G' \succ G$; according to Statement A.1.17 this implies that $t(G') \geq t(G)$. We will prove this claim by induction on the number of edges of G.

Let us choose a vertex w different from v such that $uw \in E(G)$. If such a w does not exist then G' is isomorphic to G and the claim is trivial. Thus we can assume that such a w exists. Let $h = (u, w)$. Now we can write up the identities of Fact 1:

$$M(G, x) = M(G - h, x) - M(G - \{u, w\}, x)$$

and

$$M(G', x) = M(G' - h, x) - M(G' - \{u, w\}, x).$$

Here $G' - h$ can be obtained from $G - h$ by some Kelmans transformation and these graphs have fewer edges than G; so by induction we have $G' - h \succ G - h$, i.e.,

$$M(G - h, x) \geq M(G' - h, x)$$

for all $x \geq t(G' - h)$. On the other hand, $G' - \{u, w\}$ is a spanning subgraph of $G - \{u, w\}$, thus we have $G - \{u, w\} \succ G' - \{u, w\}$ by Statement A.1.19. In other words,

$$M(G' - \{u, w\}, x) \geq M(G - \{u, w\}, x)$$

for all $x \geq t(G - \{u, w\})$. Altogether we get that

$$M(G,x) = M(G-h,x) - M(G-\{u,w\},x) \geq M(G'-h,x) - M(G'-\{u,w\},x) = M(G',x)$$

for all $x \geq \max(t(G'-h), t(G-\{u,w\}))$. Note that $t(G') \geq \max(t(G'-h), t(G-\{u,w\}))$ as both graphs are subgraphs of G (so we can use Fact 2). In the latter case we embed the graph $G - \{u, w\}$ into G' such that v goes to u in the embedding. Thus

$$M(G,x) \geq M(G',x)$$

for all $x \geq t(G')$.

Hence $G' \succ G$ and we have proved the theorem.

□

2.4 The independence polynomial

In this section we prove that the Kelmans transformation decreases the smallest root of the independence polynomial. D. Fisher and J. Ryan [28] proved that the (in)dependence polynomial always has a real root having the smallest absolute value among the roots. It will be more convenient to work with the independence polynomial of the graph G, i.e., with the dependence polynomial of $\overline{G}$.

Recall that we define the independence polynomial as

$$I(G,x) = \sum_{k=0}^{n} (-1)^k i_k(G) x^k,$$

where $i_k(G)$ denotes the number of independent sets of size k. Let $\beta(G)$ denote the smallest real root of $I(G,x)$; it is positive by the alternating sign of the coefficients of the polynomial.

Remark 2.4.1. Some authors call the polynomial $I(G,-x)$ the independence polynomial; since the transformation between the two forms is trivial it will not cause any confusion to work with this definition.

The graph parameter $\beta(G)$ is examined in various papers. The fundamental result on $\beta(G)$, due to D. Fisher and J. Ryan [28], is the following: if G_1 is a subgraph of G_2 then $\beta(G_1) \geq \beta(G_2)$. For details, see the Appendix.

We will use the following recursion formulas of the independence polynomials subsequently.

Fact 1. (Statement A.1.4 and Remark A.1.5, [44]) The polynomial $I(G,x)$ satisfies the recursion

$$I(G,x) = I(G-v,x) - xI(G-N[v],x),$$

where v is an arbitrary vertex of the graph G.

Fact 2. (Statement A.1.4 and Remark A.1.5, [44]) The polynomial $I(G,x)$ satisfies the recursion

$$I(G,x) = I(G-e,x) - x^2 I(G-N[v]-N[u],x),$$

where $e=(u,v)$ is an arbitrary edge of the graph G.

We are going to prove our result in an analogous way that we have seen at the matching polynomials.

Definition A.1.6. Let $G_1 \succ G_2$ if $I(G_2,x) \geq I(G_1,x)$ on the interval $[0,\beta(G_1)]$.

This definition seems to be unnatural, because of the "reversed" inequality, but one can prove that if G_2 is a subgraph of G_1 then $G_1 \succ G_2$ (see Statement A.1.10). Thus in the light of the following statement this claim implies Fisher and Ryan's result (see Remark 2.4.1). For details, see the Appendix.

Statement A.1.7. *The relation $\succ$ is transitive on the set of graphs and if $G_1 \succ G_2$ then $\beta(G_1) \leq \beta(G_2)$.*

Statement A.1.10. *If G_2 is a subgraph of G_1 then $G_1 \succ G_2$.*

The main result of this section is the following

Theorem 2.4.2. *The Kelmans transformation decreases the smallest root of the independence polynomial. More precisely, assume that G' is a graph obtained from G by some Kelmans transformation, then $G' \succ G$ and so $\beta(G') \leq \beta(G)$.*

Proof. We prove the statement by induction on the number of vertices. The claim is true for small graphs. Let u be the beneficiary at the Kelmans transformation, v be the co-beneficiary. We can assume that $N_G(u)\backslash N_G(v)$ is not empty, otherwise G' and G are isomorphic, so let $w \in N_G(u)\backslash N_G(v)$. Now let us use the recursion formula of Fact 1.

$$I(G,x) = I(G-w,x) - xI(G-N_G[w],x)$$

and

$$I(G',x) = I(G'-w,x) - xI(G'-N_{G'}[w],x).$$

Observe that $G'-w$ can be obtained from $G-w$ by some Kelmans transformation and so by the induction we have

$$I(G-w,x) \geq I(G'-w,x)$$

on the interval $[0, \beta(G' - w)]$. On the other hand, $G' - N_{G'}[w]$ is a subgraph of $G - N_G[w]$, thus by Statement A.1.10 we have

$$I(G' - N_{G'}[w], x) \geq I(G - N_G[w], x)$$

on the interval $[0, \beta(G - N_G[w])]$. Putting together these two inequalities we get that

$$I(G, x) \geq I(G', x)$$

on the interval $[0, \min(\beta(G' - w), \beta(G - N_G[w])]$. Note that $G' - w$ and $G - N_G[w]$ are both subgraphs of G'; in the latter case v goes to u at the injective homomorphism from $V(G - N_G[w])$ to $V(G')$. Thus we have $\beta(G') \leq \min(\beta(G' - w), \beta(G - N_G[w]))$. This proves that $G' \succ G$. □

Remark 2.4.3. Theorem 2.4.2 does not imply Theorem 2.3.5 since the Kelmans transformation on a graph G does not induce a Kelmans transformation on the line graph.

2.4.1 The number of independent sets

Theorem 2.4.4. *The Kelmans transformation increases the number of independent sets of size r and the number of cliques of size r, i.e., assume that G' is a graph obtained from G by some Kelmans transformation, then $i_r(G) \leq i_r(G')$ and $i_r(\overline{G}) \leq i_r(\overline{G'})$ for all r.*

Disclaimer: it is easier to prove this theorem on their own than to read the following proof.

Proof. Since the Kelmans transformation of the graph G is also a Kelmans transformation of its complement, it is enough to prove the statement concerning the number of cliques of size k. Let $\mathcal{C}l_k(G)$ and $\mathcal{C}l_k(G')$ be the set of cliques of size k in G and G', respectively. We will give an injective map φ from $\mathcal{C}l_k(G)$ to $\mathcal{C}l_k(G')$. This way we prove that $|\mathcal{C}l_k(G)| \leq |\mathcal{C}l_k(G')|$.

Let $S \in \mathcal{C}l_k(G)$. If $S \in \mathcal{C}l_k(G')$ then we simply define φ to be the identity map. If $S \notin \mathcal{C}l_k(G')$ then $v \in V(S)$ and there exists some $w \in N_G(v) \backslash N_G(u)$ for which $w \in V(S)$ as well. This implies that $u \notin V(S)$. In this case let $\varphi(S)$ be the clique of G' induced on the set $(S - v) \cup \{u\}$. This is indeed a clique of G' and it cannot be the clique of G so it is not the image of any other clique of G. Hence φ is injective. □

2.5 The chromatic polynomial

In this section we prove a coefficient majorization result for the chromatic polynomial, see Theorem 2.5.3 below.

Recall that we define the chromatic polynomial $ch(G, \lambda)$ of the graph G as follows [4, 56]: for a positive integer λ the value $ch(G, \lambda)$ is the number of ways that G can be well-colored with

λ colors. It is indeed a polynomial in λ:

$$ch(G,\lambda)=\sum_{k=1}^{n}(-1)^{n-k}c_k(G)\lambda^k.$$

The coefficients of the chromatic polynomial have the following nice interpretation [4].

Theorem 2.5.1. *Let G be a graph on n vertices and edge set $E(G)=\{e_1,e_2,\dots,e_m\}$. Call a subset of $E(G)$ a broken cycle if it is obtained from the edge set of a cycle by deleting the edge of highest index. Then the chromatic polynomial of G is*

$$ch(G,\lambda)=\lambda^n-c_{n-1}\lambda^{n-1}+c_{n-2}\lambda^{n-2}-\dots+(-1)^{n-1}c_1\lambda,$$

where c_i is the number of $n-i$-subsets of $E(G)$ containing no broken cycles.

Remark 2.5.2. In fact, we will only need that the coefficients of the chromatic polynomial have alternating sign. This can easily be deduced from the recursion formula of Statement 2.5.4, too.

Theorem 2.5.3. *The Kelmans transformation decreases the coefficients of the chromatic polynomial in absolute value, i.e., assume that G' is a graph obtained from G by some Kelmans transformation, then*

$$ch(G,\lambda)\gg ch(G',\lambda).$$

In other words, $c_k(G)\geq c_k(G')$ for $k=1,\dots,n-1$.

To prove this theorem we need some preparation.

Statement 2.5.4. [4, 56] *Let $e\in E(G)$ then*

$$ch(G,\lambda)=ch(G-e,\lambda)-ch(G/e,\lambda).$$

Lemma 2.5.5. *If G_1 is a spanning subgraph of G then*

$$ch(G,\lambda)\gg ch(G_1,\lambda).$$

Proof. It is enough to prove the claim for $G_1=G-e$ for which the statement is trivial by Statement 2.5.4 and Theorem 2.5.1. □

Now we are ready to prove Theorem 2.5.3.

Proof. Let us introduce the notation

$$\widehat{ch}(G,\lambda)=(-1)^{|V(G)|}ch(G,-\lambda).$$

Then $\widehat{ch}(G,\lambda)=\sum_{k=1}^{n}c_k(G)\lambda^k$ has only non-negative coefficients. Clearly, one can rewrite Statement 2.5.4 as

$$\widehat{ch}(G,\lambda)=\widehat{ch}(G-e,\lambda)+\widehat{ch}(G/e,\lambda).$$

We need to prove that $\widehat{ch}(G,\lambda) \gg \widehat{ch}(G',\lambda)$.

We prove this statement by induction on the sum of the number of edges and vertices of G. Assume that G' is obtained from G by some Kelmans transformation applied to the vertices u and v, where u is the beneficiary and v is co-beneficiary. Let $w \in N(v)\backslash N(u)$, we can assume the existence of such a vertex, otherwise $G' = G$. Let us denote the edge $(v,w) \in E(G)$ by $e = (v,w)$ and the edge $(u,w) \in E(G')$ by $f = (u,w)$. Then we have

$$\widehat{ch}(G,\lambda) = \widehat{ch}(G-e,\lambda) + \widehat{ch}(G/e,\lambda)$$

and

$$\widehat{ch}(G',\lambda) = \widehat{ch}(G'-f,\lambda) + \widehat{ch}(G'/f,\lambda).$$

Note that $G'-f$ can be obtained from $G-e$ by a Kelmans transformation, thus by induction we have

$$\widehat{ch}(G-e,\lambda) \gg \widehat{ch}(G'-f,\lambda).$$

Observe that G/e and G'/f are multigraphs, indeed if for some $t \in N_G(v)$ the vertex t were adjacent to w than tw became multiple edges in G/e. Now we erase all except one copy of all multiple edges to make G/e and G'/f simple graphs. (See the remark at the end of the proof.) Let $(G/e)^*$ and $(G'/f)^*$ be the obtained simple graphs. This way we did not change the chromatic polynomial since the value of $ch(.,\lambda)$ became unchanged for all positive integers, thus the polynomial itself must be unchanged. Another observation is that whenever we erased a multiple edge in G/e we erased a multiple edge in G'/f too. On the other hand, for if some $t \in N_G(u)\backslash N_G(v)$ the vertex t were adjacent to w then it became a multiple edge in G'/f while it is a simple edge in G/e. Let us erase all edges of the form $\{(t,w) \mid t \in N_G(u)\backslash N_G(w)\}$ from the graph $(G/e)^*$; let $(G/e)^{**}$ be the obtained graph. According to Lemma 2.5.5 we have

$$\widehat{ch}((G/e)^*,\lambda) \gg \widehat{ch}((G/e)^{**},\lambda).$$

Now our last observation is that $(G'/f)^*$ can be obtained from $(G/e)^{**}$ by some Kelmans transformation where w is the beneficiary and u is the co-beneficiary (in $(G'/f)^*$ the vertex $u \in V((G/e)^{**})$ became $v \in V((G/f)^*)$). Hence by the induction hypothesis we have

$$\widehat{ch}((G/e)^{**},\lambda) \gg \widehat{ch}((G'/f)^*,\lambda).$$

Altogether we have

$$\widehat{ch}(G,\lambda) = \widehat{ch}(G-e,\lambda) + \widehat{ch}(G/e,\lambda) = \widehat{ch}(G-e,\lambda) + \widehat{ch}((G/e)^*,\lambda) \gg$$

$$\gg \widehat{ch}(G-e,\lambda) + \widehat{ch}((G/e)^{**},\lambda) \gg \widehat{ch}(G'-f,\lambda) + \widehat{ch}((G'/f)^*,\lambda) =$$

$$= \widehat{ch}(G'-f,\lambda) + \widehat{ch}(G'/f,\lambda) = \widehat{ch}(G',\lambda).$$

By comparing the two ends of the chain of inequalities we obtained the desired result. □

Remark 2.5.6. We avoided the use of multigraphs because we have not defined the Kelmans transformation for multigraphs, although this can be done, see e.g. [10]. In some cases it would have been more convenient to use multigraphs, but in some other cases it would have led to more discussion. Since we were primarily interested in simple graphs we chose the way described in the proof.

2.6 Exponential-type graph polynomials

We call a graph polynomial $f(G, x)$ *exponential-type* if it satisfies the following identity:

$$\sum_{\substack{S_1 \cup S_2 = V(G) \\ S_1 \cap S_2 = \emptyset}} f(S_1, x) f(S_2, y) = f(G, x + y),$$

where $f(S, x) = f(G|_S, x)$.

This is a very special class of graph polynomials, till it has some notable elements: chromatic polynomial, Laplacian polynomial and the following modified matching polynomial: $\overline{M}(G, x) = \sum_{k=0}^{n} m_k(G) x^{n-k}$.

The main structure result for exponential-type graph polynomials is the following (again we refer to the Appendix). For any exponential-type graph polynomial there exists a function b from the isomorphism classes of graphs to the complex numbers such that if

$$f(G, x) = \sum_{k=1}^{n} a_k(G) x^k$$

then

$$a_k(G) = \sum_{\{S_1, S_2, \dots, S_k\} \in \mathcal{P}_k} b(S_1) b(S_2) \dots b(S_k),$$

where the summation goes over the set $\mathcal{P}_k$ of the partitions of the vertex set into exactly k sets. We denote this connection by $f(G, x) = f_b(G, x)$ (see Appendix). We can obtain an easy consequence of this result.

Lemma 2.6.1. *Assume that $b(G) \geq 0$ for all graphs G and*

$$f_b(G, x) = \sum_{k=1}^{n} a_k(G) x^k.$$

Let H_1 and H_2 be two graphs on the same vertex set V and let $u, v \in V$. Assume that the following two conditions hold:

- *if $u, v \in S$ or $u, v \notin S$ at the same time we have $b(H_1|_S) \geq b(H_2|_S)$,*
- *(cut condition) for all S for which $u, v \in S$ we have*

$$\sum_{\substack{S_1 \cap S_2 = \emptyset,\ S_1 \cup S_2 = S \\ u \in S_1, v \in S_2}} b(H_1|_{S_1}) b(H_1|_{S_2}) \geq \sum_{\substack{S_1 \cap S_2 = \emptyset,\ S_1 \cup S_2 = S \\ u \in S_1, v \in S_2}} b(H_2|_{S_1}) b(H_2|_{S_2}).$$

Then we have $a_k(H_1) \geq a_k(H_2)$ for all $1 \leq k \leq n$.

Proof. Clearly, the first condition implies that

$$\sum_{\substack{\{S_1,S_2,\dots,S_k\}\in\mathcal{P}\\ u,v\in S_1}} b(H_1|_{S_1})b(H_1|_{S_2})\dots b(H_1|_{S_k}) \geq \sum_{\substack{\{S_1,S_2,\dots,S_k\}\in\mathcal{P}\\ u,v\in S_1}} b(H_2|_{S_1})b(H_2|_{S_2})\dots b(H_2|_{S_k}).$$

Similarly, the first and the second condition together imply

$$\sum_{\substack{\{S_1,S_2,\dots,S_k\}\in\mathcal{P}\\ u\in S_1,v\in S_2}} b(H_1|_{S_1})b(H_1|_{S_2})\dots b(H_1|_{S_k}) =$$

$$= \sum_{\{S_3,\dots S_k\}} b(H_1|_{S_3})\dots b(H_1|_{S_k}) \sum_{\substack{S_1\cup S_2=S\\ u\in S_1,v\in S_2}} b(H_1|_{S_1})b(H_1|_{S_2}) \geq$$

$$\geq \sum_{\{S_3,\dots S_k\}} b(H_2|_{S_3})\dots b(H_2|_{S_k}) \sum_{\substack{S_1\cup S_2=S\\ u\in S_1,v\in S_2}} b(H_2|_{S_1})b(H_2|_{S_2}) =$$

$$\sum_{\substack{\{S_1,S_2,\dots,S_k\}\in\mathcal{P}\\ u\in S_1,v\in S_2}} b(H_2|_{S_1})b(H_2|_{S_2})\dots b(H_2|_{S_k}).$$

By adding up the two equations we obtain

$$a_k(H_1) = \sum_{\{S_1,S_2,\dots,S_k\}\in\mathcal{P}} b(H_1|_{S_1})b(H_1|_{S_2})\dots b(H_1|_{S_k}) \geq$$

$$\sum_{\{S_1,S_2,\dots,S_k\}\in\mathcal{P}} b(H_2|_{S_1})b(H_2|_{S_2})\dots b(H_2|_{S_k}) = a_k(H_2).$$

□

Remark 2.6.2. Naturally, we will use Lemma 2.6.1 for a graph G and G' obtained by Kelmans transformation and u, v beneficiary and co-beneficiary vertices. The first condition is equivalent with the fact that the Kelmans transformation increase (or decrease) the parameter $b(.)$; indeed, if $u, v \in S$ then $G'|_S$ can be obtained from $G|_S$ by the Kelmans transformation applied to u and v. If $u, v \notin S$ then simply $G'|_S = G|_S$.

One expects that it is easy (or at least not hard) to check the first condition and considerably much harder to check the cut condition. Surprisingly, there are some cases when it is easier to check the cut condition. For instance, let $b(G) = \tau(G)$ be the number of spanning trees. Then

$$r(G, u, v) = \sum_{\substack{S_1\cap S_2=\emptyset,\ S_1\cup S_2=V(G)\\ u\in S_1,v\in S_2}} b(G|_{S_1})b(G|_{S_2})$$

can be interpreted as follows. Let us put an edge e between u and v then $r(G, u, v)$ is exactly the number of spanning trees containing the edge e. But this is $\tau(G/e)$. Since G/e and G'/e are isomorphic multigraphs we have $r(G, u, v) = r(G', u, v)$.

We also could have proved the corresponding statement for the coefficients of the (modified) matching polynomial. Since $b(G) = 0$ there, except for $G = K_1, K_2$ we have $b(K_1) = b(K_2) = 1$ we have to check the first and the second conditions for graphs on at most 2 and 4(!) vertices, respectively.

2.7 Laplacian polynomial of a graph

Recall that the Laplacian matrix $L(G)$ of the graph G is $D - A$, where D is the diagonal matrix consisting of the vertex degrees and A is the adjacency matrix. We call the polynomial $L(G, x) = \det(xI - L(G))$ the Laplacian polynomial of the graph G, i.e., it is the characteristic polynomial of the Laplacian matrix of G. We will write $L(G, x)$ in the form

$$L(G,x) = \sum_{k=1}^{n} (-1)^{n-k} a_k(G) x^k,$$

where $a_k(G) \geq 0$.

The main result of this section is the following.

Theorem 2.7.1. *The Kelmans transformation decreases the coefficients of the Laplacian polynomial in absolute value, i.e., assume that G' is a graph obtained from G by some Kelmans transformation, then*

$$L(G, x) \gg L(G', x).$$

In other words, $a_k(G) \geq a_k(G')$ for $k = 1, \dots, n-1$.

To prove this theorem we use the fact from the Appendix that the Laplacian polynomial is exponential-type.

Theorem A.3.13. *The Laplacian polynomial $L(., x)$ is exponential-type with*

$$b(G) = (-1)^{|V(G)|-1} \overline{\tau}(G) = (-1)^{|V(G)|-1} |V(G)| \tau(G).$$

Remark 2.7.2. Hence $(-1)^n L(G, -x) = f_{\overline{\tau}}(G, x)$, where $\overline{\tau}(G) = |V(G)|\tau(G)$. So we can use Lemma 2.6.1 to $f_{\overline{\tau}}(G, x)$. We have to check the two conditions, the first one is the result of Satyanarayana, Schoppmann and Suffel quoted in the introduction of this chapter.

Theorem 2.7.3. [59] *The Kelmans transformation decreases the number of spanning trees, i.e., assume that G' is a graph obtained from G by some Kelmans transformation, then*

$$\tau(G) \geq \tau(G').$$

Proof. Let u and v be the beneficiary and the co-beneficiary of the Kelmans transformation, respectively.

Let R be a subset of the edge set $\{(u, w) \in E(G) \mid w \in N_G(u) \cap N_G(v)\}$. Let

$$\mathcal{T}_R(G) = \{T \mid T \text{ is a spanning tree, } R \subset E(T)\}.$$

Let $\tau_R(G) = |\mathcal{T}_R(G)|$. We will show that for any $R \subseteq \{(u, w) \in E(G) \mid w \in N(u) \cap N(v)\}$, we have $\tau_R(G) \geq \tau_R(G')$. For $R = \emptyset$ we immediately obtain the statement of the theorem.

We prove this statement by induction on the lexicographic order of

$$(e(G), |N_G(u) \cap N_G(v)| - |R|).$$

For the empty graph on n vertices the statement is trivial. Thus we assume that we already know that the Kelmans transformation decreases $\tau_R(G_1)$ if $e(G_1) < e(G)$ or $e(G_1) = e(G)$, but $|N_G(u_1) \cap N_G(v_1)| - |R_1| < |N_G(u) \cap N_G(v)| - |R|$.

Now assume that $|N_G(u) \cap N_G(v)| - |R| = 0$, in other words $R = \{(u, w) \in E(G) \mid w \in N(u) \cap N(v)\}$. Observe that $N_{G'}(v) = N_G(u) \cap N_G(v)$, but since $R \subset E(T')$ the vertex v must be a leaf in T' for any spanning tree $T' \in \mathcal{T}_R(G')$.

Now let us consider the following map. Take a spanning tree T' which contains the elements of the set R. Let us erase the edges between u and $(N_G(v) \backslash N_G(u)) \cap N_{T'}(u)$ (maybe there is no such edge in the tree) and add the edges between v and $(N_G(v) \backslash N_G(u)) \cap N_{T'}(u)$. The tree, obtained this way, is an element of $\mathcal{T}_R(G)$. This map is obviously injective; if we get an image $T \in \mathcal{T}_R(G)$ we simply erase the edges between v and $(N_G(v) \backslash N_G(u)) \cap N_T(v)$ and add the edges between u and $(N_G(v) \backslash N_G(u)) \cap N_T(v)$. Hence $\tau_R(G') \leq \tau_R(G)$.

Now assume that $|R| < |N_G(u) \cap N_G(v)|$. Let $h = (u, w)$ be an edge not in R for which $w \in N_G(u) \cap N_G(v)$. Then we can decompose $\tau_R(G)$ according to $h \in E(T)$ or not. Hence

$$\tau_R(G) = \tau_{R \cup \{h\}}(G) + \tau_R(G - h).$$

Similarly,

$$\tau_R(G') = \tau_{R \cup \{h\}}(G') + \tau_R(G' - h).$$

Note that $G' - h$ can be obtained from $G - h$ by a Kelmans transformation applied to the vertices u and v. Since it has fewer edges than G we have

$$\tau_R(G - h) \geq \tau_R(G' - h).$$

Similarly, $|N_G(u) \cap N_G(v)| - |R \cup \{h\}| < |N_G(u) \cap N_G(v)| - |R|$, so we have by induction that

$$\tau_{R \cup \{h\}}(G) \geq \tau_{R \cup \{h\}}(G').$$

Hence

$$\tau_R(G) \geq \tau_R(G').$$

In particular,

$$\tau(G) = \tau_\emptyset(G) \geq \tau_\emptyset(G') = \tau(G').$$

$\square$

Now we prove that the function $\overline{\tau}$ satisfies the second condition of Lemma 2.6.1. The proof of it will be very similar to the previous one.

Theorem 2.7.4. *Let $\overline{\tau}(G) = |V(G)|\tau(G)$, where $\tau(G)$ denotes the number of spanning trees of the graph G. Let G be a graph and let G' be the graph obtained from G by a Kelmans transformation applied to the vertices u and v. Then for all S for which $u, v \in S$ we have*

$$\sum_{\substack{S_1\cap S_2=\emptyset,\ S_1\cup S_2=S\\ u\in S_1, v\in S_2}} \overline{\tau}(G|_{S_1})\overline{\tau}(G|_{S_2}) \geq \sum_{\substack{S_1\cap S_2=\emptyset,\ S_1\cup S_2=S\\ u\in S_1, v\in S_2}} \overline{\tau}(G'|_{S_1})\overline{\tau}(G'|_{S_2}).$$

Proof. We can assume that $S = V(G)$. Let R be a subset of the edge set $\{(u,w) \in E(G) \mid w \in N(u) \cap N(v)\}$. Let

$$\mathcal{S}(G)_R = \{(T_1, T_2) \mid T_1, T_2 \text{ trees},\ u \in V(T_1),\ v \in V(T_2),$$

$$V(T_1) \cap V(T_2) = \emptyset, V(T_1) \cup V(T_2) = V(G),\ R \subseteq E(T_1)\}.$$

Note that

$$s(G,u,v) := \sum_{\substack{S_1\cap S_2=\emptyset, S_1\cup S_2=S\\ u\in S_1, v\in S_2}} \overline{\tau}(G|_{S_1})\overline{\tau}(G|_{S_2}) = \sum_{(T_1,T_2)\in\mathcal{S}(G)_\emptyset} |V(T_1)||V(T_2)|.$$

In general, we introduce the expression

$$s(G,R,u,v) = \sum_{(T_1,T_2)\in\mathcal{S}(G)_R} |V(T_1)||V(T_2)|.$$

We will show that for any $R \subseteq \{(u,w) \in E(G) \mid w \in N(u) \cap N(v)\}$ we have

$$s(G,R,u,v) \geq s(G',R,u,v).$$

We prove this statement by induction on the lexicographic order of

$$(|E(G)|, |N(u) \cap N(v)| - |R|).$$

For the empty graph on n vertices the statement is trivial. Thus we assume that we already know that the Kelmans transformation decreases $s(G_1, R_1, u_1, v_1)$ if $e(G_1) < e(G)$ or $e(G_1) = e(G)$, but $|N(u_1) \cap N(v_1)| - |R_1| < |N(u) \cap N(v)| - |R|$.

Now assume that $|N(u) \cap N(v)| - |R| = 0$, in other words, $R = \{(u,w) \in E(G) \mid w \in N(u) \cap N(v)\}$. We prove that $s(G,R,u,v) \geq s(G',R,u,v)$. Observe that $N_{G'}(v) = N(u) \cap N(v)$, but since $R \subseteq T_1$ the set $N_{G'}(v) \subseteq V(T_1)$. Hence $V(T_2) = \{v\}$. So

$$s(G',R,u,v) = (n-1)\tau_R(G'-v),$$

where $\tau_R(G'-v)$ denotes the number of spanning trees of $G'-v$ which contains the elements of the set R. Now let us consider the following map. Take a spanning tree T' of $G'-v$ which contains the elements of the set R, let us erase the edges between u and $(N_G(v)\setminus N_G(u))\cap N_{T'}(u)$ (maybe there is no such edge in the tree) and add the edges between v and $(N_G(v)\setminus N_G(u))\cap N_{T'}(u)$. The pair of trees, obtained this way, is an element of $\mathcal{S}(G)_R$. This map is obviously injective; if we get an image $(T_1,T_2)\in\mathcal{S}(G)_R$ we simply erase the edges between v and $N_{T_2}(v)$ and add the edges between u and $N_{T_2}(v)$. Since $n-1\leq k(n-k)$ for any $1\leq k\leq n-1$ we have

$$s(G',R,u,v)=\sum_{(T_1,T_2)\in\mathcal{S}(G')_R}1\cdot(n-1)\leq\sum_{(T_1,T_2)\in\mathcal{S}(G)_R}|V(T_1)||V(T_2)|=s(G,R,u,v).$$

Now assume that $|R|<|N_G(u)\cap N_G(v)|$. Let $h=(u,w)$ be an edge not in R for which $w\in N_G(u)\cap N_G(v)$. Then we can decompose $s(G,R,u,v)$ according to $h\in T_1$ where $(T_1,T_2)\in\mathcal{S}(G)_R$ or not. Hence

$$s(G,R,u,v)=s(G,R\cup\{h\},u,v)+s(G-h,R,u,v).$$

Similarly,

$$s(G',R,u,v)=s(G',R\cup\{h\},u,v)+s(G'-h,R,u,v).$$

Note that $G'-h$ can be obtained from $G-h$ by a Kelmans transformation applied to the vertices u and v. Since it has fewer edges than G we have

$$s(G-h,R,u,v)\geq s(G'-h,R,u,v).$$

Similarly, $|N_G(u)\cap N_G(v)|-|R\cup\{h\}|<|N_G(u)\cap N_G(v)|-|R|$, so we have by induction that

$$s(G,R\cup\{h\},u,v)\geq s(G',R\cup\{h\},u,v).$$

Hence

$$s(G,R,u,v)\geq s(G',R,u,v).$$

In particular,

$$\sum_{\substack{S_1\cap S_2=\emptyset,\ S_1\cup S_2=S\\ u\in S_1, v\in S_2}}\overline{\tau}(G|_{S_1})\overline{\tau}(G|_{S_2})=s(G,\emptyset,u,v)\geq s(G',\emptyset,u,v)=\sum_{\substack{S_1\cap S_2=\emptyset,\ S_1\cup S_2=S\\ u\in S_1,\ v\in S_2}}\overline{\tau}(G'|_{S_1})\overline{\tau}(G'|_{S_2}).$$

□

Proof of Theorem 2.7.1. Since the Laplace graph is of exponential-type it is enough to check the conditions of Lemma 2.6.1 for the polynomial $(-1)^n L(G,-x)$. This satisfies that $b_L(G)=\overline{\tau}(G)=|V(G)|\tau(G)\geq 0$.

If $u,v\in S$, then according Theorem 2.7.3, $\tau(G'|_S)\leq\tau(G|_S)$ and so $\overline{\tau}(G'|_S)\leq\overline{\tau}(G|_S)$. If $u,v\notin S$ then $G'|_S=G|_S$ and simply $\overline{\tau}(G'|_S)=\overline{\tau}(G|_S)$.

On the other hand, by Theorem 2.7.4 we have

$$\sum_{\substack{S_1\cap S_2=\emptyset,\ S_1\cup S_2=S\\ u\in S_1, v\in S_2}} \overline{\tau}(G|_{S_1})\overline{\tau}(G|_{S_2}) \geq \sum_{\substack{S_1\cap S_2=\emptyset,\ S_1\cup S_2=S\\ u\in S_1, v\in S_2}} \overline{\tau}(G'|_{S_1})\overline{\tau}(G'|_{S_2}).$$

Hence every condition of Lemma 2.6.1 are satisfied. Thus $a_k(G') \leq a_k(G)$ for any $1 \leq k \leq n$. □

2.8 Number of closed walks

Definition 2.8.1. The *NA-Kelmans transformation* is the Kelmans transformation applied to non-adjacent vertices.

Theorem 2.8.2. *The NA-Kelmans transformation increases the number of closed walks of length k for every $k \geq 1$. In other words, $W_k(G') \geq W_k(G)$ for $k \geq 1$.*

Proof. Let G be an arbitrary graph. Let G' be the graph obtained from G by a Kelmans transformation applied to u and v, where u is the beneficiary. Let $D(x, y, k)$ denote the number of walks from x to y of length k in G. Similarly $R(x, y, k)$ denotes the number of walks from x to y of length k in G'. If $x, y \neq v$ then for all k we have $R(x, y, k) \geq D(x, y, k)$. Indeed, if we have a walk from x to y of length k we can exchange those v's to u's in the walk whose any of the neighbor in the walk is a vertex belonging to $N_G(v)\backslash N_G(u)$. (It is one of the steps where we use that u and v are not adjacent.) This will give an injective mapping from the walks of G to the set of walks of G'. (It is not surjective since $\dots v_1 u v_2 \dots$ never appears in these "image" walks if $v_1 \in N_G(v)\backslash N_G(u)$ and $v_2 \in N_G(u)\backslash N_G(v)$.) In particular, if $x \neq u, v$ then $R(x, x, k) \geq D(x, x, k)$. On the other hand,

$$D(u, u, k) + D(v, v, k) = \sum_{u,v\in N_G(u)} D(x, y, k-2) + \sum_{x',y'\in N_G(v)} D(x', y', k-2) \leq$$

$$\leq \sum_{x,y\in N_G(u)} R(x, y, k-2) + \sum_{x',y'\in N_G(v)} R(x', y', k-2) \leq$$

$$\leq \sum_{x,y\in N_{G'}(u)} R(x, y, k-2) + \sum_{x',y'\in N_{G'}(v)} R(x', y', k-2) = R(u, u, k) + R(v, v, k).$$

Hence

$$W_k(G) = \sum_{x\in V(G)} D(x, x, k) \leq \sum_{x\in V(G)} R(x, x, k) = W_k(G').$$

□

Remark 2.8.3. The statement is not true for any Kelmans transformation. Let G be the 4-cycle, u, v are two adjacent vertices of G. Let us apply the Kelmans transformation to u and v. Then G has 32 closed walks of length 4 while G' has only 28 closed walks of length 4.

2.9 Upper bound to the spectral radius of threshold graphs

In this section we prove a simple upper bound on the spectral radius of graphs belonging to a certain class of graphs. This class contains the threshold graphs.

As an application we give a good upper bound to

$$\mu(G)+\mu(\overline{G}).$$

This problem was posed by Eva Nosal. She proved that

$$\mu(G)+\mu(\overline{G})\leq \sqrt{2}n.$$

For a long time this was the best upper bound in terms of the number of vertices. (There were other bounds in terms of the number of vertices, the chromatic number of the graph and its complement [42], or in terms of the clique sizes of the graphs [52]. However, these bounds could not be applied to improve on the constant $\sqrt{2}$.) Only very recently, V. Nikiforov [54] managed to prove that $\sqrt{2}$ is not the best possible constant. He proved that

$$\mu(G)+\mu(\overline{G})\leq (\sqrt{2}-\varepsilon)n,$$

where $\varepsilon=8\cdot 10^{-7}$.

Compared to this results Theorem 2.9.4 was a real a breakthrough. The success of the Kelmans transformation in this problem motivated the author to take a closer look at this transformation.

We mention that V. Nikiforov [54] conjectured that

$$\mu(G)+\mu(\overline{G})\leq \frac{4}{3}n.$$

This conjecture was proved by Tamás Terpai [61].

Theorem 2.9.1. *Let us assume that in the graph G the set $X=\{v_1,v_2,\dots,v_k\}$ forms a clique while $V\backslash X=\{v_{k+1},\dots,v_n\}$ forms an independent set. Furthermore, let $e(X,V\backslash X)$ denote the number of edges going between X and $V\backslash X$. Then*

$$\mu(G)\leq \frac{k-1+\sqrt{(k-1)^2+4e(X,V\backslash X)}}{2}.$$

Proof. We can assume that G is not the empty graph, for which the statement is trivial. Let $\underline{x}$ be the non-negative eigenvector belonging to $\mu=\mu(G)$. For $1\leq j\leq k$ we have

$$\mu x_j=x_1+\dots+x_{j-1}+x_{j+1}+\dots+x_k+\sum_{v_m\in N(v_j)\cap(V\backslash X)} x_m.$$

By adding up these equations we get

$$\mu\left(\sum_{j=1}^k x_j\right)=(k-1)\left(\sum_{j=1}^k x_j\right)+d_{k+1}x_{k+1}+\dots+d_nx_n.$$

For $k+1 \leq j \leq n$ we have

$$\mu x_j = \sum_{v_m \in N(v_j)} x_m.$$

Since $V \backslash X$ forms an independent set we have $\mu x_j \leq \sum_{i=1}^{k} x_i$ for $k+1 \leq j \leq n$ and so

$$\mu \left(\sum_{j=1}^{k} x_j \right) = (k-1) \left(\sum_{j=1}^{k} x_j \right) + d_{k+1} x_{k+1} + \cdots + d_n x_n \leq$$

$$\leq (k-1) \left(\sum_{j=1}^{k} x_j \right) + \frac{d_{k+1}}{\mu} \left(\sum_{j=1}^{k} x_j \right) + \cdots + \frac{d_n}{\mu} \left(\sum_{j=1}^{k} x_j \right).$$

Since $\sum_{j=k+1}^{n} d_j = e(X, V \backslash X)$ we have

$$\mu \leq k - 1 + \frac{e(X, V \backslash X)}{\mu}.$$

Hence

$$\mu(G) \leq \frac{k - 1 + \sqrt{(k-1)^2 + 4e(X, V \backslash X)}}{2}.$$

□

Remark 2.9.2. Let G be a threshold graph for which v_i dominates v_j whenever $i < j$. Let k be the least integer for which v_k and v_{k+1} are not adjacent. In this case $X = \{v_1, \ldots, v_k\}$ forms a clique while $V \backslash X = \{v_{k+1}, \ldots, v_n\}$ forms an independent set. One can prove a bit stronger inequalities for threshold graphs, namely

$$\frac{1}{\mu} \left(\sum_{j=k+1}^{n} d_j^2 \right) \leq k\mu - k(k-1),$$

and

$$\mu^2 + \mu \leq k(k-1) + \frac{1}{\mu} \left(\sum_{j=k+1}^{n} d_j^2 \right) + e(X, V \backslash X).$$

By combining these inequalities we immediately get the statement of the theorem.

Remark 2.9.3. For our purpose the inequality

$$\mu(G) \leq \frac{k + \sqrt{k^2 + 4e(X, V \backslash X)}}{2}$$

will suffice.

Theorem 2.9.4.

$$\mu(G) + \mu(\overline{G}) \leq \frac{1 + \sqrt{3}}{2} n.$$

Proof. By Theorem 2.2.1 and Remark 2.0.3 we only need to check the statement for threshold graphs. Let G be a threshold graph for which v_i dominates v_j whenever $i < j$. Let k be the least integer for which v_k and v_{k+1} are not adjacent. In this case $X = \{v_1, \dots, v_k\}$ forms a clique while $V \backslash X = \{v_{k+1}, \dots, v_n\}$ forms an independent set. Let us apply Theorem 2.9.1 with G and X and with $\overline{G}$ and $V \backslash X$. Then we have

$$\mu(G) \leq \frac{k + \sqrt{k^2 + 4e_G(X, V\backslash X)}}{2}$$

and

$$\mu(\overline{G}) \leq \frac{n - k + \sqrt{(n-k)^2 + 4e_{\overline{G}}(V\backslash X, X)}}{2}.$$

Thus we have

$$2(\mu(G) + \mu(\overline{G})) - n \leq \sqrt{k^2 + 4e_G(X, V\backslash X)} + \sqrt{(n-k)^2 + 4e_{\overline{G}}(V\backslash X, X)}.$$

By the arithmetic-quadratic mean inequality we have

$$\sqrt{k^2 + 4e_G(X, V\backslash X)} + \sqrt{(n-k)^2 + 4e_{\overline{G}}(V\backslash X, X)} \leq$$
$$\leq \sqrt{2(k^2 + 4e_G(X, V\backslash X) + (n-k)^2 + 4e_{\overline{G}}(V\backslash X, X))} =$$
$$= \sqrt{2(k^2 + (n-k)^2 + 4k(n-k))} \leq \sqrt{3}n.$$

Altogether we get

$$2(\mu(G) + \mu(\overline{G})) - n \leq \sqrt{3}n.$$

Hence

$$\mu(G) + \mu(\overline{G}) \leq \frac{1 + \sqrt{3}}{2} n.$$

□

2.10 Polynomials of the threshold graphs

In this section we give some special graph polynomials of the threshold graphs. We start with the Laplacian polynomial (which can be found implicitly in the paper [47] as well, although we give the proof here).

Theorem 2.10.1. *Let G be a threshold graph of Kelmans transformation with degree sequence $d_1 \geq d_2 \geq \dots \geq d_n$. Let t be the unique integer for which $d_t = t - 1$, i.e., for which $v_1, \dots, v_t$ induces a clique, but v_t and v_{t+1} are not connected. Then the spectra of the Laplacian matrix of G is the multiset*

$$\{d_1 + 1, d_2 + 1, \dots, d_{t-1} + 1, d_{t+1}, \dots, d_n, 0\}.$$

In other words, the Laplacian polynomial is

$$L(G, x) = x \prod_{i=1}^{t-1} (x - d_i - 1) \prod_{i=t+1}^{n} (x - d_i).$$

Proof. We will use the following well-known facts.

Fact 1. (Statement A.2.12) If we add k isolated vertices to the graph G then the Laplacian spectra of the obtained graph consists of the Laplacian spectra of the graph G and k zeros.

Fact 2. (Statement A.2.13, [32]) If the Laplacian spectra of the graph G is $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n = 0$ then the Laplacian spectra of $\overline{G}$ is $n - \lambda_1, n - \lambda_2, \ldots, n - \lambda_{n-1}, 0$.

We prove the theorem by induction on the number of vertices of the graph. The claim is trivial for threshold graphs having 1 or 2 vertices. If v_1 is not adjacent to v_n then v_n is an isolated vertex and the claim follows from the induction hypothesis and Fact 1. If v_1 and v_n are adjacent then we observe that $\overline{G}$ has the same structure and v_1 is isolated vertex in $\overline{G}$. Note that in $\overline{G}$ the vertices $v_n, v_{n-1}, \ldots, v_{t+1}, v_t$ induce a clique, but v_t and v_{t-1} are not adjacent. So we can apply the induction hypothesis to $\overline{G} \backslash \{v_1\}$ obtaining that its Laplacian spectra is $\{n - 1 - d_n + 1, n - 1 - d_{n-1} + 1, \ldots, n - 1 - d_{t+1} + 1, n - 1 - d_{t-1}, \ldots, n - 1 - d_2, 0\}$. Thus using Fact 2 and $d_1 = n - 1$ we get that the Laplacian spectra of the graph G is $\{d_1 + 1, d_2 + 1, \ldots, d_{t-1} + 1, d_{t+1}, \ldots, d_n, 0\}$. □

The threshold graphs are also chordal graphs so the roots of their chromatic polynomials are integers. The more precise (and trivial) result is the following.

Theorem 2.10.2. *Let G be a threshold graph of Kelmans transformation with degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. Let t be the unique integer for which $d_t = t - 1$, i.e., for which $v_1, \ldots, v_t$ induce a clique, but v_t and v_{t+1} are not connected. Then the chromatic polynomial of the graph G is the following*

$$ch(G, \lambda) = \prod_{i=1}^{t}(\lambda - i + 1) \prod_{i=t+1}^{n} (\lambda - d_i).$$

Proof. We can color the clique of size t in $\prod_{i=1}^{t}(\lambda - i + 1)$ ways. For $i \geq t + 1$, the vertex v_i has d_i neighbors in the clique induced by $v_1, \ldots, v_t$, so we can color it in $\lambda - d_i$ ways. □

It is also easy to determine the independence polynomial of a threshold graph.

Theorem 2.10.3. *Let G be a threshold graph of Kelmans transformation with degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. Let t be the unique integer for which $d_t = t - 1$, i.e. , for which $v_1, \ldots, v_t$ induces a clique, but v_t and v_{t+1} are not connected. Then the independence polynomial of G is*

$$I(G, x) = (1 - x)^{n-t} - x \sum_{i=1}^{t}(1 - x)^{n-1-d_i}.$$

Proof. Since every independent set can contain at most one vertex from the clique induced by the vertices of $v_1, \ldots, v_t$ we can decompose the terms of the independence polynomials as follows. Those independent sets which does not contain any of the vertex $v_1, \ldots, v_t$ contribute

$(1-x)^{n-t}$ to the sum. Those independent sets which contain the vertex v_i $(1 \leq i \leq t)$ contribute $-x(1-x)^{n-1-d_i}$ to the sum. □

Remark 2.10.4. One can consider the previous theorem as an inclusion-exclusion formula. A more general formula can be found in [25].

It remains to consider the matching polynomials of the threshold graphs. In this case the answer is a bit more complicated. Some notation is in order. First of all, let $M(K_n, x) = H_n(x)$ for brevity. Furthermore, let G be a threshold graph with degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. Let t be the unique integer for which $d_t = t-1$, i.e., for which $v_1, \ldots, v_t$ induce a clique, but v_t and v_{t+1} are not adjacent and set

$$M(G, x) = P(n, t, d_{t+1}, \ldots, d_n; x).$$

Then we have

Theorem 2.10.5.

$$P(n, t, d_{t+1}, \ldots, d_n; x) = xP(n-1, t, d_{t+1}, \ldots, d_{n-1}; x)$$

$$-d_n P(n-1, t-1, d_{t+1}-1, \ldots, d_{n-1}-1; x)$$

Furthermore,

$$P(n, t, d_{t+1}, \ldots, d_n; x) = \sum_{k=0}^{n-t} \widetilde{\sigma}_k(d_{t+1}, \ldots, d_n)(-1)^k x^{n-t-k} H_{t-k}(x),$$

where

$$\widetilde{\sigma}_k(r_1, \ldots, r_m) = \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq m} (r_{i_1} - k + 1)(r_{i_2} - k + 2) \ldots (r_{i_{k-1}} - 1) r_{i_k}.$$

Proof. The recursion follows from the recursion formula for the matching polynomial applied to the edges incident to v_n: if $e = (v_i, v_n) \in E(G)$ then $G - \{v_i, v_n\}$ is a threshold graph with the matching polynomial $P(n-1, t-1, d_{t+1}-1, \ldots, d_{n-1}-1; x)$. If $d_n = 0$ then the second term vanishes and so it does not cause any problem that $P(n-1, t-1, d_{t+1}-1, \ldots, d_{n-1}-1; x)$ is not the matching polynomial of $G - v_n$ and maybe meaningless. The other formula for the matching polynomial easily follows from the recursion formula. □

2.11 Concluding remarks

In this last section we wish to make some remarks on the use of the Kelmans transformation. As one can see the threshold graphs of these transformations are very special, so the use of this transformation is restricted to those problems where the extremal graph is conjectured to belong to this class of graphs. But if it is the case then the Kelmans transformation is probably the right tool to attack the problem. One of its main strengths is that it is very simple to work with. The other strength of this transformation is that it is very compatible with the deletion-contraction algorithms; in most of the proofs we used only some special recursion formula for the corresponding polynomial.

Although the Kelmans transformation could handle various problems, the reason why it worked maybe totally different. We try to explain it through two examples. If we are looking for the graph maximizing the spectral radius among graphs with prescribed number of edges then we know from Rowlinson's result [58] that the extremal graph is as "clique-like" as it is possible. The Kelmans transformation works properly because it makes the graphs more "clique-like". Now if we consider the problem of finding the graph maximizing the largest root of the matching polynomial among graphs with prescribed number of edges, the situation is completely different. We believe that the Kelmans transformation works because it generates some large-degree vertices. We conjecture that in this case the extremal graph will be as "star-like" as it is possible: it has as many vertices of degree $n-1$ as it is possible and one more vertex of the clique part of the threshold graph has some additional edges.

2.12 Afterlife

Tamás Terpai [61] managed to prove Nikiforov's original conjecture, namely he proved that

$$\mu(G)+\mu(\overline{G})\leq \frac{4}{3}n-1.$$

He used analytic tools to prove the statement.

Chapter 3

On a poset of trees: applications of the generalized tree shift

In this chapter we survey the applications of the so-called generalized tree shift. This graph transformation was developed by the author so as to attack an extremal graph theoretic problem of V. Nikiforov on the minimum number of closed walks. Nikiforov conjectured that the minimal number of the closed walks of length ℓ attained at the path among trees on a fixed number of vertices; Nikiforov's conjecture was motivated by the corresponding conjecture of J. A. de la Peña, I. Gutnam and J. Rada concerning the so-called Estrada index. This graph transformation can be applied to trees and the image of the tree at this transformation is also a tree. If we say that the image is "greater" than the original tree, then this way we obtain a partially ordered set on the set of trees on a fixed number of vertices: the induced poset of the generalized tree shift. It will turn out that the the minimal element of this induced poset is the path on n vertices while its maximal element is the star on n vertices. The main strength of this transformation lies in the fact that surprisingly many graph parameters behave the same way along this induced poset.

Definition 3.0.1. Let T be a tree and let x and y be vertices such that all the interior points of the path xPy (if they exist) have degree 2 in T. The *generalized tree shift* (GTS) of T is the tree T' obtained from T as follows: let z be the neighbor of y lying on the path xPy, let us erase all the edges between y and $N_T(y)\backslash\{z\}$ and add the edges between x and $N_T(y)\backslash\{z\}$. See Figure 3.1.

In what follows we call x the beneficiary and y the candidate (for being a leaf) of the generalized tree shift. Observe that we can exchange the role of the beneficiary and the candidate, the resulting trees will be isomorphic. Hence the resulting tree T' only depends on the tree T and the path xPy.

Note that if x or y is a leaf in T then $T' \cong T$, otherwise the number of leaves in T' is the number of leaves in T plus one. In this latter case we call the generalized tree shift proper.

Remark 3.0.2. Note that x and y need not have degree 2.

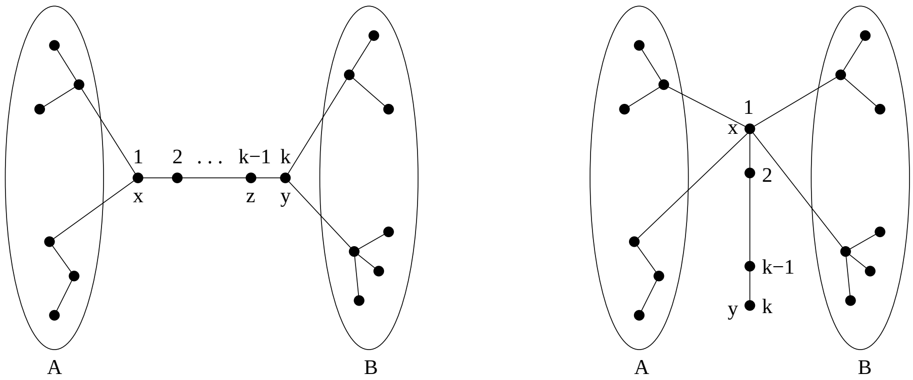

Figure 3.1: The generalized tree shift.

Notation: Throughout this chapter we will assume that the path xPy has exactly k vertices. In the following we call the vertices of the path xPy $1, 2, \ldots, k$ if the path consists of k vertices in such a way that x will be 1 and y will be k. The set $A \subset V(T)$ consists of the vertices which can be reached with a path from k only through 1, and similarly the set $B \subset V(T)$ consists of those vertices which can be reached with a path from 1 only through k. For the sake of simplicity, let A and B denote the corresponding sets in T'. The set of neighbors of 1 in A is called A_0, and similarly B_0 is the set of neighbors of 1 in $B \subset V(T')$ and the set of neighbors of k in $B \subset V(T)$. Let H_1 be the tree induced by the vertices of $A \cup \{1\}$ in T, similarly let H_2 denote the tree induced by the vertices of $B \cup \{k\}$ in T. Note that H_1 and H_2 are both subtrees of T' as well.

Definition 3.0.3. Let us say that $T' > T$ if T' can be obtained from T by some proper generalized tree shift. The relation $>$ induces a poset on the trees on n vertices, since the number of leaves of T' is greater than the number of leaves of T, more precisely the two numbers differ by one. Hence the relation $>$ is indeed extendable.

One can always apply a proper generalized tree shift to any tree which has at least two vertices that are not leaves. This shows that the only maximal element of the induced poset is the star. The following theorem shows that the only minimal element of the induced poset, i.e., the smallest element is the path.

Theorem 3.0.4. *Every tree different from the path is the image of some proper generalized tree shift.*

Proof. Let T be a tree different from the path, i.e., it has at least one vertex having degree greater or equal to 3. Let v be a vertex having degree one. Furthermore, let w be the closest vertex to v which has degree at least 3. Then the interior vertices (if they exist) of the path

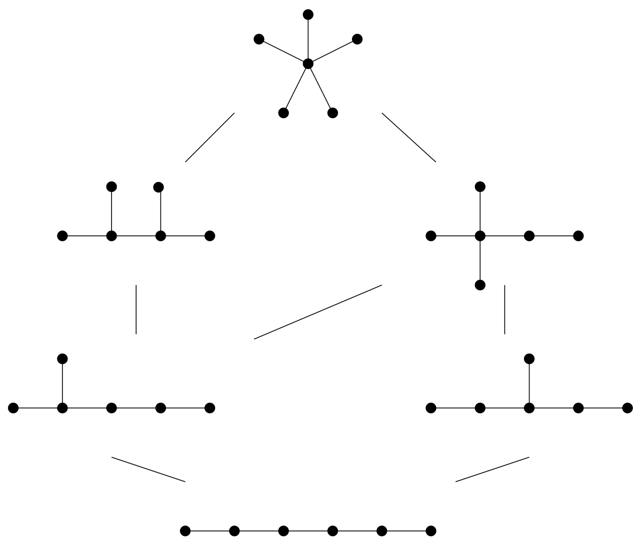

Figure 3.2: The poset of trees on 6 vertices.

induced by v and w have degree 2. The vertex w has at least two neighbors different from the one which lies on the path induced by v and w, so we can decompose these neighbors into two non-empty sets, A_0 and B_0. Let T^* be the tree given by erasing the edges between w and B_0 and adding the edges between v and B_0. Then T can be obtained from T^* by the GTS, where w is the beneficiary and v is the candidate. Since A_0 and B_0 are non-empty, this is a proper generalized tree shift. □

Corollary 3.0.5. *The star is the greatest, the path is the smallest element of the induced poset of the generalized tree shift.*

Remark 3.0.6. One can define a poset on trees induced by the original Kelmans transformation in the same way we defined the poset induced by GTS. Then it is true that the star is the greatest element of the poset induced by the original Kelmans transformation, but it is not true that the path is the only minimal element of this poset. The graph in Figure 3.3 is not the image of any Kelmans transformation. This explains why we needed to generalize this concept.

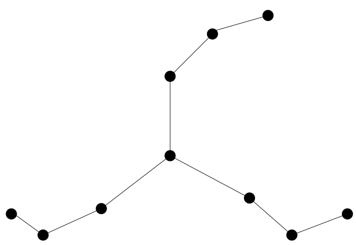

Figure 3.3: A tree which is not the image of Kelmans transformation.

3.1 Some elementary properties of GTS

Let $d(x, y)$ denote the distance of the vertices x and y. The Wiener-index of a graph is $\sum_{x,y} d(x, y)$.

Theorem 3.1.1. *The proper generalized tree shift decreases the Wiener-index.*

Proof. Let T be a tree and T' its image by a GTS. Let d_T and $d_{T'}$ be the distance in the corresponding graphs.

Clearly,

$$d_{T'}(i, a) + d_{T'}(k + 1 - i, a) = d_T(i, a) + d_T(k + 1 - i, a)$$

for all $a \in A$ and

$$d_{T'}(i, b) + d_{T'}(k + 1 - i, b) = d_T(i, b) + d_T(k + 1 - i, b)$$

for all $b \in B$, where the vertex $i \in \{1, 2, \ldots, k\}$ lies on the path xPy in the trees T and T'.

Trivially, $d_{T'}(a, a') = d_T(a, a')$ for $a, a' \in A$, $d_{T'}(b, b') = d_T(b, b')$ for $b, b' \in B$ and $d_T(a, b) = d_{T'}(a, b) + (k - 1)$ for $a \in A$ and $b \in B$.

Altogether we have

$$\sum_{x,y} d_T(x, y) = \sum_{x,y} d_{T'}(x, y) + (k - 1)|A||B|.$$

Hence the generalized tree shift decreases $\sum_{x,y} d(x, y)$. □

Corollary 3.1.2. *The path maximizes, the star minimizes the Wiener-index among the trees on n vertices.*

Proof. It follows from the previous theorem and the fact that the path is the only minimal, the star is the only maximal element of the induced poset of the generalized tree shift. □

Remark 3.1.3. Corollary 3.1.2 was known [45].

A bit more advanced property of the generalized tree shift is the following.

Theorem 3.1.4. *The generalized tree shift increases the spectral radius of the tree.*

Proof. Let u and v be the beneficiary and the candidate of the generalized tree shift, respectively. First of all, recall that if we change the role of the beneficiary and the candidate then the resulting tree will not change up to isomorphism.

Let $\underline{x}$ be the non-negative eigenvector of unit length corresponding to the largest eigenvalue of the tree T. By the previous paragraph we can assume that $x_u \geq x_v$.

Furthermore, let $A(T)$ and $A(T')$ be the adjacency matrices of the tree T and T'. Then

$$\mu(T) = \underline{x}^T A(T)\underline{x} = \underline{x}^T A(T')\underline{x} - 2(x_u - x_v) \sum_{w \in B_0} x_w \leq \underline{x}^T A(T')\underline{x} \leq$$

$$\leq \max_{||\underline{y}||=1} \underline{y}^T A(T')\underline{y} = \mu(T').$$

Hence $\mu(T) \leq \mu(T')$.

$\square$

Corollary 3.1.5. *The path minimizes, the star maximizes the spectral radius of the adjacency matrix among the trees on n vertices.*

Remark 3.1.6. Corollary 3.1.5 was known, it was proved by L. Lovász and J. Pelikán [46]. In fact, they proved their theorem by the aid of some graph transformation which is a special case of the generalized tree shift.

We mention that Nikiforov's inequality [52]

$$\mu(G) \leq \sqrt{2e(G)\left(1 - \frac{1}{\omega(G)}\right)}$$

also implies that the star has maximal spectral radius among trees since we have $e(G) = n - 1$ and $\omega(G) = 2$ and the greatest eigenvalue of the star is exactly $\sqrt{n-1}$. (It was Nosal who proved that for triangle-free graphs $\mu(G) \leq \sqrt{e(G)}$ holds, later Nikiforov [53] proved that in Nosal's inequality equality holds if and only if the graph is complete bipartite with some isolated vertices.)

Theorem 3.1.7. *The generalized tree shift increases the spectral radius of the complement of a tree.*

Proof. Let u and v be the beneficiary and the candidate of the generalized tree shift, respectively. Let $\underline{x}$ be the non-negative eigenvector of unit length corresponding to the largest eigenvalue of the graph $\overline{T}$. As before, we can assume that $x_v \geq x_u$.

Furthermore, let $A(\overline{T})$ and $A(\overline{T'})$ be the adjacency matrix of the $\overline{T}$ and $\overline{T'}$. Then

$$\mu(\overline{T}) = \underline{x}^T A(\overline{T'})\underline{x} - 2(x_v - x_u) \sum_{w \in B_0} x_w \leq \underline{x}^T A(\overline{T'})\underline{x} \leq$$

$$\leq \max_{||\underline{y}||=1} \underline{y}^T A(\overline{T'})\underline{y} = \mu(\overline{T'}).$$

Hence $\mu(\overline{T}) \leq \mu(\overline{T'})$. $\square$

Corollary 3.1.8. *If T is a tree on n vertices, P_n and S_n are the path and the star on n vertices and $\mu(G)$ is the spectral radius of a graph then*

$$\mu(\overline{P_n}) \leq \mu(\overline{T}) \leq \mu(\overline{S_n}).$$

3.2 Graph polynomials and the generalized tree shift

In this section we give a general overview how to use the generalized tree shift in the situations when we would like to prove that certain graph polynomial has the largest coefficients for the star and smallest coefficients for the path among the trees on n vertices, or we would like to prove that the largest real root of the polynomial is maximal for the star and minimal for the path.

Assume that given a graph polynomial $f(G,x)$. We will see that in many cases we have an identity of the following kind:

$$f(T',x) - f(T,x) = c_1 h(P_k,x) h(H_1,x) h(H_2,x),$$

where $h(G,x) = c_2 f(G,x) + c_3 g(G|v,x)$ and c_1, c_2, c_3 are rational functions of x and $g(G|v,x)$ is some graph polynomial depending on G and some special vertex v. (Recall that H_1 and H_2 are the subtrees of T and T' induced by the vertex set $A \cup \{1\}$ and $B \cup \{k\}$, respectively.) Generally, the graph polynomial $g(G|v,x)$ is very strongly related to $f(G,x)$, in many cases it will be $f(H,x)$ for some subgraph H of G. This means that the difference $f(T',x) - f(T,x)$ factorizes to polynomials of trees which are subtrees of both T and T'. Then we use some monotonicity property of the studied parameter to deduce that the generalized tree shift increases (decreases) this parameter. Clearly, it yields the desired result for the extremality of the star and the path. We have to emphasize that the monotonicity of the parameter is indeed crucial in many applications. Sometimes it will be more tedious to settle the suitable monotonicity property than to prove the proper identity for $f(T',x) - f(T,x)$. (Although we settle many monotonicity property in the Appendix.)

How will we obtain the above identity for $f(T',x) - f(T,x)$? There is a very straightforward way of doing that. We only need to compute a recursion formula for $M_1 : M_2$ (this graph was defined in the notation).

Observe that $T = (H_1 : P_k) : H_2$, where we identify $1 \in V(H_1)$ and $1 \in V(P_k)$ and then we identify $k \in V(P_k)$ and $k \in V(H_2)$. While for the image of T at the generalized tree shift applied to the tree T and P_k, we have $T' = (H_1 : H_2) : P_k$, where we identify $1 \in V(H_1)$ and $1 \in V(H_2)$ and then we identify $1 \in V(H_1 : H_2)$ and $1 \in V(P_k)$. So if we have some recursion formula for $M_1 : M_2$ then we can express

$$f(T,x) = h_1(f(P_k,x), g(P_k|1,x), f(H_1,x), g(H_1|1,x), f(H_2,x), g(H_2|k,x))$$

and

$$f(T',x) = h_2(f(P_k,x), g(P_k|1,x), f(H_1,x), g(H_1|1,x), f(H_2,x), g(H_2|k,x)).$$

Although this strategy would be very straightforward, the amount of computation we need to perform heavily depends on the polynomial $f(G,x)$ and sometimes it is indeed a huge work. To avoid this, we will prove a theorem which directly computes $f(T,x) - f(T',x)$ from the recursion formula of $f(M_1 : M_2)$.

3.3 General lemma

Theorem 3.3.1. *(General lemma.) Assume that the graph polynomials f and g satisfy the following recursion formula:*

$$f(M_1 : M_2, x) = c_1 f(M_1, x) f(M_2, x) + c_2 f(M_1, x) g(M_2|u_2, x) +$$

$$+ c_2 g(M_1|u_1, x) f(M_2, x) + c_3 g(M_1|u_1, x) g(M_2|u_2, x),$$

where c_1, c_2, c_3 are rational functions of x. Assume that $c_2 f(K_2) + c_3 g(K_2|1) \neq 0$. Then

$$f(T) - f(T') = c_4 (c_2 f(P_k) + c_3 g(P_k|1))(c_2 f(H_1) + c_3 g(H_1|1))(c_2 f(H_2) + c_3 g(H_2|k)),$$

where

$$c_4 = \frac{g(P_3|1) - g(P_3|2)}{(c_2 f(K_2) + c_3 g(K_2|1))^2}.$$

Proof. Since $T = ((H_1|1) : (P_k|1)|k) : (H_2|k)$ we have

$$f(T) = c_1 f(H_1 : P_k) f(H_2) + c_2 f(H_1 : P_k) g(H_2|k) =$$

$$+ c_2 g(H_1 : P_k|k) f(H_2) + c_3 g(H_1 : P_k|k) g(H_2|k).$$

Similarly, $T' = ((H_1|1) : (P_k|1)|1) : (H_2|1)$ so

$$f(T') = c_1 f(H_1 : P_k) f(H_2) + c_2 f(H_1 : P_k) g(H_2|1) +$$

$$+ c_2 g(H_1 : P_k|1) f(H_2) + c_3 g(H_1 : P_k|1) g(H_2|1).$$

Note that $g(H_2|1) = g(H_2|k)$, since 1 and k denote the same vertex, only their names are different in the different trees. Hence

$$f(T) - f(T') = (c_2 f(H_2) + c_3 g(H_2|k))(g(H_1 : P_k|k) - g(H_1 : P_k|1)).$$

Now let us consider

$$\frac{f(T) - f(T')}{(c_2 f(H_1) + c_3 g(H_1|1))(c_2 f(H_2) + c_3 g(H_2|k))} = \frac{g(H_1 : P_k|k) - g(H_1 : P_k|1)}{c_2 f(H_1) + c_3 g(H_1|1)}.$$

The left hand side is symmetric in H_1 and H_2 so if we switch them we obtain that

$$\frac{g(H_1 : P_k|k) - g(H_1 : P_k|1)}{c_2 f(H_1) + c_3 g(H_1|1)} = \frac{g(H_2 : P_k|k) - g(H_2 : P_k|1)}{c_2 f(H_2) + c_3 g(H_2|1)}.$$

Hence this expression is the same for every graph H_1. In particular, we can apply it to K_2:

$$\frac{g(H_1 : P_k|k) - g(H_1 : P_k|1)}{c_2 f(H_1) + c_3 g(H_1|1)} = \frac{g(K_2 : P_k|k) - g(K_2 : P_k|1)}{c_2 f(K_2) + c_3 g(K_2|1)}.$$

In fact, applying the above computation for $H_1 = H_2 = K_2$ we obtain that

$$\frac{f(P_{k+2}) - f(Q_{k+2})}{(c_2 f(K_2) + c_3 g(K_2|1))^2} = \frac{g(K_2 : P_k|k) - g(K_2 : P_k|1)}{c_2 f(K_2) + c_3 g(K_2|1)},$$

where Q_{k+2} is the tree obtained from P_{k+1} by attaching a pendant edge to the second vertex. This will be the GTS-transform of P_{k+2} if we apply it to $H_1 = H_2 = K_2$ and the path P_k. Note that $Q_{k+2} = P_3 : P_k$, where we identified the middle vertex of P_3 and the endvertex of P_k. On the other hand, $P_{k+2} = P_3 : P_k$, where we identified the endvertices of P_3 and P_k. Hence

$$f(Q_{k+2}) = c_1 f(P_3) f(P_k) + c_2 g(P_3|2) f(P_k) + c_2 f(P_3) g(P_k|1) + c_3 g(P_3|2) g(P_k|1).$$

Similarly,

$$f(P_{k+2}) = c_1 f(P_3) f(P_k) + c_2 g(P_3|1) f(P_k) + c_2 f(P_3) g(P_k|1) + c_3 g(P_3|1) g(P_k|1).$$

Hence

$$f(P_{k+2}) - f(Q_{k+2}) = (g(P_3|1) - g(P_3|2))(c_2 f(P_k) + c_3 f(P_k|1)).$$

Putting all together we obtain that

$$f(T) - f(T') = c_4 (c_2 f(P_k) + c_3 g(P_k|1))(c_2 f(H_1) + c_3 g(H_1|1))(c_2 f(H_2) + c_3 g(H_2|k)),$$

where

$$c_4 = \frac{g(P_3|1) - g(P_3|2)}{(c_2 f(K_2) + c_3 g(K_2|1))^2}.$$

□

Remark 3.3.2. Throughout this chapter we will refer to Theorem 3.3.1 as General Lemma.

3.4 The adjacency polynomial

In this section we concern with the characteristic polynomial of the adjacency matrix. We have already seen that the GTS increases the spectral radius of the adjacency matrix. The main result of this section that it decreases the coefficients in absolute value.

Theorem 3.4.1. *The generalized tree shift decreases the coefficients of the characteristic polynomial in absolute value, i.e., if the tree T' is obtained from the tree T by some generalized tree shift then*

$$\phi(T, x) \gg \phi(T', x).$$

(Recall that $\phi(T, x) \gg \phi(T', x)$ means that all the coefficients of $\phi(T, x)$ in absolute value is at least as large as the corresponding coefficient of $\phi(T', x)$ in absolute value.)

Theorem A.1.20. [46] *For an arbitrary forest T we have*

$$\phi(T,x)=\sum_{k=0}^{n}(-1)^k m_k(T)x^{n-2k},$$

where $m_k(T)$ denotes the number of ways one can choose k independent edges of the forest T. Consequently,

$$\phi(T,x)=\phi(T-e,x)-\phi(T-\{u,v\},x)$$

holds for an arbitrary edge $e=(u,v)$.

Remark 3.4.2. We need to prove that $m_k(T)\geq m_k(T')$ for every $1\leq k\leq n$. One can do it by purely combinatorial tools, but in order to show our strategy in work we chose an algebraic way.

Lemma 3.4.3. *With the notation introduced in the introduction, for the trees T and T' we have*

$$\phi(T,x)-\phi(T',x)=\phi(P_{k-2},x)(\phi(H_1,x)-x\phi(H_1-\{1\},x))(\phi(H_2,x)-x\phi(H_2-\{1\},x)).$$

To prove this lemma we need the following formula for the characteristic polynomial of $M_1:M_2$.

Lemma 3.4.4. *For the graphs $M_1:M_2$ we have*

$$\phi(M_1:M_2,x)=\phi(M_1,x)\phi(M_2-u_2,x)+\phi(M_1-u_1,x)\phi(M_2,x)-x\phi(M_1-u_1,x)\phi(M_2-u_2,x).$$

Proof. This is Corollary 3.3 in Chapter 4 of [30]. Another proof can be given by copying the argument of Lemma 3.5.5. □

Proof of Lemma 3.4.3. By the previous lemma we can apply the General Lemma for $f(G,x)=\phi(G,x)$, $g(G|v,x)=\phi(G-v,x)$ and $c_1=0,c_2=1,c_3=-x$.

We have $\phi(K_2,x)-x\phi(K_1,x)=(x^2-1)-x^2=-1$ and

$$\phi(P_3-\{1\},x)-\phi(P_3-\{2\},x)=(x^2-1)-x^2=-1.$$

Finally,

$$x\phi(P_{k-1},x)-\phi(P_k,x)=\phi(P_{k-2},x).$$

Hence

$$\phi(T,x)-\phi(T',x)=\phi(P_{k-2},x)(\phi(H_1,x)-x\phi(H_1-\{1\},x))(\phi(H_2,x)-x\phi(H_2-\{1\},x)).$$

□

From this one can easily deduce Theorem 3.4.1 as follows.

Proof of Theorem 3.4.1. Note that from Theorem A.1.20 we have

$$(-i)^n\phi(ix) = \sum_{r=0}^{\lfloor n/2 \rfloor} m_r(G)x^{n-2r},$$

where i is the square root of -1. Hence

$$\sum_{r=0}^{n}(m_r(T) - m_r(T'))x^{n-2r} = (-i)^n(\phi(T, ix) - \phi(T', ix)) =$$

$$= (-i)^{k-2}\phi(P_{k-2}, ix)((-i)^{a+1}\phi(H_1, ix) - (-i)^{a+1}(ix)\phi(H_1 - \{1\}, ix))\cdot$$
$$\cdot((-i)^{b+1}\phi(H_2, ix) - (-i)^{b+1}(ix)\phi(H_2 - \{1\}, ix)),$$

where $|V(H_1)| = a + 1$, $|V(H_2)| = b + 1$ and $|V(T)| = |V(T')| = n = a + b + k$. Note that $x\phi(H_j - \{1\}, x)$ is the characteristic polynomial of the forest H_j^* which can be obtained from H_j by deleting the edges incident to the vertex 1 (but we do not delete the vertex). Hence

$$\sum_{r=0}^{n}(m_r(T) - m_r(T'))x^{n-2r} =$$

$$= \left(\sum_{r=0}^{n} m_r(P_{k-2})x^{n-2r}\right)\left(\sum_{r=0}^{n}(m_r(H_1) - m_r(H_1^*))x^{n-2r}\right)\left(\sum_{r=0}^{n}(m_r(H_2) - m_r(H_2^*))x^{n-2r}\right).$$

Since $m_r(H_j) \geq m_r(H_j^*)$, all the coefficients of the right hand side are non-negative. Hence $m_r(T) \geq m_r(T')$. ☐

Remark 3.4.5. Theorem 3.1.4 can be deduced from Lemma 3.4.3 as well.

3.5 The Laplacian characteristic polynomial

Let $L(G)$ be the Laplacian matrix of G (so $L(G)_{ii} = d_i$ and $-L(G)_{ij}$ is the number of edges between i and j if $i \neq j$); recall that the Laplacian polynomial of the graph G is the polynomial $L(G, x) = \det(xI - L(G))$, i.e., it is the characteristic polynomial of the Laplacian matrix of G.

Let $L(G|u)$ be the matrix obtained from $L(G)$ by deleting the row and the column corresponding to the vertex u (warning: this is not $L(G - u)$ because of the diagonal elements). Furthermore, let $L(G|u, x)$ denote the characteristic polynomial of $L(G|u)$.

We will subsequently use the following two classical facts, for details see [32] or the Appendix.

Statement A.2.2. *The eigenvalues of $L(G)$ are non-negative real numbers, at least one of them is 0. Hence we can order them as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n = 0$.*

Corollary A.2.3. *The Laplacian polynomial can be written as*

$$L(G, x) = x^n - a_{n-1}x^{n-1} + a_{n-2}x^{n-2} - \cdots + (-1)^{n-1}a_1 x,$$

where $a_1, a_2, \ldots, a_{n-1}$ are positive integers.

Recall that we also use the notation $\lambda_{n-1}(G) = a(G)$ for the so-called algebraic connectivity of the graph G. We have also introduced the notation $\theta(G)$ for the Laplacian spectral radius $\lambda_1(G)$.

The main result of this section is the following.

Theorem 3.5.1. *The generalized tree shift decreases the coefficients of the Laplacian polynomial in absolute value, i.e., if T' is obtained from T by a generalized tree shift then*

$$L(T, x) \gg L(T', x)$$

or in other words $a_k(T) \geq a_k(T')$ for $k = 1, \ldots, n-1$. Furthermore, $\theta(T') \geq \theta(T)$ and $a(T') \geq a(T)$.

Corollary 3.5.2. *Let $L(G, x) = \sum_{k=1}^{n}(-1)^{n-k}a_k(G)x^k$. Then*

$$a_k(P_n) \geq a_k(T) \geq a_k(S_n).$$

for any tree T on n vertices and $k = 1, \ldots, n-1$. Furthermore,

$$\theta(P_n) \leq \theta(T) \leq \theta(S_n),$$

and

$$a(P_n) \leq a(T) \leq a(S_n).$$

Remark 3.5.3. All parts of Corollary 3.5.2 are known. The first statement concerning the coefficients of the Laplacian polynomial was conjectured in [36] and was proved by B. Zhou and I. Gutnam [68] by the aid of a surprising connection between the Laplacian polynomial and the adjacency polynomial of trees. A different proof was given by B. Mohar [49] using graph transformations.

The maximality of the star concerning the Laplacian spectral radius is trivial since $\theta(S_n) = n$, because $\overline{S_n}$ is not connected and this is the maximal value for a graph on n vertices. The minimality of the path is proved in [37].

The first statement concerning the algebraic connectivity (the minimality of the path) was proved by Grone and Merris [34], the second statement was proved by Merris [48]. Guo [35] gave new proofs for both parts by using graph transformations.

Again we will prove a product formula for $L(T, x) - L(T', x)$.

Lemma 3.5.4. *With our usual notation we have*

$$L(T,x) - L(T',x) = \frac{1}{x}L(P_{k-1},x)(L(H_1,x) - xL(H_1|1,x))(L(H_2,x) - xL(H_2|k,x)).$$

Lemma 3.5.5. *As usual, let $M_1 : M_2$ denote the graph obtained from M_1, M_2 by identifying the vertices u_1 and u_2. Then*

$$L(M_1 : M_2, x) = L(M_1,x)L(M_2|u_2,x) + L(M_2,x)L(M_1|u_1,x)-$$

$$-xL(M_1|u_1,x)L(M_2|u_2,x).$$

Proof. Let $|V(M_1)| = n_1$ and $|V(M_2)| = n_2$. Furthermore, let d_1 and d_2 be the degree of u_1 and u_2 in M_1 and M_2, respectively.

Let the rows and columns of $A = L(M_1 : M_2)$ ordered in such a way that the first n_1 rows and columns correspond to the vertices of M_1, while the last n_2 rows and columns correspond to the vertices of M_2. Hence, the n_1-th row and column correspond to the vertex $u_1 = u_2$.

The key observation is that if we consider the expansion of $\det(xI - A)$, none of the non-zero terms contain $a_{i,n_1}, a_{n_1,j}$ together, where $i < n_1 < j$. Indeed, a non-zero product should contain $n_1 - 1$ non-zero elements from the first $n_1 - 1$ columns and together with $a_{i,n_1}, a_{n_1,j}$, this would be $n_1 + 1$ elements from the first n_1 rows.

Similarly, none of the non-zero terms contain $a_{i,n_1}, a_{n_1,j}$ together, where $i > n_1 > j$.

So we can divide the non-zero terms of $\det(xI - A)$ into three classes. The first class contains those terms in which $x - a_{n_1,n_1} = x - d_1 - d_2$ appears. Their sum is clearly

$$(x - d_1 - d_2)L(M_1|u_1,x)L(M_2|u_2,x).$$

The second class contains those non-zero terms which contain an element $-a_{i,n_1}$ where $i < n_1$. These terms should contain $-a_{n_1,j}$ for some $j < n_1$. These terms contribute $\det(B_1)L(M_2|u_2,x)$ to the determinant, where B_1 is the matrix obtained from $xI - L(M_1)$ by replacing $x - a_{n_1,n_1}$ with 0. Then

$$\det(B_1) = L(M_1,x) - (x - d_1)L(M_1|u_1,x).$$

Finally, the third class contain those non-zero terms which contain an element $-a_{i,n_1}$, where $i > n_1$. These terms should contain $-a_{n_1,j}$ for some $j > n_1$. These terms contribute the sum $\det(B_2)L(M_1|u_1,x)$ where B_2 is the matrix obtained from $xI - L(M_2)$ by replacing $x - a_{n_1,n_1}$ with 0. Then

$$\det(B_2) = L(M_2,x) - (x - d_2)L(M_2|u_2,x).$$

Putting all these together we get

$$L(M_1 : M_2, x) = (x - d_1 - d_2)L(M_1|u_1,x)L(M_2|u_2,x)+$$

$$+(L(M_1,x) - (x - d_1)L(M_1|u_1,x))L(M_2|u_2,x) + (L(M_2,x) - (x - d_2)L(M_2|u_2,x))L(M_1|u_1,x)$$

$$= L(M_1,x)L(M_2|u_2,x) + L(M_2,x)L(M_1|u_1,x) - xL(M_1|u_1,x)L(M_2|u_2,x).$$

□

Proof of Lemma 3.5.4. By the previous Lemma we can apply the General Lemma with $f(G,x) = L(G,x)$, $g(G|v,x) = L(G|v,x)$ and $c_2 = 1, c_3 = -x$.

In this case, $L(K_2,x) - xL(K_2|1,x) = x(x-2) - x(x-1) = -x$ and $L(P_3|1,x) - L(P_3|2,x) = ((x-2)(x-1)-1) - (x-1)^2 = -x$. Furthermore, expanding the matrix of $L(P_k,x)$ according to the first row, we have

$$L(P_k,x) = (x-1)L(P_{k-1}|1,x) - L(P_{k-2}|1,x).$$

Hence

$$L(P_k,x) - xL(P_{k-1},x) = -L(P_{k-1}|1,x) - L(P_{k-2},x) = -L(P_{k-1},x).$$

Putting all together we get that

$$L(T,x) - L(T',x) = \frac{1}{x}L(P_{k-1},x)(L(H_1,x) - xL(H_1|1,x))(L(H_2,x) - xL(H_2|k,x)).$$

□

Now we are ready to prove Theorem 3.5.1. For the sake of convenience we repeat the corresponding part of the theorem which we prove.

Theorem 3.5.1 (First part.)

$$L(T,x) \gg L(T',x).$$

Proof. Let $|V(A)| = a$, $|V(B)| = b$, then $|V(T)| = |V(T')| = a+b+k$. Because of the alternating sign of the coefficients we have to prove that all the coefficients of

$$(-1)^{a+b+k}(L(T,-x) - L(T',-x))$$

are non-negative. Let $\widehat{L}(G,x) = (-1)^{|V(G)|}L(G,-x)$ and $\widehat{L}(G|v,x) = (-1)^{|V(G)|-1}L(G,-x)$, then $\widehat{L}(G,x)$ and $\widehat{L}(G|v,x)$ have only non-negative coefficients.

By Lemma 3.5.4 we have

$$\widehat{L}(T,x) - \widehat{L}(T',x) = (-1)^{a+b+k}(L(T,-x) - L(T',-x)) =$$

$$= (-1)^{a+b+k}\frac{L(P_{k-1},-x)}{-x}(L(H_1,-x) + xL(H_1|1,-x))(L(H_2,-x) + xL(H_2|1,-x)) =$$

$$= \frac{(-1)^{k-1}L(P_{k-1},-x)}{x}((-1)^{a+1}L(H_1,-x) - x(-1)^a L(H_1|1,-x))\cdot$$

$$\cdot((-1)^{b+1}L(H_2,-x) - x(-1)^b L(H_2|1,-x)) =$$

$$= \frac{1}{x}\widehat{L}(P_{k-1},x)(\widehat{L}(H_1,x) - x\widehat{L}(H_1|1,x))(\widehat{L}(H_2,x) - x\widehat{L}(H_2|1,x)).$$

We know that all coefficients of $\widehat{L}(P_{k-1},x)$ are non-negative. We show that the coefficients of the polynomials $\widehat{L}(H_1,x) - x\widehat{L}(H_1|1,x)$ and $\widehat{L}(H_2,x) - x\widehat{L}(H_2|1,x)$ are also non-negative. Clearly, it is enough to show it for the former one.

For any matrix B we have

$$f(B,x)=\det(xI-B)=\sum_{r=0}^{n}(-1)^{n-r}(\sum_{|S|=r}\det(B_S))x^r,$$

where the matrix B_S is obtained from by deleting the rows and columns corresponding to the elements of the set S. In other words,

$$\widehat{f}(B,x)=(-1)^n\det(-xI-B)=\det(xI+B)=\sum_{r=0}^{n}(\sum_{|S|=r}\det(B_S))x^r.$$

Hence

$$\widehat{L}(H_1,x)-x\widehat{L}(H_1|1,x))=\sum_{r=0}^{n}\left(\sum_{|S|=r,"1"\notin S}^{n}\det(L(H_1)_S)\right)x^r.$$

Since $L(H_1)$ is a positive semidefinite matrix, all subdeterminants of it are non-negative. This proves that the coefficients are indeed non-negative.

□

Remark 3.5.6. We have already shown that the generalized tree shift decreases the Wiener-index of a tree (see Theorem 3.1.1). One can consider Theorem 3.5.1 as a generalization of this fact since the signless coefficient of x^2 in the Laplacian polynomial is just the Wiener-index ([66] or Corollary A.2.10 in the Appendix).

Theorem 3.5.1 (Second part.)

$$a(T')\geq a(T).$$

For the proof some preparation is needed. We will use the following fundamental lemmas. These are proved in the Appendix under the name Lemma A.2.14 and Corollary A.2.16.

Lemma A.2.14. *(Interlacing lemma) Let G be a graph and e an edge of it. Let $\lambda_1\geq\lambda_2\geq\dots\lambda_{n-1}\geq\lambda_n=0$ be the roots of $L(G,x)$ and let $\tau_1\geq\tau_2\geq\dots\tau_{n-1}\geq\tau_n=0$ be the roots of $L(G-e,x)$. Then*

$$\lambda_1\geq\tau_1\geq\lambda_2\geq\tau_2\geq\dots\geq\lambda_{n-1}\geq\tau_{n-1}.$$

Corollary A.2.16. *Let T_1 be a tree and T_2 be its subtree. Then $a(T_1)\leq a(T_2)$.*

For the sake of simplicity, we introduce the polynomials

$$h(G,x)=(-1)^{n-1}\frac{1}{x}L(G,x)\quad\text{and}\quad r(G,x)=(-1)^{n-1}L(G|u,x),$$

where G is a graph on n vertices. It will be convenient to use the notation $a(p(x))$ for the smallest positive root of the polynomial $p(x)$.

The slight advantage of these polynomials is that they are non-negative at 0, more precisely $r(G,0)$ is the number of spanning trees while $h(G,0)$ is n times the number of spanning trees. So for a tree T we have $h(T,0)=n$ and $r(T,0)=1$.

Now we are ready to prove the second part of Theorem 3.5.1.

Proof. Let us rewrite the formula of Lemma 3.5.4 in terms of the polynomials h and r. For the sake of brevity, let $h(H_i,x)=h_i(x)$ and $r(H_i,x)=r_i(x)$. Since $V(H_1)=a+1$, $V(H_2)=b+1$, $V(P_k)=k$ we have

$$(-1)^{a+b+k}x(h(T,x)-h(T',x))=$$
$$(-1)^{k-1}h(P_{k-1},x)((-1)^a xh_1(x)-x(-1)^a r_1(x))((-1)^b xh_2(x)-x(-1)^b r_2(x)).$$

Hence

$$h(T',x)=h(T,x)+xh(P_{k-1},x)(h_1(x)-r_1(x))(h_2(x)-r_2(x)).$$

Since all of these polynomials are positive in 0 we have

$$a(T')\geq \min(a(T),a(P_{k-1}),a(h_1-r_1),a(h_2-r_2)).$$

We only need to show that

$$\min(a(T),a(P_{k-1}),a(h_1-r_1),a(h_2-r_2))=a(T).$$

Clearly, $a(P_{k-1})\geq a(T)$ because P_{k-1} is a subtree of T, so we can apply Corollary A.2.16. Next we show that $a(h_1-r_1)\geq a(T)$. In fact, it will turn out that $a(h_1-r_1)\geq a(h_1)$; but then we are done since H_1 is a subtree of T so $a(h_1)\geq a(T)$.

Now we prove that $a(h_1-r_1)\geq a(h_1)$. The roots of the polynomial h_1 are the roots of $L(H_1,x)$ without 0: $\lambda_1\geq\dots\geq\lambda_a>0$. The roots of the polynomial r_1 are the roots of $L(H_1|1,x)$: $\lambda'_1\geq\dots\geq\lambda'_a>0$. By the interlacing theorem for symmetric matrices, we have

$$\lambda_1\geq\lambda'_1\geq\lambda_2\geq\lambda'_2\geq\dots\geq\lambda_a\geq\lambda'_a>0.$$

Assume for a moment that these roots are all different. Since h_1-r_1 is positive in 0, namely $h_1(0)-r_1(0)=(a+1)-1=a$ we get that h_1-r_1 is positive in the interval $[\lambda'_j,\lambda_j]$ if $a-j$ is odd and negative if $a-j$ is even, because the sign of h_1 and r_1 are different at these intervals. So there must be a root of h_1-r_1 in the interval $(\lambda_j,\lambda'_{j-1})$ for $j=1,\dots,a-1$. But h_1-r_1 is a polynomial of degree $a-1$, so we have found all of its roots. Hence there cannot be any root in the interval $[0,\lambda_a]$. Clearly, this argument with a slight modification still holds if some roots coincide: one can consider the intervals of length 0 as infinitely small intervals. Hence $a(h_1-r_1)\geq a(h_1)$ and similarly $a(h_2-r_2)\geq a(h_2)$. Hence $a(T')\geq a(T)$.

□

Theorem 3.5.1 (Third part.)

$$\theta(T') \geq \theta(T).$$

Disclaimer: the proof of this part is very similar to the proof of the previous part.

Here we need the other corollary of Lemma A.2.14.

Corollary A.2.15. *Let G_2 be a subgraph of G_1 then $\theta(G_2) \leq \theta(G_1)$.*

Proof. We will show that

$$L(T,x) - L(T',x) = \frac{1}{x} L(P_{k-1},x)(L(H_1,x) - xL(H_1|1,x))(L(H_2,x) - xL(H_2|k,x)) \geq 0$$

for $x \geq \theta(T')$ implying that $\theta(T') \geq \theta(T)$.

It is enough to show that $L(H_1,x) - xL(H_1|1,x) \leq 0$ for $x \geq \theta(H_1)$. Then by symmetry, we have $L(H_2,x) - xL(H_2|k,x) \leq 0$ for $x \geq \theta(H_2)$. Thus $L(T,x) - L(T',x) \geq 0$ for $x \geq \max(\theta(P_k), \theta(H_1), \theta(H_2))$. Since P_k, H_1, H_2 are all subgraphs of T' we have $\theta(T') \geq \max(\theta(P_k), \theta(H_1), \theta(H_2))$ by Corollary A.2.15. Hence $L(T,x) - L(T',x) \geq 0$ for $x \geq \theta(T')$.

Now let us prove that $L(H_1,x) - xL(H_1|1,x) \leq 0$ for $x \geq \theta(H_1)$. First of all, let us observe that $L(H_1,x) - xL(H_1|1,x)$ is a polynomial of degree a with main coefficient $-d_1$, where $|V(H_1)| = a+1$ and d_1 is the degree of the vertex 1. Let the roots of the polynomial $L(H_1,x)$ be $\lambda_1 \geq \cdots \geq \lambda_a = \lambda_{a+1} = 0$. The roots of the polynomial $L(H_1|1,x)$ are $\lambda'_1 \geq \cdots \geq \lambda'_a \geq 0$. By the interlacing theorem for symmetric matrices, we have

$$\lambda_1 \geq \lambda'_1 \geq \lambda_2 \geq \lambda'_2 \geq \cdots \geq \lambda_a \geq \lambda'_a \geq 0.$$

Assume for a moment that these roots are all different. Then $L(H_1,x) - xL(H_1|1,x)$ is positive in the interval $[\lambda'_j, \lambda_j]$ if j is odd and negative if j is even since both terms have the same sign. Hence there must be a root in the interval $(\lambda_{j+1}, \lambda'_j)$ for $j = 1, \ldots, a-1$ and 0 is also a root of the polynomial $L(H_1,x) - xL(H_1|1,x)$. This way we find all roots of this polynomial, thus $L(H_1,x) - xL(H_1|1,x) \leq 0$ if $x > \lambda'_1$, in particular if $x > \lambda_1$. Clearly, this argument also works if some λ_i, λ'_i coincide since the interlacing property still holds. ☐

3.6 The independence polynomial

Recall that we define the independence polynomial as

$$I(G,x) = \sum_{k=0}^{n} (-1)^k i_k(G) x^k,$$

where $i_k(G)$ denotes the number of independent sets of size k and $\beta(G)$ denotes the smallest real root of $I(G,x)$.

The main result of this section is the following.

Theorem 3.6.1. *Let T be a tree and T' is a tree obtained from T by a generalized tree shift. Then $I(T',x) \gg I(T,x)$ or in other words, $i_k(T') \geq i_k(T)$ for all $k \geq 1$. Furthermore, $\beta(T') \leq \beta(T)$.*

The first statement of the theorem is quite straightforward. The second statement needs some preparation, more precisely the preparation of the suitable monotonicity property. This is done in the Appendix; we will quote the statements from the Appendix which we will use.

Fact 1. (Statement A.1.4 and Remark A.1.5, [44]) The polynomial $I(G,x)$ satisfies the recursion

$$I(G,x) = I(G-v,x) - xI(G-N[v],x),$$

where v is an arbitrary vertex of the graph G.

Fact 2. (Statement A.1.4 and Remark A.1.5, [44]) The polynomial $I(G,x)$ satisfies the recursion

$$I(G,x) = I(G-e,x) - x^2 I(G-N[u]-N[v],x),$$

where $e = uv$ is an arbitrary edge of the graph G.

The following definition –together with the statements following it– will be the main tool to prove the second statement of Theorem 3.6.1. These statements are proved in the Appendix in a bit more general framework.

Definition A.1.6. Let $G_1 \succ G_2$ if $I(G_2,x) \geq I(G_1,x)$ on the interval $[0,\beta(G_1)]$.

Statement A.1.7. *The relation $\succ$ is transitive on the set of graphs and if $G_1 \succ G_2$ then $\beta(G_1) \leq \beta(G_2)$.*

Statement A.1.10. *If G_2 is a subgraph of G_1 then $G_1 \succ G_2$.*

Lemma 3.6.2. *We have*

$$I(M_1 : M_2, x) = I(M_1 - u_1, x)I(M_2 - u_2, x) - xI(M_1 - N[u_1], x)I(M_2 - N[u_2]).$$

Equivalently,

$$I(M_1 : M_2) = I(M_1)I(M_2) + xI(M_1)I(M_2 - N[u_2]) + xI(M_1 - N[u_1])I(M_2) +$$

$$+ (x^2 - x)I(M_1 - N[u_1])I(M_2 - N[u_2]).$$

Proof. In the first formula we simply separated those terms which contain the vertex $u_1 = u_2$ (second term) from the ones not containing $u_1 = u_2$ (first term).

The second formula simply follows from the first one by using the identity

$$I(M_j - u_j, x) = I(M_j, x) + xI(M_j - N[u_j], x)$$

for $j = 1, 2$. □

Lemma 3.6.3. *Let T be a tree and T' be obtained from T by a generalized tree shift. Then with the usual notation we have*

$$I(T, x) - I(T', x) = xI(P_{k-3})(I(A, x) - I(A - A_0, x))(I(B, x) - I(B - B_0, x)),$$

where we define $I(P_0, x) = I(P_{-1}, x) = 1$.

Proof. By the previous lemma we can use the General Lemma applied to $f(G, x) = I(G, x)$ and $g(G|v, x) = I(G - N[v], x)$ and $c_2 = x$, $c_3 = x^2 - x$.

Then $I(P_3 - N[1], x) - I(P_3 - N[2], x) = (1 - x) - 1 = -x$ and $xI(K_2, x) + (x^2 - x)I(K_2 - N[1], x) = x(1 - 2x) + (x^2 - x)1 = -x^2$. Furthermore,

$$xI(P_k) + (x^2 - x)I(P_{k-2}, x) = x(I(P_{k-1}, x) - xI(P_{k-2}, x)) + (x^2 - x)I(P_{k-2}, x) =$$

$$= x(I(P_{k-1}, x) - I(P_{k-2}, x)) = -x^2 I(P_{k-3}, x).$$

Finally,

$$x(I(H_1 - 1, x) + xI(H_1 - N[1], x)) + (x^2 - x)I(H_1 - N[1], x) =$$
$$= x(I(H_1 - 1, x) - I(H_1 - N[1], x) = x(I(A, x) - I(A - A_0, x)).$$

Similar statement holds for $xI(H_2, x) + (x^2 - x)I(H_2 - N[1], x)$. Putting all together we get that

$$I(T, x) - I(T', x) = xI(P_{k-3}, x)(I(A, x) - I(A - A_0, x))(I(B, x) - I(B - B_0, x)).$$

□

Now we are ready to prove Theorem 3.6.1.

Theorem 3.6.1. *Let T be a tree and T' be a tree obtained from T by a generalized tree shift. Then $I(T', x) \gg I(T, x)$ or in other words $i_k(T') \geq i_k(T)$ for all $k \geq 1$. Furthermore, $T' \succ T$ and so $\beta(T') \leq \beta(T)$.*

Proof. By Lemma 3.6.3 we have

$$I(T', -x) - I(T, -x) = xI(P_{k-3}, -x)(I(A, -x) - I(A - A_0, -x))(I(B, -x) - I(B - B_0, -x)).$$

Since on the left hand side we multiply polynomials of positive coefficients, we have $I(T', x) \gg I(T, x)$.

Now we prove the second statement. Since $A - A_0$ is a subgraph of A we have

$$I(A, x) - I(A - A_0, x) \leq 0$$

on the interval $[0, \beta(A)]$. Similarly,

$$I(B, x) - I(B - B_0, x) \leq 0$$

on the interval $[0, \beta(B)]$. Finally $I(P_{k-3}, x) \geq 0$ on the interval $[0, \beta(T')]$ since $T' \succ P_{k-3}$ because P_{k-3} is a subgraph of T'. It is also true that $\beta(A), \beta(B) \geq \beta(T')$ because of the same reason. Hence

$$I(T, x) - I(T', x) = xI(P_{k-3})(I(A, x) - I(A - A_0, x))(I(B, x) - I(B - B_0, x)) \geq 0$$

on the interval $[0, \beta(T')]$, i.e., we have $T' \succ T$ (and so $\beta(T') \leq \beta(T)$).

□

3.7 Edge cover polynomial

The concept of the edge cover polynomial was introduced by Saieed Akbari and Mohammad Reza Oboudi [1]. The edge cover polynomial is defined as follows.

Definition 3.7.1. Let G be a graph on n vertices and m edges. Let $e_k(G)$ denote the number of ways one can choose k edges that cover all vertices of the graph G. We call the polynomial

$$E(G, x) = \sum_{k=1}^{m} e_k(G) x^k$$

the *edge cover polynomial* of the graph G. Clearly, if the graph G has an isolated vertex then the edge cover polynomial is 0.

Let $\xi(G)$ denote the smallest real root of the edge cover polynomial.

Unfortunately, the parameter $\xi(G)$ is not a monotone parameter of graphs, not even for trees. Surprisingly, in spite of this fact, one can use the generalized tree shift to prove that the path and the star are the extremal cases. (Although, the star is not the only tree for which $\xi(T) = 0$.)

Theorem 3.7.2. *Let T be a tree on n vertices. Then*

$$\xi(P_n) \leq \xi(T) \leq \xi(S_n).$$

Furthermore, for any $1 \leq k \leq n - 1$ we have

$$e_k(S_n) \leq e_k(T) \leq e_k(P_n).$$

As usual, we prove a lemma connecting $E(T,x)$ and $E(T',x)$.

Lemma 3.7.3. *Let T be a tree and T' be the tree obtained from the tree T by a generalized tree shift. Then*

$$E(T,x) - E(T',x) = \frac{1}{x} E(P_k,x)E(H_1,x)E(H_2,x).$$

Lemma 3.7.4.

$$E(M_1 : M_2) = E(M_1)E(M_2) + E(M_1)E(M_2 - u_2) + E(M_1 - u_1)E(M_2).$$

Proof. The terms of $E(M_1 : M_2)$ are separated according to the vertex $u_1 = u_2$ is covered in the graph M_1, M_2 or both. □

Proof of Lemma 3.7.3. According to the previous lemma we can apply the General Lemma to $f(G,x) = E(G,x)$ and $g(G|v,x) = E(G - v,x)$ and $c_2 = 1$, $c_3 = 0$.

Then $E(P_3 - 1,x) - E(P_3 - 2,x) = x - 0 = x$ and $c_2 E(K_2,x) + c_3 E(K_2 - 1,x) = x$. Hence

$$E(T,x) - E(T',x) = \frac{1}{x} E(P_k,x)E(H_1,x)E(H_2,x).$$

□

Proof of Theorem 3.7.2. Since all the coefficients of the edge cover polynomial are non-negative we have $\xi(T) \leq 0 = \xi(S_n)$. (Note that $E(S_n,x) = x^{n-1}$.)

To prove the extremality of the path, we make the observation that

$$E(P_n,x) = \sum_{k=0}^{n} \binom{n-2-k}{k} x^{n-1-k}.$$

Indeed, $E(P_n,x) = x(E(P_{n-1},x) + E(P_{n-2},x))$ and $E(P_1,x) = 0, E(P_2,x) = x$. Thus $E(P_n,x)$ is a simple transform of the Chebysev polynomial of the second kind. This implies that

$$\xi(P_n) = -4\cos^2 \frac{\pi}{n-1}$$

if $n \geq 3$. In particular, $-\xi(P_n) > -\xi(P_{n-1}) > \cdots > -\xi(P_2)$.

Let $\lambda \geq -\xi(P_n)$ and set $c(T) = (-1)^{n-1}E(T,-\lambda)$. Clearly, $c(P_n) > 0$. We show that for all tree on n vertices we have $c(T) \geq c(P_n) > 0$. We prove it by induction on the number of vertices. By Lemma 3.7.3 we have

$$c(T') - c(T) = \frac{1}{\lambda} c(P_k)c(H_1)c(H_2).$$

By the induction hypothesis all terms on the right hand side are positive; indeed, $c(H_1) > c(P_{a+1}) > 0$ because $\lambda > -\xi(P_n) > -\xi(P_{a+1})$. Thus $c(T') > c(T)$. Since the smallest element of the poset induced by the generalized tree shift is the path on n vertices, this implies that $c(T) > c(P_n)$ indeed holds. Hence $E(T,x)$ has no root in the interval $(-\infty, \xi(P_n))$.

The second claim is trivial from Lemma 3.7.3 and from the fact that the star is the largest, the path is the smallest element of the induced poset of the generalized tree shift.

□

Remark 3.7.5. Although, we have no monotonicity for $\xi(T)$ in general, the weak monotonicity for the paths was enough to prove the statement.

In [21] one can find a strengthening of Theorem 3.7.2.

3.8 Walks in trees

In this section we prove Theorem 3.8.6 on the number $W_\ell(G)$ of closed walks of length ℓ which was already mentioned in the introduction. The importance of the parameter $W_k(G)$ lies in the fact that

$$W_k(G) = TrA^k = \sum_{i=1}^{n} \mu_i^k,$$

where the μ_i's $(i = 1, \dots, n)$ are the eigenvalues of the adjacency matrix A.

To prove our result, we need some preparation.

Definition 3.8.1. Let $\hat{G}_1$ be the tree consisting of a path on k vertices and two vertices adjacent to one of the endpoints of the path. Let $\hat{G}_2$ be the tree consisting of a path on k vertices and two vertices which are adjacent to different endpoints of the path; this is simply a path on $k+2$ vertices. We will refer to these graphs as the reduced graphs of the generalized tree shift. (See Figure 3.4.)

Notation: The vertices of the path in each reduced graph will be denoted by $1, 2, \dots, k$. The other two vertices are a and b. In $\hat{G}_1$ vertex 1 will be adjacent to a and b, in $\hat{G}_2$ vertex 1 will be adjacent to vertex a and vertex k will be adjacent to vertex b.

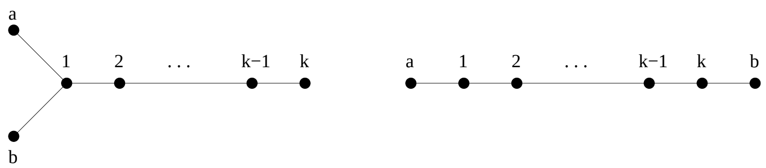

Figure 3.4: Reduced graphs of the generalized tree shift.

Definition 3.8.2. Let $\mathcal{R}(\ell, i, j, m, n)$ be the set of those walks of length ℓ in $\hat{G}_1$ which start at vertex i, finish at vertex j and visit vertex a exactly m times, vertex b exactly n times. Similarly let $\mathcal{D}(\ell, i, j, m, n)$ be the set of those walks of length ℓ in $\hat{G}_2$ which start at vertex i, finish at vertex j and visit vertex a exactly m times, vertex b exactly n times. The cardinality of $\mathcal{R}(\ell, i, j, m, n)$ and $\mathcal{D}(\ell, i, j, m, n)$ are denoted by $R(\ell, i, j, m, n)$ and $D(\ell, i, j, m, n)$, respectively.

Symmetry properties of the function R and D. Since we can "reflect" any walk of $\hat{G}_1$ in the "horizontal axis" of $\hat{G}_1$, i.e., we can exchange the a's and b's in any walk we have

$$R(\ell, i, j, m, n) = R(\ell, i, j, n, m)$$

for all ℓ, i, j, m, n.

Similarly, we can "reflect" any walk of $\hat{G}_2$ in the "vertical symmetry axis" of $\hat{G}_2$ and so we have

$$D(\ell, i, j, m, n) = D(\ell, k+1-i, k+1-j, n, m)$$

for all ℓ, i, j, m, n.

Lemma 3.8.3. *$R(\ell, 1, j, m, n) \geq D(\ell, 1, j, m, n)$, where $1 \leq j \leq k$.*

Proof. First we prove the statement in the case $m = 0$, $j = k$. Let $w_1 w_2 \dots w_{\ell+1}$ be a walk from 1 to k in $\hat{G}_2$ in which b occurs n times. Let us define $v_i = f(w_i)$ as follows:

$$f(w_i) = \begin{cases} k+1-s \text{ if } w_{\ell+2-i} = s, \\ \quad b \quad \text{if} \quad w_{\ell+2-i} = b. \end{cases}$$

Then $v_1 v_2 \dots v_{l+1}$ is a walk of length ℓ from 1 to k in $\hat{G}_1$ which contains b exactly n times. Hence we have proved that

$$R(\ell, 1, k, 0, n) = D(\ell, 1, k, 0, n)$$

since this algorithm gives a bijection between $\mathcal{R}(\ell, 1, k, 0, n)$ and $\mathcal{D}(\ell, 1, k, 0, n)$.

Now let j be arbitrary, but still $m = 0$, i. e., the walks do not visit a. If $n = 0$ then

$$R(\ell, 1, j, 0, 0) = D(\ell, 1, j, 0, 0)$$

trivially, because of the identical map between the vertices of $1, 2 \dots, k$ of $\hat{G}_1$ and $\hat{G}_2$. If $n \geq 1$ then a walk $w_1 w_2 \dots w_{\ell+1}$ in $\hat{G}_2$ surely visit the vertex k, let the time of the last visit of the vertex k be t. Then let us encode $w_1 w_2 \dots w_t$ by the function f and let $v_1 v_2 \dots v_t w_{t+1} \dots w_{\ell+1}$ be the corresponding walk to $w_1 \dots w_{l+1}$ in $\hat{G}_1$. This way we managed to give an injection from $\mathcal{D}(\ell, 1, j, 0, n)$ to $\mathcal{R}(\ell, 1, j, 0, n)$. (Note: this mapping is no more bijective: those walks in $\hat{G}_1$ which do not visit k are not in the image of the mapping.)

Now let us consider the general case. Let us do the following: repeat those sequences of the walk $w_1 \dots w_{\ell+1}$ of $\mathcal{D}(\ell, 1, j, n, m)$, where the walk has the form $1a1a \dots a1$ and between two parts of this form we encode the same way as in the previous case. Then it is trivially an injective mapping from $\mathcal{D}(\ell, 1, j, m, n)$ to $\mathcal{R}(\ell, 1, j, m, n)$.

Hence $R(\ell, 1, j, m, n) \geq D(\ell, 1, j, m, n)$. □

Lemma 3.8.4. *For all $1 \leq i, j \leq k$ and for all non-negative integers ℓ, m, n the following inequality holds*

$$R(\ell, i, j, m, n) + R(\ell, k+1-i, k+1-j, m, n) \geq$$

$$\geq D(\ell, i, j, m, n) + D(\ell, k+1-i, k+1-j, m, n).$$

Proof. We prove it by induction on ℓ. The claim is trivial for $\ell = 0, 1$.

We can assume that $i \le k + 1 - i$. We distinguish two cases.

Case 1. Assume $i \ge 2$. Let $w_1 w_2 \dots w_{\ell+1}$ be a walk of $R(\ell, i, j, m, n)$, i.e., $w_1 = i$, $w_{\ell+1} = j$. Then $w_2 = i + 1$ or $w_2 = i - 1$, thus we can decompose the set $\mathcal{R}(\ell, i, j, m, n)$ into the sets $\mathcal{R}(\ell - 1, i - 1, j, m, n)$ and $\mathcal{R}(\ell - 1, i + 1, j, m, n)$ respected to $w_2 \dots w_{\ell+1}$ starting from $i - 1$ or $i + 1$. Similarly, we can decompose the other sets with respect to their first step.

$$R(\ell, i, j, m, n) + R(\ell, k + 1 - i, k + 1 - j, m, n) =$$

$$R(\ell - 1, i - 1, j, m, n) + R(\ell - 1, i + 1, j, m, n)+$$

$$+R(\ell - 1, k - i, k + 1 - j, m, n) + R(\ell - 1, k + 2 - i, k + 1 - j, m, n)$$

and similarly,

$$D(\ell, i, j, m, n) + D(\ell, k + 1 - i, k + 1 - j, m, n) =$$

$$D(\ell - 1, i - 1, j, m, n) + D(\ell - 1, i + 1, j, m, n)$$

$$+D(\ell - 1, k - i, k + 1 - j, m, n) + D(\ell - 1, k + 2 - i, k + 1 - j, m, n).$$

By induction we have

$$R(\ell - 1, i - 1, j, m, n) + R(\ell - 1, k + 2 - i, k + 1 - j, m, n) \ge$$

$$\ge D(\ell - 1, i - 1, j, m, n) + D(\ell - 1, k + 2 - i, k + 1 - j, m, n)$$

and

$$R(\ell - 1, i + 1, j, m, n) + R(\ell - 1, k - i, k + 1 - j, m, n) \ge$$

$$\ge D(\ell - 1, i + 1, j, m, n) + D(\ell - 1, k - i, k + 1 - j, m, n).$$

By adding up the two inequalities we get the desired inequality

$$R(\ell, i, j, m, n) + R(\ell, k + 1 - i, k + 1 - j, m, n) \ge$$

$$\ge D(\ell, i, j, m, n) + D(\ell, k + 1 - i, k + 1 - j, m, n).$$

Case 2. Assume $i = 1$. Then we see that

$$R(\ell, 1, j, m, n) + R(\ell, k, k + 1 - j, m, n) =$$

$$= R(\ell - 1, a, j, m, n) + R(\ell - 1, b, j, m, n)+$$

$$+R(\ell - 1, 2, j, m, n) + R(\ell, k - 1, k + 1 - j, m, n)$$

while

$$D(\ell, 1, j, m, n) + D(\ell, k, k + 1 - j, m, n) =$$

$$= D(\ell-1,a,j,m,n) + D(\ell-1,2,j,m,n)$$

$$+D(\ell-1,b,k+1-j,m,n) + D(\ell-1,k-1,k+1-j,m,n).$$

By induction we have

$$R(\ell-1,2,j,m,n) + R(\ell-1,k-1,k+1-j,m,n) \geq$$

$$\geq D(\ell-1,2,j,m,n) + D(\ell-1,k-1,k+1-j,m,n).$$

Furthermore, by Lemma 3.8.3 we have

$$R(\ell-1,a,j,m,n) = R(\ell-2,1,j,m-1,n) \geq$$

$$\geq D(\ell-2,1,j,m-1,n) = D(\ell-1,a,j,m,n)$$

and by the symmetry properties and Lemma 3.8.3,

$$R(\ell-1,b,j,m,n) = R(\ell-2,1,j,m,n-1) = R(\ell-2,1,j,n-1,m) \geq$$

$$D(\ell-2,1,j,n-1,m) = D(\ell-2,k,k+1-j,m,n-1) = D(\ell-1,b,k+1-j,m,n).$$

By adding up the three inequalities we obtain the required inequality

$$R(\ell,1,j,m,n) + R(\ell,k,k+1-j,m,n) \geq$$

$$\geq D(\ell,1,j,m,n) + D(\ell,k,k+1-j,m,n).$$

Hence we completed the proof of the inequality. □

Corollary 3.8.5. *The following inequalities hold*

$$R(\ell,a,a,m,n) \geq D(\ell,a,a,m,n)$$

and

$$R(\ell,b,b,m,n) \geq D(\ell,b,b,m,n)$$

and

$$\sum_{i=1}^{k} R(\ell,i,i,m,n) \geq \sum_{i=1}^{k} D(\ell,i,i,m,n).$$

Proof. To obtain the first inequality we use Lemma 3.8.3.

$$R(\ell,a,a,m,n) = R(\ell-2,1,1,m-2,n) \geq$$

$$\geq D(\ell-2,1,1,m-2,n) = D(\ell,a,a,m,n).$$

Similarly, by Lemma 3.8.3 and the symmetry properties we have

$$R(\ell,b,b,m,n) = R(\ell-2,1,1,m,n-2) = R(\ell-2,1,1,n-2,m) \geq$$

$$\geq D(\ell-2,1,1,n-2,m) = D(\ell-2,k,k,m,n-2) = D(\ell,b,b,m,n).$$

To obtain the third inequality we put $i = j$ into the previous lemma

$$R(\ell,i,i,m,n) + R(\ell,k+1-i,k+1-i,m,n) \geq$$

$$\geq D(\ell,i,i,m,n) + D(\ell,k+1-i,k+1-i,m,n).$$

Summing these inequalities for $i = 1,\ldots,k$, and dividing by two we get

$$\sum_{i=1}^{k} R(\ell,i,i,m,n) \geq \sum_{i=1}^{k} D(\ell,i,i,m,n).$$

□

Theorem 3.8.6. *The proper generalized tree shift increases the number of closed walks of length t.*

Proof. Let G_2 be a tree and G_1 a tree obtained from G_2 by a generalized tree shift. We give an injective mapping from the closed walks of length t of G_2 to the closed walks of length t of G_1. We can decompose a closed walk of G_2 into parts which are entirely in A, entirely in B or entirely in the path $\{1,2,\ldots,k\}$ of G_2. By substituting a or b instead of the parts walking in A, respectively in B we get a walk of $\hat{G}_2$. By the previous corollary we know that there is an injective mapping from the closed walks of length ℓ with given number of a's and b's of $\hat{G}_2$ to the closed walks of length ℓ with given number of a's and b's of $\hat{G}_1$. Moreover, we can ensure that those walks which start with a or b have the image starting with a or b, respectively. Now by substituting back the a's and b's by the parts of walks going in A or B, respectively, we get an injective mapping from the closed walks of length t of G_2 to the closed walks of length t of G_1. □

Vladimir Nikiforov observed (private communication) that Theorem 3.8.6 already implies known and new results in a simple manner. We can give a new proof of the theorem that the generalized tree shift increases the spectral radius.

Corollary 3.8.7. *The proper generalized tree shift increases the spectral radius.*

Proof. Let T be a tree and T' a tree obtained from T by a generalized tree shift. Then

$$\mu(T') = \lim_{k\to\infty} W_{2k}(T')^{1/(2k)} \geq \lim_{k\to\infty} W_{2k}(T)^{1/(2k)} = \mu(T)$$

by the identity $W_{2k} = \sum_{i=1}^{n} \mu_i^{2k}$ and Theorem 3.8.6. □

Definition 3.8.8. [26, 27] The Estrada index of the graph G is defined as the sum

$$EE(G) = \sum_{i=1}^{n} e^{\mu_i}.$$

Corollary 3.8.9. *The proper generalized tree shift increases the Estrada index.*

Proof. We have

$$\sum_{i=1}^{n} e^{\mu_i} = \sum_{i=1}^{n}\sum_{t=0}^{\infty} \frac{\mu_i^t}{t!} = \sum_{t=0}^{\infty} \frac{1}{t!} \sum_{i=1}^{k} \mu_i^t = \sum_{t=0}^{\infty} \frac{W_t}{t!},$$

proving the statement. □

Corollary 3.8.10. *The path minimizes, the star maximizes the Estrada index among all trees on n vertices.*

Remark 3.8.11. The statement in Corollary 3.8.10 concerning the Estrada index was conjectured in the paper [23].

Remark 3.8.12. The author recently learned that H. Deng [24] also proved the conjecture concerning the Estrada index. His proof goes in a very similar fashion. He uses two different transformations for proving the minimality of the path and the maximality of the star; both transformations are special cases of the generalized tree shift.

3.9 The generalized tree shift and related transformations of trees

Originally, the author developed the generalized tree shift to overcome a certain weakness of the Kelmans transformation. However, it turned out that the generalized tree shift is indeed the generalization of many transformations for trees found in the literature. In this section we survey some of them.

In [46] L. Lovász and J. Pelikán proved that the star has the largest, the path has the smallest spectral radius among trees on n vertices. Their proof for settling the minimality of the path used a certain transformation of trees. This transformation is nothing else than the generalized tree shift applied in the case when the degree of the candidate vertex is 2, so it moves one edge. We also mention that they used the same ordering for the polynomials that we used for the independence polynomial and for the matching polynomial in the previous chapter.

In [49] Bojan Mohar defined the operation σ and π. Both transformations are special cases of the generalized tree shift; more precisely, the inverse of π is the special case of the generalized tree shift. In the language of the generalized tree shift, the inverse of π-transformation is nothing else than the generalized tree shift when H_2 himself is a path. The σ-transformation is the generalized tree shift when H_2 is a star and $k = 2$ (so the path has no interior vertices). Surprisingly, Hanyuan Deng [24] used exactly the same transformations for proving the extremality of the star and the path at the Estrada index. In fact, he also solved the problem for the number of closed walks as well. They needed two transformations, one for settling the extremality of the star and one for settling the extremality of the path.

In [35] Guo studied the algebraic connectivity of graphs, the transformation "separating an edge" is the generalized tree shift applied to adjacent vertices x, y. (In fact, he defined it for every graph, but Theorem 2.1 of [35] shows that it was useful only when the separated edge was a cut edge.) In this paper Guo used another transformation also called "grafting an edge". This transformation is not the special case of the generalized tree shift, but surprisingly they have a nontrivial common special transformation. In the language of the generalized tree shift this special case is when the graph H_2 is a path. Then the generalized tree shift acts as if the graph H_1 had been shifted from the end of a long path to the middle of this path. Guo showed that this can be refined such a way that the graph H_1 is closer and closer to the center of the path the algebraic connectivity becomes greater and greater. This suggests that maybe one can refine the poset induced by the generalized tree shift.

We mention that a more and more refined poset of trees could have a serious application. In biology one often measures molecules by some parameter. In this case it is invaluable that the star maximizes, the path minimizes this parameter since these are not the graph of molecules in general. Still a graph transformation could be useful to compare molecules in a fast way or to give a hint where to find the proper molecule.

3.10 Concluding remarks

In this section we collected the parameters of trees into a table which increase or decrease by applying the generalized tree shift. The common property of this parameters is that they are all monotone parameters of trees. In fact, most of them are monotone properties of all graphs.

We hope that the many examples could convince everybody that this transformation is much more natural than it seems to be for the first sight. The simple form of the General Lemma is also a clue of this naturality.

	Parameter	Change	Maximum
1	largest eigenvalue of the adjacency matrix	increasing	star
2	coefficients of the adjacency characteristic polynomial	decreasing	path
3	number of closed walks of length ℓ (ℓ fix)	increasing	star
4	number of walks of length ℓ (ℓ fix) [5]	increasing	star
5	algebraic connectivity	increasing	star
6	largest real root of the Laplacian polynomial	increasing	star
7	coefficients of the Laplacian characteristic polynomials	decreasing	path
8	smallest real root of the independence polynomial	decreasing	path
9	coefficients of the independence polynomial	increasing	star
10	coefficients of the edge cover polynomial	decreasing	path

3.11 Afterlife

The generalized tree shift gained some attention by Béla Bollobás and Mykhaylo Tyomkyin [5]. In their paper they gave a simpler proof of the result that the GTS increases the number of closed walks of length ℓ. They also proved that the GTS increases the number of (arbitrary) walks of length ℓ. (Although they used the name KC-transformation for the generalized tree shift.) They also considered other extremal graph theoretic problems concerning trees.

Chapter 4

Density Turán problem

This part is based on a joint work with Zoltán L. Nagy. The following problem was studied in Zoltán L. Nagy's master thesis [50]. A very closely related variant of this problem was mentioned in the book Extremal Graph Theory [3] on page 324.

Given a simple, connected graph H, define the blown-up graph $G[H]$ of H as follows. Replace all vertices $v_i \in V(H)$ by a cluster A_i and connect vertices between the clusters A_i and A_j (not necessarily all) if v_i and v_j were adjacent in H. As usual, we define the density between A_i and A_j as

$$d(A_i, A_j) = \frac{e(A_i, A_j)}{|A_i||A_j|},$$

where $e(A_i, A_j)$ denotes the number of edges between the clusters A_i and A_j. We say that the graph H is a transversal of $G[H]$ if H is the subgraph of $G[H]$ such that we have a homomorphism $\varphi : V(H) \to V(G[H])$ for which we have $\varphi(v_i) \in A_i$ for all $v_i \in V(H)$. We will also use the terminology that H is the factor of $G[H]$.

The density Turán problem asks to determine the critical edge density d_{crit} which ensures the existence of the subgraph H of $G[H]$ as a transversal. What does it mean? Assume that for all $e = (i, j) \in E(H)$ we have $d(A_i, A_j) > d_{crit}$ then no matter how the graph $G[H]$ looks like, it induces the graph H such that $v_i \in A_i$. On the other hand, for any $d < d_{crit}$ there exists a blown-up graph $G[H]$ such that $d(A_i, A_j) > d$ for all $(i, j) \in E(H)$ and it does not contain H as a transversal. Clearly, the critical edge density of the graph H is the largest one of the critical edge densities of its components. Thus we can and will assume that H is a connected graph throughout this chapter.

It will turn out that it is useful to consider the following more general problem. Assume that a density γ_e is given for every edge $e \in E(H)$. Now the problem is to decide whether the densities $\{\gamma_e\}$ ensure the existence of the subgraph H as a transversal or one can construct a blown-up graph $G[H]$ such that $d(A_i, A_j) \geq \gamma_{ij}$, yet the graph H does not appear in $G[H]$ as a transversal. This more general approach allows us to use inductive proofs.

In the next section we give a survey of Zoltán L. Nagy's results. Then we solve the above mentioned more general problem for trees. As a corollary it will turn out that the critical edge density is related to the largest eigenvalue of the adjacency matrix of the tree. Later for every graph H we give an upper bound to the critical edge density in terms of the largest real root of the matching polynomial. We will also construct blown-up graphs in terms of the largest eigenvalues of the adjacency matrices of the so-called *monotone-path trees*.

4.1 Diamonds and Zoltán Nagy's results

In this section we motivate some key definitions through an example (diamond) and we grasp the opportunity to survey Zoltán Lóránt Nagy's theorems.

The diamond is the unique simple graph on 4 vertices and 5 edges, generally denoted by K_4^-.

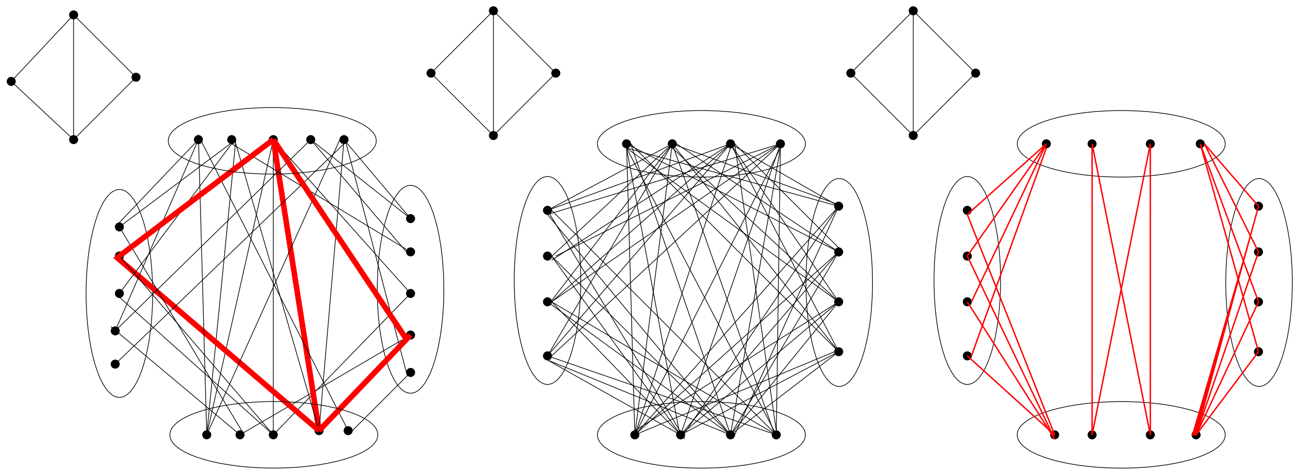

Figure 4.1: Blown-up graphs of diamonds.

In the above figure, the first blown-up graph of the diamond contains the diamond as a transversal. The second blown-up graph does not contain the diamond as a transversal although the edge density is 3/4 between any two clusters. So as to see it, we gave the *complement of the blown-up graph with respect to the complete blown-up graph*; in what follows we will simply call this graph the *complement graph* and we will denote it by $\overline{G[H]|H}$. In the "complement language" the claim is the following: if one chooses one vertex from each cluster then we cannot avoid choosing both ends of a red edge. This is true indeed: whichever vertex we choose from the "right" and "left" clusters we cannot choose the rightmost and leftmost vertices of the upmost and downmost clusters; so we have to choose a vertex from the middle of these clusters, but they are all connected by red edges.

We also see that this construction was a bit redundant in the sense that each vertex from the right and left clusters had the same role. This motivates the following definition.

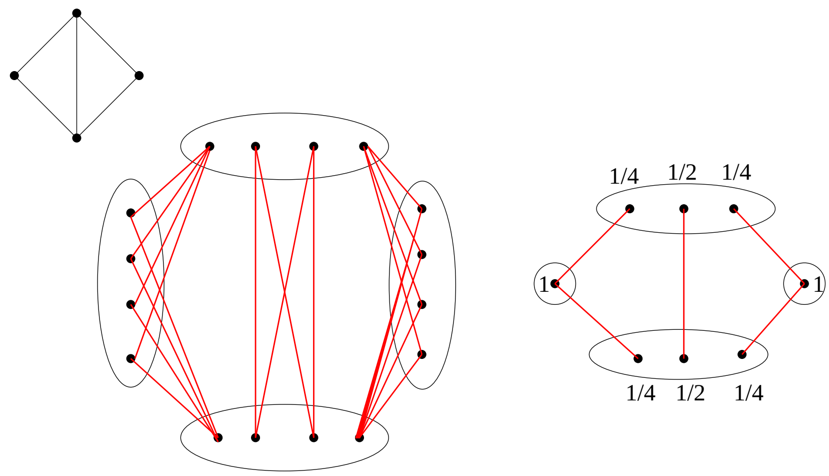

Figure 4.2: Weighted blown-up graph.

Definition 4.1.1. A weighted blown-up graph is a blown-up graph where a non-negative weight $w(u)$ is assigned to each vertex u such that the total weight of each cluster is 1. The density between two clusters is

$$d_{ij} = \sum_{\substack{(u,v)\in E \\ u\in A_i, v\in A_j}} w(u)w(v).$$

This definition also has the advantage that now we can allow irrational weights as well. (But this does not change the problem since we can approximate any irrational weight by rational weights and then we blow up the construction with the common denominator of the weights.) The following result of Zoltán L. Nagy also shows that the problem in this framework is much more convenient.

Theorem 4.1.2 (Zoltán L. Nagy, [50, 51])**.** *If there is a construction of a blown-up graph $G[H]$ not containing H then there is a construction of a weighted blown-up graph $G'[H]$ not containing H, where*

- *each edge density is at least as large as in $G[H]$,*
- *the cluster V_i contains at most as many vertices as the degree of the vertex v_i in the graph H.*

The importance of this theorem lies in the fact that if we are looking for the critical edge density we only have to check those constructions where each cluster contains a bounded number of vertices. So in fact, we have to check a finite number of configurations and we only have to decide that which configuration has a weighting providing the greatest density. In general, the number of possible configurations is very large, till it has some notable consequence. For instance, there is a "best" construction in the sense that if we have construction for $\gamma_e - \varepsilon$ for every ε then we have a construction with edge densities γ_e. Indeed, we have a compact space (finite number of configurations) and the edge densities are continuous functions of the weights.

With a small extra idea one can prove the following important corollary of this theorem.

Theorem 4.1.3 (Zoltán L. Nagy, [50, 51])**.** *There is a weighted blown-up graph $G[H]$ not containing H where each edge density is exactly the critical edge density.*

From this theorem one can deduce the following one.

Theorem 4.1.4 (Zoltán L. Nagy, [50, 51])**.** *If H_1 is a subgraph of H_2 then for the critical edge densities we have*

$$d_{crit}(H_1) \leq d_{crit}(H_2).$$

If H_2 is connected and H_1 is a proper subgraph of H_2 then the inequality is strict.

4.2 Trees

In this section we study the case when the graph H is a tree.

Theorem 4.2.1. *Let T be a tree, v_n is an endnode of T. Assume that for each edge of T a density $\gamma_e = 1 - r_e$ is given. Let T' be a tree obtained from T by deleting the endvertex v_n (together with the edge $e_{n-1,n} = v_{n-1}v_n$). Let the densities γ'_e's be defined as follows:*

$$\gamma'_e = \begin{cases} \gamma_e = 1 - r_e & \textit{if } e \textit{ is not incident to } v_{n-1}, \\ 1 - \frac{r_e}{1 - r_{e_{n-1,n}}} & \textit{if } e \textit{ is incident to } v_{n-1}. \end{cases}$$

Then the set of densities γ_e ensure the existence of the factor T if and only if all γ'_e's are between 0 and 1 and the set of densities γ'_e ensure the existence of the factor T'.

Remark 4.2.2. Clearly, this theorem provides us with an efficient algorithm to decide whether a given set of densities ensures the existence of a factor (see Algorithm 4.2.3).

Proof. First we prove that if all the γ'_e's are indeed densities and they ensure the existence of the factor T' then the original γ_e's ensure the existence of a factor T.

Assume that $G[T]$ is a blown-up of T such that the density between A_i and A_j is at least γ_{ij}, where A_i is the blown-up of the vertex v_i of T. We need to show that it contains a factor T.

Let us define

$$R = \{v \in A_{n-1} \mid \ v \text{ is incident to some edge going between } A_{n-1} \text{ and } A_n\}.$$

First of all we show that the cardinality of R is large:

$$|R||A_n| \geq e(R, A_n) = \gamma_{n-1,n}|A_{n-1}||A_n|.$$

Thus $|R| \geq \gamma_{n-1,n}|A_{n-1}|$.

Next we show that many edges are incident to R. Let v_k be adjacent to v_{n-1}. Then we can bound the number of edges between R and A_k as follows:

$$e(R, A_k) \geq e(A_{n-1}, A_k) - (|A_{n-1}| - |R|)|A_k| = |R||A_k| + (\gamma_{k,n-1} - 1)|A_k||A_{n-1}| \geq$$

$$|R||A_k| + (\gamma_{k,n-1} - 1)\frac{1}{\gamma_{n-1,n}}||R||A_k| =$$

$$= (1 - \frac{r_{k-1,n}}{1 - r_{n-1,n}})|R||A_k| = \gamma'_{k,n-1}|R||A_k|.$$

Now delete the vertex set A_n and $A_{n-1}\backslash R$ from $G[T]$. Then the obtained graph is a blown-up of T' with edge densities ensuring the factor T'. But this factor can be extended to a factor T because of the definition of R.

Now we prove that if some $\gamma'_{k,n-1} < 0$, then there exists a construction for a blown-up of T having no factor of T. In fact $\gamma'_{k,n-1} < 0$ means that $\gamma_{k,n} + \gamma_{n-1,n} < 1$ and so we can easily reach that some construction does not induce the path $u_k u_{n-1} u_n$ where $u_i \in A_i$ $(i \in \{k, n-1, n\})$.

Now assume that all γ'_e's are proper densities, but there is a construction $G'[T']$ with edge-densities at least γ'_e's, but which does not induce a factor T'. In this case we can easily construct a blown-up $G[T]$ of the tree not inducing T by setting $A_{n-1} = R^* \cup A'_{n-1}$ with an appropriate weight of $R^* = \{v^*_{n-1}\}$ and taking an $A_n = \{v_n\}$ which we connect to all elements of A'_{n-1}, but we do not connect to v^*_{n-1}. □

Algorithm 4.2.3. ***Step 0.*** *Given a tree a T_0 and edge densities γ^0_e. Set $T := T_0$ and $r_e = 1-\gamma^0_e$.*
Step 1. *Consider $(T, \underline{r_e})$.*

- *If $|V(T)| = 2$ and $0 \leq r_e < 1$ then **STOP**: the densities γ^0_e ensure the existence of the transversal T_0.*

- *If $|V(T)| \geq 2$ and there exists an edge for which $r_e \geq 1$ then **STOP**: the densities γ^0_e do not ensure the existence of the transversal T_0.*

Step 2. *If $|V(T)| \geq 3$ and $0 \leq r_e < 1$ for all edge $e \in E(T)$ then **do** pick a vertex v of degree 1, let u be its unique neighbor. Let $T' := T - v$ and*

$$r'_e = \begin{cases} r_e \text{ if } e \text{ is not incident to } u, \\ \frac{r_e}{1-r_{(u,v)}} \text{ if } e \text{ is incident to } u. \end{cases}$$

Jump to Step 1. with $(T, \underline{r_e}) := (T', \underline{r'_e})$.

In what follows we analyse the above mentioned algorithm. The following concept will be the key tool.

Definition 4.2.4. Let x_e's be variables assigned to each edge of a graph. The *multivariate matching polynomial* F is defined as follows:

$$F(\underline{x_e}, t) = \sum_{M \in \mathcal{M}} (\prod_{e \in M} x_e)(-t)^{|M|},$$

where the summation goes over the matchings of the graph including the empty matching.

Remark 4.2.5. Clearly, if L_G denotes the line graph of the graph G we have

$$F(\underline{x_e}, t) = I((L_G, \underline{x_e}); t)$$

or in other words,

$$t^n F(\underline{x_e}, \frac{1}{t^2}) = M((G, \underline{x_e}); t).$$

The following lemma is a straightforward generalization of the well-known fact that for trees the matching polynomial and the characteristic polynomial of the adjacency matrix coincide. We quote it from the Appendix.

Theorem A.1.20. *Let T be a tree on n vertices. Let us define the following matrix of size $n \times n$. The entry $a_{i,j} = 0$ if the vertices v_i and v_j are not adjacent and $a_{i,j} = \sqrt{x_e}$ if $e = v_i v_j \in E(T)$. Let $\phi(\underline{x_e}, t)$ be the characteristic polynomial of this matrix. Then*

$$\phi(\underline{x_e}, t) = t^n F(\underline{x_e}, \frac{1}{t^2})$$

where $F(\underline{x_e}, t)$ is the multivariate matching polynomial.

Statement A.1.15. *Let $t_w(G)$ denote the largest real root of the polynomial $M((G, \underline{w}); t)$. Let G_1 be a subgraph of G then we have*

$$t_w(G_1) \leq t_w(G).$$

Corollary 4.2.6. *Let T be a tree and assume that for each edge $e \in E(T)$ a weight $w_e > 0$ is assigned. Furthermore, let T' be a subtree of T with the induced edge weights. Then the polynomial $F_T(\underline{w_e}, t)$ has a smaller positive root than the polynomial $F_{T'}(\underline{w_e}, t)$.*

Lemma 4.2.7. *Let T be a weighted tree with $\gamma_e = 1 - tr_e$ weights. Assume that after running the Algorithm 4.2.3 we get the two node tree with edge weight 0. Then t is the root of the multivariate matching polynomial $F(\underline{r_e}, s)$ of the tree T.*

Proof. We prove the statement by induction on the number of vertices of the tree. If the tree consists of two vertices then $0 = 1 - tr_e$ means exactly that t is the root of the multivariate matching polynomial of the tree.

Now assume that the statement is true for trees on at most $n-1$ vertices. Let T be a tree on n vertices and assume that we execute the algorithm for the pendant edge $e_{n-1,n} = (v_{n-1}, v_n)$ in the first step, where the degree of the vertex v_n is 1. Let $T' = T - v_n$. Now we continue executing the algorithm obtaining the two node tree with edge weight 0. By induction we get that $F_{T'}(\underline{r'_e}, t) = 0$.

We can expand $F_{T'}$ according to whether a monomial contains $x_{k,n-1}$ ($e_{k,n-1} \in E(T')$) or not. Each monomial can contain at most one of the variables $x_{k,n-1}$ ($v_k \in N(v_{n-1})$). Thus

$$F_{T'}(\underline{x_e}, s) = Q_0(\underline{x_e}, s) - \sum_{v_k \in N(v_{n-1})} s x_{k,n-1} Q_k(\underline{x_e}, s),$$

where Q_0 consists of those terms which contain no $x_{k,n-1}$ and $-s x_{k,n-1} Q_k$ consists of those terms which contain $x_{k,n-1}$, i.e., these terms correspond to the matchings containing the edge (v_k, v_{n-1}). Observe that

$$F_T(\underline{x_e}, s) = (1 - s x_{n-1,n}) Q_0(\underline{x_e}, s) - \sum_{v_k \in N(v_{n-1})} s x_{k,n-1} Q_k(\underline{x_e}, s)$$

by the same argument.

Since

$$0 = F_{T'}(\underline{r'_e}, t) = Q_0(\underline{r_e}, t) - \sum_{v_k \in N(v_{n-1})} \frac{r_{k,n-1}}{1 - t r_{n-1,n}} Q_k(\underline{r_e}, t)$$

we have

$$0 = (1 - t r_{n-1,n}) F_{T'}(\underline{r'_e}, t) = (1 - t r_{n-1,n}) Q_0(\underline{r_e}, t) - \sum_{v_k \in N(v_{n-1})} r_{k,n-1} Q_k(\underline{r_e}, t) = F_T(\underline{r_e}, t).$$

Hence t is the root of $F_T(\underline{r_e}, s)$. □

Theorem 4.2.8. *Let T be a tree and let $\gamma_e = 1 - r_e$ be edge densities. Then the edge densities ensure the existence of the tree T as a transversal if and only if for the multivariate matching polynomial we have*

$$F(\underline{r_e}, t) > 0$$

for all $t \in [0, 1]$.

Remark 4.2.9. We mention that the really hard part of this theorem is that if

$$F(\underline{r_e}, t) > 0$$

for all $t \in [0, 1]$ then the edge densities $\gamma_e = 1 - r_e$ ensure the existence of the tree T as a transversal. Later we will prove that this is true for every graph H, see Theorem 4.3.3.

Proof. We prove the theorem by induction on the number of vertices. We will use Theorem 4.2.1. First we show that if the edge densities ensure the existence of the factor T then

$$F(\underline{r_e}, t) > 0$$

for all $t \in [0, 1]$.

Clearly,

$$F(\underline{r_e}, t) = F(\underline{r_e t}, 1).$$

It is also trivial that the densities $\gamma_e = 1 - r_e$ ensure the existence of a factor T then the densities $\gamma_e = 1 - tr_e$ ($t \in [0, 1]$) ensure the existence of factor T. Hence we only need to prove that if the densities $\gamma_e = 1 - r_e$ ensure the existence of factor T then $F(\underline{r_e}, 1) > 0$.

By induction and Theorem 4.2.1 we have $F_{T'}(\underline{r'_e}, 1) > 0$. Now we repeat the argument of Lemma 4.2.7.

As before, we can expand $F_{T'}$ according to whether a monomial contains $x_{k,n-1}$ ($e_{k,n-1} \in E(T')$) or not. Each monomial can contain at most one of the variables $x_{k,n-1}$ ($v_k \in N(v_{n-1})$). Thus

$$F_{T'}(\underline{x_e}, t) = Q_0(\underline{x_e}, t) - \sum_{v_k \in N(v_{n-1})} t x_{k,n-1} Q_k(\underline{x_e}, t),$$

where Q_0 consists of those terms which contain no $x_{k,n-1}$ and $-tx_{k,n-1}Q_k$ consists of those terms which contain $x_{k,n-1}$, i.e., these terms correspond to the matchings containing the edge (v_k, v_{n-1}). We have

$$F_T(\underline{x_e}, t) = (1 - tx_{n-1,n})Q_0(\underline{x_e}, t) - \sum_{v_k \in N(v_{n-1})} x_{k,n-1} Q_k(\underline{x_e}, t)$$

by the same argument.

Hence

$$0 < F_{T'}(\underline{r'_e}, 1) = Q_0(\underline{r_e}, 1) - \sum_{v_k \in N(v_{n-1})} \frac{r_{k,n-1}}{1 - r_{n-1,n}} Q_k(\underline{r_e}, 1).$$

So we get that

$$0 < (1 - r_{n-1,n})F_{T'}(\underline{r'_e}, 1) = (1 - r_{n-1,n})Q_0(\underline{r_e}, 1) - \sum_{v_k \in N(v_{n-1})} r_{k,n-1} Q_k(\underline{r_e}, 1) = F_T(\underline{r_e}, 1).$$

This completes one direction of the statement.

Now we assume that $F(\underline{r_e}, t) > 0$ for all $t \in [0, 1]$. We prove by contrary that the edge densities γ_e's ensure the existence of factor T. Assume that the Algorithm 4.2.3 stops with some $r_{\text{violating edge}} \geq 1$. In the next step we show that for some $t \in [0, 1]$ we can ensure that the algorithm stops with $r_{\text{violating edge}}(t) = 1$ when we start with the edge densities $\gamma_e = 1 - tr_e$.

First of all, let us examine what happens if we decrease the r_e's. If $0 < r_e \leq r_e^*$ and $0 < r_f \leq r_f^*$ then

$$\frac{r_e}{1-r_f} \leq \frac{r_e^*}{1-r_f^*}.$$

Hence all r_i's decrease under the algorithm if we decrease t.

If we set $t = 0$ then for the edge densities $\gamma_e = 1 - tr_e$ the algorithm gives 1 for all densities which show up. Since changing t continuously all densities will change continuously we can choose an appropriate $t \in [0,1]$ for which running our algorithm with tr_e's instead of r_e's we can assume that the algorithm stops with $r_{\text{violating edge}}(t) = 1$.

Now consider those vertices and edges together with the violating edge which were deleted under executing the algorithm. These edges form a forest. Consider the components of this forest which contains the violating edge. Let us call this subtree T_1. According to Lemma 4.2.7 our chosen t is the root of the matching polynomial of T_1 (clearly, only the deleted edges modified the weight of the violating edge). On the other hand, we know from Corollary 4.2.6 that the matching polynomial of T has a smaller root than the matching polynomial of T_1. This means that the matching polynomial of T has a root in the interval $[0,1]$ contradicting the condition of the theorem.

□

Corollary 4.2.10. *Let T be a tree and assume that all edge densities γ_e satisfy $\gamma_e > 1 - \frac{1}{\mu(T)^2}$ where $\mu(T)$ is the largest eigenvalue of the adjacency matrix of T. Then γ's ensure the existence of factor T. If all $\gamma = 1 - \frac{1}{\mu(T)^2}$ then there exist a weighted blown-up of T not containing T as a transversal. In other words,*

$$d_{crit}(T) = 1 - \frac{1}{\mu(T)^2}.$$

Proof. We can assume that all edge densities are equal to $1 - d > 1 - \frac{1}{\mu^2}$. In this case $dt < \frac{1}{\mu(T)^2}$ for all $t \in [0,1]$ and so

$$0 < \phi_T\left(\frac{1}{\sqrt{dt}}\right) = (dt)^{-n/2} F_T(\underline{dt}, 1) = (dt)^{-n/2} F_T(\underline{d}, t)$$

by Theorem A.1.20. By Theorem 4.2.8 this implies that the set of edge densities $\{\gamma_e\}$ ensure the existence of factor T. Theorem 4.2.8 also implies that there exist a weighted blown-up with weights $\gamma = 1 - \frac{1}{\mu(T)^2}$ of T not containing T as a transversal. □

⋆ ⋆ ⋆

In this section we give an elegant structure theorem concerning the critical edge density of trees.

Statement 4.2.11. [50, 51] *Let T be a tree. Let us consider the following blown-up graph $G[T]$ of T. Let the cluster A_i consist of the vertices v_{ij} where $j \in N(i)$. If $(i,j) \in E(T)$ then*

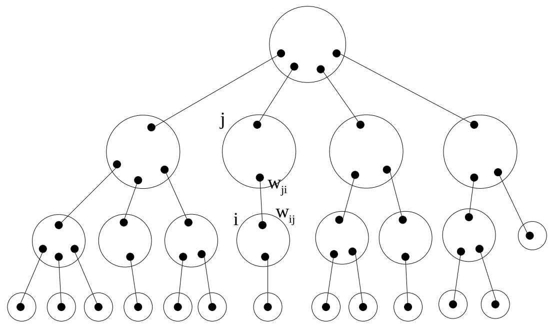

Figure 4.3: A special blown-up graph of a tree.

we connect all vertices of A_i *and* A_j *except* v_{ij} *and* v_{ji}*. Then* $G[T]$ *does not contain* T *as a transversal.*

Proof. We have to prove that one cannot avoid choosing both endvertex of a complementary edge (v_{ij}, v_{ji}) if one chooses one vertex from each cluster. This is indeed true since the set of all vertices of $G[T]$ can be decomposed to $(n-1)$ such pairs. Since we have to choose n vertices we have to choose both vertex from such a pair. $\square$

We show that we can give weights to the vertices of the above constructed $G[T]$ such that the density will be $1 - \frac{1}{\mu^2}$ where $\mu = \mu(T)$. The following weighting was the idea of András Gács.

Recall that there exists a non-negative eigenvector $\underline{x}$ belonging to the largest eigenvalue μ of T. So if v_i's are the vertices of T we have

$$\mu x_i = \sum_{j \in N(i)} x_j$$

for all i. Now let us define the weight w_{ij} of the vertex v_{ij} of $G[T]$ as follows: $w_{ij} = \frac{x_j}{\mu x_i} \geq 0$. Then we have

$$w(A_i) = \sum_{j \in N(i)} w_{ij} = \sum_{j \in N(i)} = \frac{x_j}{\mu x_i} = 1.$$

Furthermore,

$$d(A_i, A_j) = 1 - w_{ij} w_{ji} = 1 - \frac{x_j}{\mu x_i} \frac{x_i}{\mu x_j} = 1 - \frac{1}{\mu^2}.$$

Remark 4.2.12. A theorem of Zoltán Nagy already showed that there exist a unique weighting of the above constructed $G[T]$ where each density is the same and this must be the critical edge density. Hence András Gács's weighting already proved that the critical edge density of the tree is $1 - \frac{1}{\mu^2}$.

Remark 4.2.13 (Historical remark.)**.** Zoltán Nagy already proved in his master thesis that the critical edge density of a tree satisfies the inequality

$$1 - \frac{1}{\Delta} \leq d_{crit}(T) < 1 - \frac{1}{4(\Delta - 1)},$$

where Δ is the largest degree.

This inequality reminded me to the following inequality concerning the spectral radius of a tree:

$$\sqrt{\Delta} \leq \mu(T) < 2\sqrt{\Delta - 1}.$$

I asked to check Zoltán whether it is coincidence or not and after we found that for small trees $d(T) = 1 - \frac{1}{\mu(T)^2}$, we conjectured that it was always true. This was confirmed by András by his weighting the same afternoon while we took a walk in St. Andrews. This result prompted me to join the research.

4.3 Application of the Lovász local lemma and its extension

Theorem 4.3.1. *(Lovász local lemma, symmetric case.) Let $A_1, A_2, \dots, A_n$ be events in an arbitrary probability space. Suppose that each event A_i is mutually independent of all other events, but at most $\Delta \geq 2$ of them. Furthermore, assume that for each i,*

$$\mathbb{P}r(A_i) \leq \frac{1}{e(\Delta + 1)},$$

where e is the base of the natural logarithm. Then

$$\mathbb{P}r(\cap_{i=1}^{n} \overline{A_i}) > 0.$$

Theorem 4.3.2. *Let Δ be the largest degree of the graph H and let d be the critical edge density. Then*

$$d_{crit}(H) \leq 1 - \frac{1}{e(2\Delta - 1)},$$

where e is the base of the natural logarithm.

Proof. We prove by contradiction. Assume that there exists a blown-up graph $G[H]$ of the graph H with edge densities greater than $1 - \frac{1}{e(2\Delta-1)}$ which does not induce H.

We can assume that all classes of the blown-up graph $G[H]$ contains exactly N vertices. Indeed, we can approximate each weight by a rational number so that every edge densities are still larger than $1 - \frac{1}{e(2\Delta-1)}$. Then we "blow up" the construction by the common denominator of all weights.

Let us choose a vertex from each class with equal probability $1/N$ independently of each other. Let f be an edge of the complement of the graph $G[H]$ with respect to H. Let A_f be the event that we have chosen both endnodes of the edge f (clearly, a bad event we would like to avoid). Then $\mathbb{P}r(A_f) = 1/N^2$ and A_f is independent from all events $A_{f'}$ where the edge f' has endvertices in different classes. Thus A_f is independent from all, but at most $(2\Delta - 1)rN^2$ bad events where $d = 1 - r$. Since $r < \frac{1}{e(2\Delta-1)}$ the condition of Lovász local lemma is satisfied and gives that

$$\mathbb{P}r(\cap_{f \in E(\overline{G[H]|H})} A_f) > 0.$$

which means that that $G[H]$ induces the graph H (with positive probability) contradicting the assumption. □

Now we use a generalisation of the Lovász local lemma to improve on the bound of Theorem 4.3.2.

Theorem A.1.11. (Scott-Sokal [60]) *Assume that given a graph G and there is an event A_i assigned to each node i. Assume that A_i is totally independent of the events $\{A_k \mid (i,k) \in E(\overline{G})\}$. Set $\mathbb{P}r(A_i) = p_i$.*

(a) *Assume that $I((G, \underline{p}), t) > 0$ for all $t \in [0,1]$. Then we have*

$$\mathbb{P}r(\cap_{i \in V(G)} \overline{A_i}) \geq I((G, \underline{p}), 1) > 0.$$

(b) *Assume that $I((G, \underline{p}), t) = 0$ for some $t \in [0,1]$. Then there exists a probability space and a family of events B_i with $\mathbb{P}r(B_i) \geq p_i$ and with dependency graph G such that*

$$\mathbb{P}r(\cap_{i \in V(G)} \overline{B_i}) = 0.$$

Theorem 4.3.3. *Assume that for the graph H we have $F_H(\underline{r_e}, t) > 0$ for all $t \in [0,1]$ and some weights $r_e \in [0,1]$ assigned to each edge. Then the densities $\gamma_e = 1 - r_e$ ensure the existence of H as a transversal.*

Proof. As before, we choose a vertex from each cluster independently of each other. We choose the vertex u from the cluster V_i of the graph $G[H]$ with probability $w(u)$. We would like to show that we do not choose both endvertices of an edge of the complement $\overline{G[H]|H}$ with positive probability. Let $f = (u_1, u_2)$ be an edge of the complement of the graph $G[H]$ respected to H. Let A_f be the event that we have chosen both endnodes of the edge f (clearly, a bad event we would like to avoid). Then $\mathbb{P}r(A_f) = w(u_1)w(u_2)$ and A_f is independent from all events $A_{f'}$ where the edge f' has endvertices in different classes. Now let us consider the weighted independence polynomial of the graph determined by the vertices A_f in which we connect A_f and $A_{f'}$ if there exists a cluster containing one endvertices of both f and f'. In this graph, the events A_f where f goes between the fixed clusters V_i, V_j not only form a clique but it is also true that they are connected to the same set of events. Hence we can replace them by one vertex of weight

$$\sum_{(u_1,u_2)\in E(\overline{G[H]}(V_i\cup V_j))} w(u_1)w(u_2) = r_{ij}$$

without changing the weighted independence polynomial. But then the obtained weighted independence polynomial is

$$I((L_H, \underline{r_e}), t) = F_H(\underline{r_e}, t) > 0$$

for $t \in [0,1]$. Then by the Scott-Sokal theorem we have

$$\mathbb{P}r(\cap_{f\in E(\overline{G[H]|H})}\overline{A_f}) \geq F((H, \underline{r_e}), 1) > 0.$$

□

Corollary 4.3.4. *Let Δ be the largest degree of the graph H and $t(H)$ be the largest root of the matching polynomial. Then for the critical edge density d_{crit} we have*

$$d_{crit}(H) \leq 1 - \frac{1}{t(H)^2}.$$

In particular,

$$d_{crit}(H) < 1 - \frac{1}{4(\Delta-1)}.$$

Proof. Let $\gamma_e = 1 - r$ for every edge $e \in E(H)$, where $r < \frac{1}{t(H)^2}$ then

$$F_H(\underline{r}, t) = \sum_{k=0}^{n}(-1)^k m_k(H) r^k t^k = (rt)^{n/2} M(H, \frac{1}{\sqrt{rt}}) > (rt)^{n/2} M(H, t(H)) = 0$$

for $t \in [0,1]$. Hence the set of densities $\{\gamma_e\}$ ensures the existence of the graph H. Thus $d_{crit}(H) \leq 1 - r$ for every $r < \frac{1}{t(H)^2}$. Hence

$$d_{crit}(H) \leq 1 - \frac{1}{t(H)^2}.$$

The second claim follows from the fact that $t(H) < 2\sqrt{\Delta - 1}$. (This is Corollary A.1.27, see also [41].) □

Remark 4.3.5. We invite the reader to compare it with the trivial bound

$$d_{crit}(H) \geq 1 - \frac{1}{\Delta}.$$

4.4 Construction: star decomposition of the complement

In this section we examine a large class of blown-up graphs which do not induce a given graph as a transversal. Assume that $H = H_1 \cup \{v_n\}$ and we have a blown-up graph of H_1 which does not induce H_1 as a transversal. We can construct a blown-up graph of H not inducing H as follows. Let $A_n = \{w_n\}$ be the blown-up of v_n. Furthermore, assume that $N_H(v_n) = \{v_1, v_2, \dots, v_k\}$ with the corresponding clusters $A'_1, \dots, A'_k$ in the blown-up of H_1. Then let $A_i = A'_i \cup \{w_i\}$ if $1 \le i \le k$ and we leave unchanged all other clusters. Let us connect w_n to each elements of A'_i $(1 \le k \le n)$ and connect w_i with every possible neighbor except w_n. All other pairs of vertices remain adjacent or non-adjacent as in the blown-up of H_1.

Now it is clear why we call this construction star decomposition, see Figure 4.4.

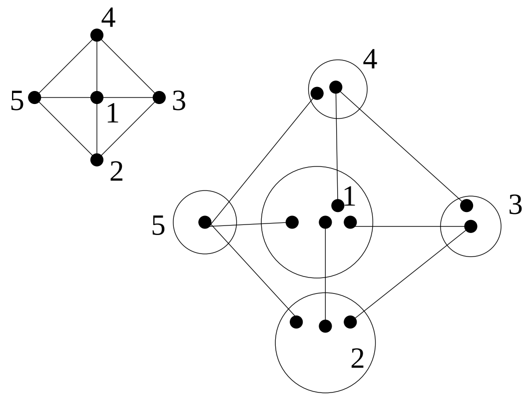

Figure 4.4: Star decomposition of the complement of the wheel.

This new blown-up graph will not induce H as a transversal since if we try to choose the elements of the transversal we have to choose w_n, but then we cannot choose any of the vertices w_i $(1 \le k \le n)$. Hence we have to choose all other vertices of the transversal from the blown-up of H_1, but according to the assumption this blown-up graph does not induce the graph H_1 as a transversal, thus the new blown-up graph does not induce H as a transversal.

Although we gave a construction of a blown-up of the graph H not inducing H, this is only the half of a real construction since we can vary the weights of the vertices of the blown-up graph. Of course, we would like to choose the weights optimally. But what does it mean? Assume that we are given densities for all edges of H and we wish to make a construction iteratively as we described in the previous paragraph and now we would like to choose the weights so that the edge-densities are at least as large as the required edge-densities. To quantify this argument we need some definitions.

Definition 4.4.1. A proper labeling of the vertices of the graph H is a bijective function f from $\{1, 2, \dots, n\}$ to the set of vertices such that the vertex set $\{f(1), \dots, f(k)\}$ induces a connected subgraph of H for all $1 \le k \le n$.

Definition 4.4.2. Given a weighted graph H with a proper labeling f, where the weights on the edges are between 0 and 1. The *weighted monotone-path tree* of H is defined as follows. The vertices of this graph are the paths of the form $f(i_1)f(i_2)\dots f(i_k)$ where $1 = i_1 < i_2 < \dots < i_k$ and two such paths are connected if one is the extension of the other with exactly one new vertex. The weight of the edge connecting $f(i_1)f(i_2)\dots f(i_{k-1})$ and $f(i_1)f(i_2)\dots f(i_k)$ is the weight of the edge $f(i_{k-1})f(i_k)$ in the graph H.

The monotone-path tree is the same without weights.

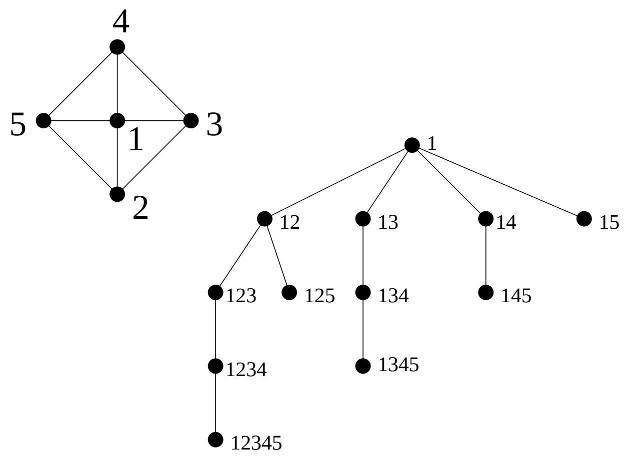

Figure 4.5: A monotone-path tree of the wheel on 5 vertices.

Theorem 4.4.3. *Let H be a properly labeled graph with edge densities γ_e and let $T_f(H)$ be its weighted monotone-path tree with weights γ_e. Assume that these densities do not ensure the existence of the factor $T_f(H)$. Then there is a construction of a blown-up graph of H not inducing H as a transversal and all densities between the clusters are at least as large as the given densities.*

Remark 4.4.4. So this theorem provides a necessary condition for the densities ensuring the existence of factor H. In fact, this gives as many necessary conditions as many proper labelings the graph H has. The advantage of this theorem is that we already know the case of trees substantially.

Proof. We prove the statement by induction on the number of vertices of H. For $n = 1, 2$ the claim is trivial since $H = T_f(H)$. Now assume that we already know the statement till $n - 1$ and we need to prove it for $|V(H)| = n$.

We know from Theorem 4.2.1 that γ_e ensure the existence of factor $T = T_f(H)$ if the corresponding γ'_e ensure the existence of factor T'. Let us apply this theorem as follows. We delete all vertices (monotone-paths) of $T_f(H)$ which contains the vertex $f(n)$. The remaining tree will be a weighted path tree of $H_1 = H - \{f(n)\}$ where the new labeling is simply the restriction of f to the set $\{1, 2, \ldots, n-1\}$. (We will denote this restriction by f as well.) By induction there exists a blown-up graph of H_1 not inducing H_1 as a transversal and all densities between the clusters are at least $\gamma_e(T_f(H_1))$ where we can also assume that the total weight of each cluster is 1.

Now we can do the the construction described in the beginning of this section. Let $f(n) = u$ and $N_H(u) = \{u_1, \ldots, u_k\}$. Let the weight of the new vertex $w_i \in A_i$ be $(1-\gamma_{uu_i})$ and the weights of the other vertices of the cluster be γ_{uu_i} times the original one. Clearly, between the clusters A_n and A_i $(1 \leq i \leq k)$, the weight is just γ_{uu_i} as required. What about the other densities? First of all let us examine γ'_e's. Let us consider the adjacent vertices $f(1)\ldots f(i)$ and $f(1)\ldots f(i)f(j)$ of $T_f(H_1)$. If both $f(i), f(j) \in N_H(u)$ then we deleted the vertices $f(1)\ldots f(i)f(n)$ and $f(1)\ldots f(i)f(j)f(n)$ from $T_f(H)$ changing $\gamma_e = 1 - r_e$ to $1 - \frac{r_e}{\gamma_{f(n)f(i)}\gamma_{f(n)f(j)}}$. If only one of the vertices $f(i)$ or $f(j)$ was connected to $f(n)$ then we can still easily follow the change: $\gamma'_e = 1 - \frac{r_e}{\gamma_{f(n)f(i)}}$ if $f(i)$ was connected to $f(n)$. If none of them was connected to $f(n)$ then there is no change. But in all cases we do exactly the inverse of this operation at the blown-up graphs ensuring that the new densities are at least γ_e.

□

Remark 4.4.5. When we consider the more general problem then it is true that, in fact, we consider only one graph, the complete graph. Indeed, if there is no edge between the vertices u and v in H then we can consider it as if we require $\gamma_{u,v} = 1$ in the complete graph. This raises the question why we only considered the proper labelings since this has no meaning for complete graphs. The answer is simple: we can consider the weighted monotone-path tree of the complete graph for arbitrary labelings, but there will be a better (or at least as good as the original) labeling which is proper for the graph H.

Indeed, assume that for some ordering f, $f(k)$ is not connected to the graph induced by vertices $f(1), \ldots, f(k-1)$. Then we can factorize

$$F((T_f(K_n), \underline{r}); t) = F((T_f(S_1), \underline{r}); t)F((T_f(S_2), \underline{r}); t)^m,$$

where $S_1 = K_n - f(k)$ and S_2 is the complete graph induced by the vertices $f(k), f(k+1), \ldots, f(n)$ and $m = 2^{k-2}$. Indeed, if there is a weighted tree T with an edge $e \in E(T)$ of weight 0 and deleting e the tree T falls into the parts T_1, T_2, then

$$F((T, \underline{r}); t) = F((T_1, \underline{r}); t)F((T_2, \underline{r}); t).$$

Since $r(f(i), f(k)) = 0$ for all $i < k$ we have that the weight is 0 on each edge $(f(1)f(i_2)\ldots f(i_r), f(1)f(i_2)\ldots f(i_r)f(k))$ for $1 < i_2 < \cdots < i_r < k$. Thus there are 2^{k-2} such pairs of monotone-paths we obtain that $m = 2^{k-2}$.

This means that the smallest root of $F((T_f(K_n), \underline{r}); t)$ is the smallest root of $F((T_f(S_1), \underline{r}); t)$ or $F((T_f(S_1), \underline{r}); t)$. In both cases we would be able to give a "better" labeling: in the first case we put the vertex $f(k)$ to the end of the labeling, in the second case we put the vertices $f(k+1), \ldots, f(n)$ to the beginning of the labeling and let us extend it with a vertex adjacent to one of these vertices. If H was connected then it is a strictly better labeling, although it is not surely proper labeling. But if it is not proper we can iterate this step. If H was connected (which we assume in this chapter) then the final labeling is proper and better than the original one.

Now the following conjecture is a natural one after the case of trees. (However, we will see that it is false.)

Conjecture 4.4.6 (General Star Decomposition Conjecture)**.** Let H be a graph with edge densities γ_e. Assume that for each proper labeling f the weights as densities of the weighted monotone-path tree ensure the existence of the graph $T_f(H)$. Then the given densities ensure the existence of the graph H.

Corollary 4.4.7. *Let $S(H)$ be the set of proper labelings of the graph H. The critical density of the graph H is at least*

$$\max_{f \in S(H)} \left\{ 1 - \frac{1}{\mu(T_f(H))^2} \right\}.$$

Remark 4.4.8. If each edge density is equal to $1 - \frac{1}{\mu(T_f(H))^2}$ then there is a straightforward connection between the weights of the constructed blown-up graph and the eigenvector of the tree $T_f(H)$ belonging to the eigenvalue $\mu(T_f(H))$. This connection is very similar to the one given by András Gács.

Conjecture 4.4.9 (Uniform Star Decomposition Conjecture)**.** Let $S(H)$ be the set of proper labelings of the graph H. The critical density of the graph H satisfies

$$d_{crit} = \max_{f \in S(H)} \left\{ 1 - \frac{1}{\mu(T_f(H))^2} \right\}.$$

Remark 4.4.10. So the General Star Decomposition Conjecture asserts that for every graph and every weighting (or edge densities) the best we can do is to choose a good order of the vertices and construct the "stars". The Uniform Star Decomposition Conjecture is clearly a special case of this conjecture when all edge densities are the same for every edge.

The General Star Decomposition Conjecture is true for the triangle in the sense that for every weighting the star decomposition of a suitable labeling gives the best construction or shows that there is no suitable blown-up graph; this is a theorem of Adrian Bondy, Jian Shen, Stéphan Thomassé and Carsten Thomassen [6]. As we have seen this conjecture is also true for trees. Zoltán L. Nagy can prove that it is also true for cycles. Although, in the next section we will show that the General Star Decomposition Conjecture is in general false. I think it makes very unlikely that the Uniform Star Decomposition Conjecture is true. Till it is a meaningful question whether for which graphs one or both conjectures hold. For instance, the author believes that the Uniform Star Decomposition Conjecture is true for complete graphs and complete bipartite graphs.

4.5 Counterexample to the General Star Decomposition Conjecture

Our counterexample is a weighted bow-tie given by the following figure. Although it seems that it is a star decomposition, it is not a star decomposition in the sense we constructed it. For instance, there is no cluster which contains exactly one vertex (and there is no "redundancy".) This is indeed a good construction: whatever we choose from the middle cluster we cannot choose its neighbors (since it is the complement), but then we have to choose the other vertices from the corresponding clusters, but they are connected in the complement.

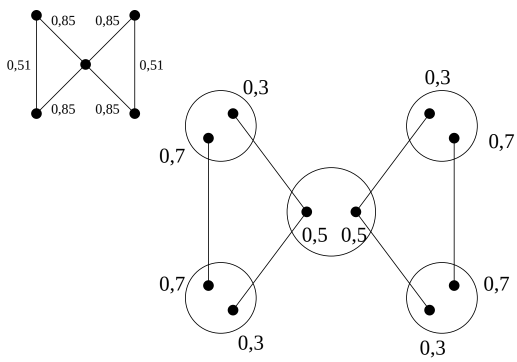

Figure 4.6: Weighted bow-tie and its weighted blown-up graph of the complement.

We will show that the given construction of the blown-up graph is the best possible in the following sense. If for some blown-up graph the edge densities are at least as large as the required densities and one of them is strictly greater, then it induces the bow-tie as a transversal. We will also show that no star decomposition can attain the same densities. Before we prove this we need some preparation. The first lemma appeared in [6] and asserts that the General Star Decomposition Conjecture is true for the triangle.

Lemma 4.5.1. [6] *Let α, β, γ be the edge densities between the clusters of a blown-up graph of the triangle. If*

$$\alpha\beta + \gamma > 1, \ \beta\gamma + \alpha > 1, \ \gamma\alpha + \beta > 1$$

then the blown-up graph contains a triangle as a transversal.

Remark 4.5.2. If we write $\alpha = 1 - r_1$, $\beta = 1 - r_2$ and $\gamma = 1 - r_3$, then the conditions of the lemma can be rewritten as $1 - r_1 - r_2 - r_3 + r_i r_j > 0$ $(1 \leq i, j \leq 3)$. One can easily prove that it is equivalent to the statement that the multivariate matching polynomials of the monotone-path trees have no root in the interval $[0,1]$. (There are three different monotone-path trees, each of them is a path on 4 vertices, on the edges the weights are α, β, γ; the difference between them is that which weight is on the middle edge.)

Next we prove a lemma which can be considered as a generalization of Theorem 4.2.1.

Lemma 4.5.3. *Let H_1, H_2 be two graphs and let $u_1 \in V(H_1)$ and $u_2 \in V(H_2)$. As usual we denote by $H_1 : H_2$ the graph obtained by identifying the vertices u_1, u_2 in $H_1 \cup H_2$. Let $0 < m_1, m_2 < 1$ such that $m_1 + m_2 \leq 1$. Furthermore, assume that an edge density $\gamma_e = 1 - r_e$ is assigned to every edge. If the edge densities*

$$\gamma'_e = \begin{cases} \gamma_e = 1 - r_e & \text{if } e \in E(H_1) \text{ is not incident to } u_1, \\ 1 - \frac{r_e}{m_1} & \text{if } e \in E(H_1) \text{ is incident to } u_1, \end{cases}$$

ensure the existence of a transversal H_1 and the edge densities

$$\gamma'_e = \begin{cases} \gamma_e = 1 - r_e & \text{if } e \in E(H_2) \text{ is not incident to } u_2, \\ 1 - \frac{r_e}{m_2} & \text{if } e \in E(H_2) \text{ is incident to } u_2. \end{cases}$$

ensure the existence of a transversal H_2, then the edge densities $\{\gamma_e\}$ ensure the existence of a transversal $H_1 : H_2$.

Proof. Let $G[H_1 : H_2]$ be a weighted blown-up graph of $H_1 : H_2$ with edge density $\{\gamma_e\}$. Let

$$R_1 = \{v \in A_{u_1=u_2} \mid \ v \text{ can be extended to a transversal } H_1 \subset G[H_1]\}$$

and

$$R_2 = \{v \in A_{u_1=u_2} \mid \ v \text{ can be extended to a transversal } H_2 \subset G[H_2]\}.$$

We show that

$$\sum_{v \in R_1} w(v) > 1 - m_1 \quad \text{and} \quad \sum_{v \in R_2} w(v) > 1 - m_2.$$

But then since $m_1 + m_2 < 1$ there would be some $v \in R_1 \cap R_2$ which we could extend to a transversal of H_1 and H_2 as well and thus we could find a transversal $H_1 : H_2$. Naturally, it is enough to prove that $\sum_{v \in R_1} w(v) > 1 - m_1$, because of the symmetry. We prove it by contradiction. Assume that $\sum_{v \in R_1} w(v) = 1 - t \leq 1 - m_1$. Let us erase all vertices belonging to R_1 from $A_{u_1=u_2}$ and let us give the weight $\frac{w(u)}{t}$ to the remaining vertices $u \in A_{u_1=u_2} - R_1$. Then we obtained a weighted blown-up graph $G'[H_1]$ in which every edge density is at least γ'_e ($e \in E(H_1)$). But then the assumption of the lemma ensures the existence of a transversal H_1 which contradicts the construction of $G'[H_1]$. □

Now we are ready to prove that the above given construction is best possible.

Statement 4.5.4. *Let $V(H) = \{v_1, v_2, v_3, v_4, v_5\}$ and $E(H) = \{v_1v_2, v_1v_3, v_1v_4, v_1v_5, v_2v_3, v_4v_5\}$. Furthermore, assume that for the edge densities of the blown-up graph $G[H]$ satisfy the following inequalities: $\gamma_{12}, \gamma_{13}, \gamma_{14}, \gamma_{15} \geq 0,85$, $\gamma_{23}, \gamma_{45} \geq 0,51$ and at least one of the inequalities is strict. Then $G[H]$ contains H as a transversal.*

Proof. We can assume that at least one of the strict inequality $\gamma_{12} > 0,85$ or $\gamma_{23} > 0,51$ holds. Let us apply the Lemma 4.5.3 with $H_1 = H(v_1, v_2, v_3)$ and $H_2 = H(v_1, v_4, v_5)$, $u_1 = u_2 = v_1$, densities γ_{ij} and $m_1 = 1/2 - \varepsilon$, $m_2 = 1/2 + \varepsilon$ where ε is a very small positive number chosen later. Then

$$\gamma'_{ij}\gamma'_{jk} + \gamma_{ik} - 1 = 1 - r'_{12} - r'_{13} - r'_{23} + r'_{ij}r'_{jk} > 0$$

for any permutation i, j, k of $\{1, 2, 3\}$. Indeed, since $0,3 = \frac{0,15}{0,5}$ we have

$$1 - 0,3 - 0,3 - 0,49 + 0,3 \cdot 0,49 > 1 - 0,3 - 0,3 - 0,49 + 0,3 \cdot 0,3 = 0$$

and one of the r_{ij}'s is strictly smaller than $0,3$ or $0,49$ and so for small enough ε, the expression $1 - r'_{12} - r'_{13} - r'_{23} + r'_{ij}r'_{jk}$ is positive. Hence by Lemma 4.5.1 it ensures the existence of a triangle transversal. For the other triangle, $r'_{14} = \frac{r_{14}}{1/2+\varepsilon} < 0,3$ and similarly, $r'_{15} < 0,3$ and $r_{45} \leq 0,49$. Again by Lemma 4.5.1 it ensures the existence of a triangle transversal. By Lemma 4.5.3 we obtain that there exists a transversal H in $G[H]$. □

Statement 4.5.5. *There is no weighted blown-up graph of the bow-tie arising from star decomposition which is at least as good as the weighted blown-up graph in the Figure 4.6.*

Proof. Because of the symmetry and since we only need to consider the star decompositions where the labeling is proper, we only have to consider two star decompositions (see Remark 4.4.5). Because of Statement 4.5.4, all edge densities must be exactly the required one. This makes the whole computation a routine work.

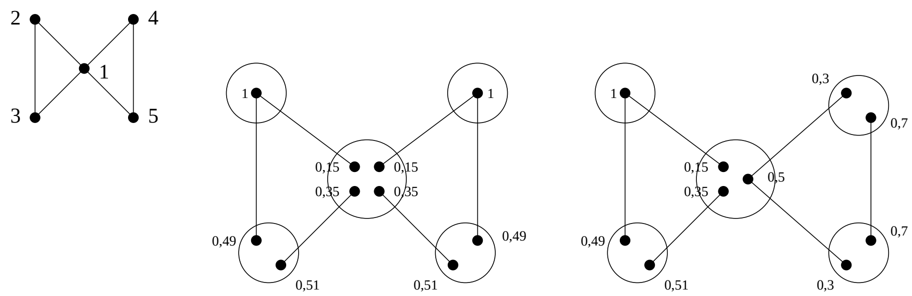

Figure 4.7: Star decompositions of bow-ties.

In both cases one can determine the weights so as that finally $0,51 \cdot 0,35 \neq 0,15$ gives the contradiction.

□

4.6 Complete bipartite graphs

Let $d_{crit}(K_{n,m}) = d(n,m)$ be the critical edge density of the complete bipartite graph $K_{n,m}$. Let $d_c(n,m)$ be the best edge density coming from the star decomposition ("c abbreviates constructed" in d_c).

If one starts to do the star decomposition to $K_{n,m}$ then the following recursion holds:

$$d_c(n,m) = \frac{1}{2 - d_c(n,m-1)} \text{ or } \frac{1}{2 - d_c(n-1,m)}$$

according to which class contains the vertex $f(n+m)$. Although we have two possibilities the recursion has only one solution, namely

$$d_c(n,m) = 1 - \frac{1}{n+m-1}$$

since $d(1,1) = d_c(1,1) = 0$. From this we already gain an interesting fact.

Theorem 4.6.1. *For any proper labeling f of the graph $K_{n,m}$ the tree $T_f(K_{n,m})$ has spectral radius $\sqrt{n+m-1}$.*

Remark 4.6.2. In this case a proper labeling simply means that $f(1)$ and $f(2)$ are elements of different classes in the bipartite graph.

For different proper labelings these trees can look very differently, but as the theorem shows their spectral radiuses are the same.

Conjecture 4.6.3. $d_{crit}(K_{n,m}) = d_c(n,m) = 1 - \frac{1}{n+m-1}$.

Remark 4.6.4. Of course, Conjecture 4.4.9 implies Conjecture 4.6.3, but the author has the feeling that Conjecture 4.6.3 is true while Conjecture 4.4.9 may not hold.

Chapter 5

Integral trees

An integral tree is a tree for which the eigenvalues of its adjacency matrix are all integers [40]. Many different classes of integral trees have been constructed in the past decades [8, 9, 12, 13, 63, 64, 67]. Most of these classes contain infinitely many integral trees, but till now only examples of trees of bounded diameters were known. The largest diameter of known integral trees was 10. In this chapter we construct integral trees of arbitrarily large diameters. In fact, we prove the following much stronger theorem.

Theorem 5.0.5. *For every finite set S of positive integers there exists a tree whose positive eigenvalues are exactly the elements of S. If the set S is different from $\{1\}$ then the constructed tree will have diameter $2|S|$.*

Clearly, there is only one tree with set S of positive eigenvalues for $S = \{1\}$, the tree on two vertices with spectrum $\{-1, 1\}$ (and its diameter is 1).

The structure of this chapter is the following. In the next section we will define a class of trees recursively. All trees belonging to this class will turn out to be *almost-integral*, i.e., all of their eigenvalues are square roots of integers. We will find integral trees in this class of trees by special choice of parameters introduced later.

5.1 Construction of trees

Definition 5.1.1. For given positive integers $r_1, \dots, r_k$ we construct the trees

$$T_1(r_1), T_2(r_1, r_2), \dots, T_k = T_k(r_1, \dots, r_k)$$

recursively as follows. We will consider the tree T_i as a bipartite graph with color classes A_{i-1}, A_i. The tree $T_1(r_1) = (A_0, A_1)$ consists of the classes of size $|A_0| = 1, |A_1| = r_1$ (so it is a star on r_1+1 vertices). If the tree $T_i(r_1, \dots, r_i) = (A_{i-1}, A_i)$ is defined then let $T_{i+1}(r_1, \dots, r_{i+1}) = (A_i, A_{i+1})$ be defined as follows. We connect each vertex of A_i with r_{i+1} new vertices of degree 1. Then for the resulting tree the color class A_{i+1} will have size $|A_{i+1}| = r_{i+1}|A_i| + |A_{i-1}|$, the color class A_i does not change.

One should not confuse these trees with the balanced trees. These trees are very far from being balanced.

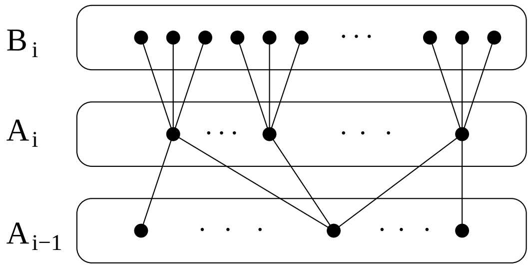

Figure 5.1: Let $A_{i+1} = A_{i-1} \cup B_i$, where each element of A_i has exactly r_{i+1} neighbors of degree 1 in B_i.

5.2 Monotone-path trees

In this section we would like to reveal the fact that the trees defined in Definition 5.1.1 are nothing else than the monotone-path trees of complete bipartite graphs.

Assume that the ordering of $K_{m,n} = (X_1, X_2, E)$ is the following: 1 is in X_1, $2, 3, \dots, r_1 + 1$ is in X_2, $r_1 + 2, r_1 + 3, \dots, r_1 + r_2 + 1$ is in X_1, etc. (Probably, it would have been better to start with vertex 0, but we decided to follow the notation of the previous chapter.)

One can imagine this as follows: we toss a coin, if we threw head for the i-th flipping then we put i in the first class, if we threw tail then we put it in the second class. Now $r_1, r_2, \dots$ are the length of the *runs*.

The tree T_i is nothing else than the monotone-path tree of the complete bipartite graph induced by the first $1 + r_1 + \dots + r_i$ vertices. Then we construct T_{i+1} from T_i as follows. Let us consider those monotone-paths $\underline{p}$ which end in the class X_j, where $j \equiv i + 1 \pmod 2$. We can extend such a monotone-path $\underline{p}$ in r_{i+1} ways by putting one of the vertex of $(1 + r_1 + \dots + r_i) + 1, (1 + r_1 + \dots + r_i) + 2, \dots, (1 + r_1 + \dots + r_i) + r_{i+1}$. On the other hand, we cannot extend the monotone-paths that end in the class containing these vertices. This shows that the constructed trees are indeed the monotone-path trees.

Remark 5.2.1. To be honest, the monotone-path tree was the original construction. It was András Gács who convinced me not to introduce the concept of monotone-path trees in the paper [16].

We have already seen in the previous chapter that the largest eigenvalue of these trees is $\sqrt{m+n-1}$ independently of the ordering. The other eigenvalues will depend on the order, but as it will turn out, they are also square roots of integers.

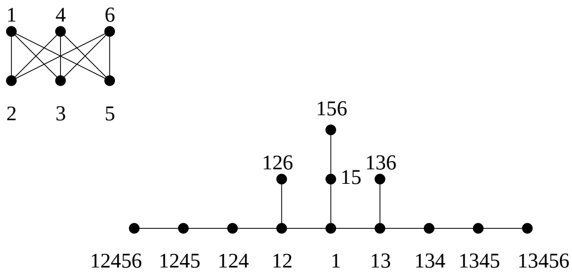

Figure 5.2: A monotone-path tree of $K_{3,3}$.

Now we see that the tree in the figure is $T(2,1,1,1)$ as the runs are $\{2,3\},\{4\},\{5\},\{6\}$. Its spectrum is

$$\{\sqrt{5},\sqrt{3},\sqrt{2},1^2,0^3,-1^2,-\sqrt{2},-\sqrt{3},-\sqrt{5}\}.$$

The exponents are the multiplicities of the eigenvalues.

5.3 Analysis of the constructed trees

To analyze the trees $T_k(r_1,\dots,r_k)$ introduced in Definition 5.1.1 we will need the following concept.

Definition 5.3.1. Let us define the following sequence of expressions.

$$Q_0(.) = 1$$

$$Q_1(x_1) = x_1$$

and

$$Q_j(x_1,\dots,x_j) = x_j Q_{j-1}(x_1,\dots,x_{j-1}) + Q_{j-2}(x_1,\dots,x_{j-2})$$

for all $3 \le j \le k$. We will also use the convention $Q_{-1} = 0$. We will call these expressions *continuants*. Sometimes if the $\underline{x} = (x_1,\dots,x_k)$ is clear from the context then we will simply write Q_j instead of $Q_j(x_1,\dots,x_j)$.

Remark 5.3.2. The first few continuants are

$$Q_2(x_1,x_2) = 1 + x_1x_2, \quad Q_3(x_1,x_2,x_3) = x_1 + x_3 + x_1x_2x_3$$

$$Q_4(x_1,x_2,x_3,x_4) = 1 + x_1x_2 + x_1x_4 + x_3x_4 + x_1x_2x_3x_4.$$

The expressions $Q_j(x_1,\dots,x_j)$ often show up in the study of some Euclidean type algorithms. For instance,

$$x_k + \cfrac{1}{x_{k-1} + \cfrac{1}{x_{k-2} + \cfrac{1}{\ddots + \cfrac{1}{x_1}}}} = \frac{Q_k(x_1,\dots,x_k)}{Q_{k-1}(x_1,\dots,x_{k-1})}.$$

For more details on continuants see [33].

Lemma 5.3.3. *Let $T_k(r_1,\dots,r_k)$ be the constructed tree with color classes (A_{k-1},A_k). Then $|A_{k-1}| = Q_{k-1}(r_1,\dots,r_{k-1})$ and $|A_k| = Q_k(r_1,\dots,r_k)$.*

Proof. This is a trivial induction. □

Lemma 5.3.4. *If $r_1 \geq 2$ then the diameter of $T_k(r_1,\dots,r_k)$ is $2k$.*

Proof. Note that each vertex is at distance at most k from the only element v_0 of the set A_0. Thus the diameter is at most $2k$. On the other hand, if we go from v_0 to two different leaves through two different elements of A_1 which are at distance k from v_0 (so these are the elements of $A_k \backslash A_{k-2}$) then these two leaves must be at distance $2k$ apart. □

Remark 5.3.5. Note that $T_j(1,r_2,r_3,\dots,r_j) = T_{j-1}(r_2+1,r_3,\dots,r_j)$. Hence all constructed trees different from the tree on two vertices have a representation $T_k(r_1,\dots,r_k)$ in which $r_1 \geq 2$.

The next lemma will be the main tool to determine the spectrum of the tree $T_k(r_1,\dots,r_k)$. Before we state it we introduce the following notation.

Definition 5.3.6. Let $Sp(G)$ denote the spectrum of the graph G. Let N_G^+ denote the number of positive eigenvalues of G and $N_G(t)$ denotes the multiplicity of the eigenvalue t.

Lemma 5.3.7. *Let $G = (A,B,E)$ be a bipartite graph with eigenvalue $\lambda \neq 0$ of multiplicity m. Let G' be obtained from G by joining each element of B with r new vertices of degree 1, so that the obtained graph has $|A| + (r+1)|B|$ vertices. Then $\pm\sqrt{\lambda^2 + r}$ are eigenvalues of G' of multiplicity m. Furthermore, the rest of the eigenvalues of the new graph are $\pm\sqrt{r}$ with multiplicity $|B| - N_G^+$ and 0 with multiplicity $|A| + (r-1)|B|$ and there is no other eigenvalue.*

Proof. Since G and G' are both bipartite graphs we only need to deal with the non-negative eigenvalues. Let $0 < \mu \neq \sqrt{r}$ be an eigenvalue of the graph G' of multiplicity m. We prove that $\sqrt{\mu^2 - r}$ is an eigenvalue of G of multiplicity m. (Note that it means that $0 < \mu < \sqrt{r}$ cannot occur since the eigenvalues of a graph are real numbers.)

Let $\underline{x}$ be an eigenvector belonging to μ. We will construct an eigenvector $\underline{x'}$ to $\sqrt{\mu^2 - r}$ in the graph G. Let $v_i \in B$ and its new neighbors $w_{i1},\dots,w_{ir}$. Then

$$x(v_i) = \mu x(w_{i1}) = \mu x(w_{i2}) = \dots = \mu x(w_{ir}).$$

Since $\mu \neq 0$ we have $x(w_{i1}) = \cdots = x(w_{ir})$. Moreover, for each $v_i \in B$ and $u_j \in A$ we have

$$\mu x(v_i) = \sum_{v_i \sim u_k} x(u_k) + r x(w_{i1})$$

and

$$\mu x(u_j) = \sum_{u_j \sim v_l} x(v_l).$$

Since $x(v_i) = \mu x(w_{i1})$ we can rewrite these equations as

$$(\mu^2 - r) x(w_{i1}) = \sum_{v_i \sim u_k} x(u_k)$$

and

$$\mu x(u_j) = \sum_{u_j \sim v_l} \mu x(w_{l1}).$$

In the second equation we can divide by μ since it is not 0. Hence it follows that

$$\sqrt{\mu^2 - r} \cdot (\sqrt{\mu^2 - r} \cdot x(w_{i1})) = \sum_{v_i \sim u_k} x(u_k)$$

and

$$\sqrt{\mu^2 - r} \cdot x(u_j) = \sum_{u_j \sim v_l} (\sqrt{\mu^2 - r} \cdot x(w_{l1})).$$

Thus the vector $\underline{x}'$ which is equal to $\sqrt{\mu^2 - r} \cdot x(w_{i1})$ on the vertices of B and $x(u_j)$ on the elements of A is an eigenvector of the graph G with eigenvalue $\sqrt{\mu^2 - r}$. Clearly, this vector is not $\underline{0}$, otherwise $\underline{x}$ should have been $\underline{0}$. It also implies that if the vectors $\underline{x}_1, \dots, \underline{x}_h$ are independent eigenvectors belonging to μ then the constructed eigenvectors $\underline{x'}_1, \dots, \underline{x'}_h$ are also independent. Note that this construction can be reversed if $\sqrt{\mu^2 - r} \neq 0$ implying that for $\mu \neq \sqrt{r}$ the multiplicity of μ in G' is the same as the multiplicity of $\sqrt{\mu^2 - r}$ in G.

We can easily determine the multiplicity of the eigenvalues 0 and $\sqrt{r}$ as follows:

$$e(G) + r|B| = e(G') = \sum_{\mu > 0, \mu \in Sp(G')} \mu^2 = \sum_{\lambda > 0, \lambda \in Sp(G)} (\lambda^2 + r) + N_{G'}(\sqrt{r}) r =$$

$$= e(G) + N_G^+ r + N_{G'}(\sqrt{r}) r.$$

Hence $N_{G'}(\sqrt{r}) = |B| - N_G^+$. Finally, the multiplicity of 0 as an eigenvalue of G' can be determined as follows:

$$N_{G'}(0) = |A| + (r+1)|B| - 2N_{G'}^+ =$$

$$= |A| + (r+1)|B| - 2N_G^+ - 2N_{G'}(\sqrt{r}) = |A| + (r+1)|B| - 2|B|.$$

□

Theorem 5.3.8. *Let $r_1 \geq 2, r_i \geq 1$ integers. The set of different eigenvalues of the tree $T_k(r_1, r_2, \ldots, r_k)$ is the set*

$$\{\pm\sqrt{r_k}, \pm\sqrt{r_k + r_{k-1}}, \pm\sqrt{r_k + r_{k-1} + r_{k-2}}, \ldots, \pm\sqrt{r_k + \cdots + r_1}, 0\}.$$

Furthermore, the multiplicity of 0 *is*

$$Q_k(r_1, \ldots, r_k) - Q_{k-1}(r_1, \ldots, r_{k-1})$$

and the multiplicity of the eigenvalues $\pm\sqrt{r_k + r_{k-1} + \cdots + r_j}$ are

$$Q_{j-1}(r_1, \ldots, r_{j-1}) - Q_{j-2}(r_1, \ldots, r_{j-2}),$$

where Q_i's are the continuants.

Proof. We will use the short notation Q_j for $Q_j(r_1, \ldots, r_j)$. We prove the theorem by induction on k. The statement is true for $k = 1$. Assume that it is true for $n = k - 1$. We need to prove it for $n = k$. By the induction hypothesis the tree $T_{k-1}(r_1, \ldots, r_{k-1})$ has spectrum

$$\{\pm\sqrt{r_{k-1}}, \pm\sqrt{r_{k-1} + r_{k-2}}, \ldots, \pm\sqrt{r_{k-1} + \cdots + r_1}, 0\}.$$

Furthermore, the multiplicity of the eigenvalues $\pm\sqrt{r_{k-1} + \cdots + r_j}$ are $Q_{j-1} - Q_{j-2}$. Now let us apply Lemma 5.3.7 with $G = T_{k-1}(r_1, \ldots, r_{k-1})$ and $r = r_k$. Then $G' = T_k(r_1, \ldots, r_k)$ has spectrum

$$\{\pm\sqrt{r_k}, \pm\sqrt{r_k + r_{k-1}}, \pm\sqrt{r_k + r_{k-1} + r_{k-2}}, \ldots, \pm\sqrt{r_k + \cdots + r_1}, 0\}.$$

Furthermore, the multiplicity of the eigenvalues $\pm\sqrt{r_k + r_{k-1} + \cdots + r_j}$ are $Q_{j-1} - Q_{j-2}$ for $j \leq k - 1$. The multiplicity of $\sqrt{r_k}$ is

$$Q_{k-1} - ((Q_{k-2} - Q_{k-3}) + (Q_{k-3} - Q_{k-4}) + \cdots + (Q_0 - Q_{-1})) = Q_{k-1} - Q_{k-2}.$$

Finally, the multiplicity of 0 is

$$(r_k - 1)Q_{k-1} + Q_{k-2} = Q_k - Q_{k-1}.$$

□

Remark 5.3.9. Note that if $r_1 \geq 2$ then the tree $T_k(r_1, \ldots, r_k)$ has $2k + 1$ different eigenvalues and diameter $2k$. Since the number of different eigenvalues is at least the diameter plus one for any graph [32] these trees have the largest possible diameter among graphs having restricted number of different eigenvalues.

Theorem 5.0.5 *For every set S of positive integers there exists a tree whose positive eigenvalues are exactly the elements of S. If the set S is different from $\{1\}$ then the constructed tree will have diameter $2|S|$.*

Proof. Let $S = \{n_1, n_2, \ldots, n_{|S|}\}$, where $n_1 < n_2 < \cdots < n_{|S|}$. Then apply the previous theorem with

$$r_{|S|} = n_1^2, r_{|S|-1} = n_2^2 - n_1^2, \ldots, r_1 = n_{|S|}^2 - n_{|S|-1}^2.$$

If the set is different from $\{1\}$ then $r_1 \geq 2$ and in this case the diameter of the tree is $2|S|$ by Lemma 5.3.4. $\square$

Example 1. Let $S = \{1, 2, 4, 5\}$ then $r_4 = 1, r_3 = 3, r_2 = 12, r_1 = 9$. The resulting tree has 781 vertices and the spectrum is

$$\{-5, -4^8, -2^{100}, -1^{227}, 0^{109}, 1^{227}, 2^{100}, 4^8, 5\}.$$

Here the exponents are the multiplicities of the eigenvalues.

Example 2. Let $S = \{1, 2, 3, 4, 5, 6\}$ then $r_6 = 1, r_5 = 3, r_4 = 5, r_3 = 7, r_2 = 9, r_1 = 11$. The resulting tree has 27007 vertices and the spectrum is

$$\{\pm 6, \pm 5^{10}, \pm 4^{89}, \pm 3^{611}, \pm 2^{2944}, \pm 1^{8021}, 0^{3655}\}$$

The diameter of this tree is 12.

Remark 5.3.10. Recently Andries E. Brouwer (private communication) found a very elegant (and very short!) proof that $T(n_k^2 - n_{k-1}^2, n_{k-1}^2 - n_{k-2}^2, \ldots, n_2^2 - n_1^2, n_1^2)$ are integral trees. It is really worth reading this proof. This proof is outlined on Brouwer's homepage [7] or a bit more detailed version of this proof can be found at [17].

5.4 Afterlife

Recently, E. Ghorbani, A. Mohammadian and B. Tayfeh-Rezaie [29] managed to construct integral trees of odd diameters. In their work they built on the trees constructed in this chapter.

Chapter 6

Appendix

The aim of this appendix is to provide a concise background to the materials included in my thesis. Many things appearing here are well-known or an easy modification of it are well-known. Still I hope that the Reader will find this appendix useful.

A.1 Independence polynomial and matching polynomial

In this section we define the notion of the weighted independence polynomial and weighted matching polynomial and study its fundamental properties. This two polynomials have an intimate relationship, that is why we treat them together.

A.1.1 Weighted independence polynomial

Definition A.1.1. Let G be a graph and assume that a positive weight function $w : V(G) \to \mathbb{R}^+$ is given. Then let

$$I((G,\underline{w});t) = \sum_{S\in\mathcal{I}} \left(\prod_{u\in S} w_u\right)(-t)^{|S|},$$

where the summation goes over the set $\mathcal{I}$ of all independent set S of the graph G including the empty set. When $\underline{w} = \underline{1}$ we simply write $I(G,t)$ instead of $I((G,\underline{1});t)$ and we call $I(G,t)$ the independence polynomial of G.

Remark A.1.2. Clearly,

$$I(G,t) = \sum_{k=1}^{n} i_k(G)(-1)^k t^k,$$

where $i_k(G)$ denotes the number of independent sets of size k in the graph G. We have to mention that in the literature the polynomial $I(G,-t)$ is called the independence polynomial. Since the relationship between these two forms is very simple, it will not cause any confusion.

Note that $I((G,\underline{w});0) = 1$ and $I((G,t\underline{w}),1) = I((G,\underline{w}),t)$. The following simple facts follow from separating the terms including vertex u or vertices u and v, respectively.

Statement A.1.3. *Let $u \in V(G)$ be an arbitrary vertex. Then*

$$I((G, \underline{w}); t) = I((G - u, \underline{w}); t) - w_u t I((G - N[u], \underline{w}); t),$$

where we denoted the functions w restricted to $V(G-u)$ and $V(G-N[u])$ by w as well.

Statement A.1.4. *The polynomial $I((G, \underline{w}), x)$ satisfies the recursion*

$$I((G, \underline{w}); t) = I((G - e, \underline{w}); t) - w_u w_v t^2 I((G - N[v] - N[u], \underline{w}); t),$$

where $e = (u, v)$ is an arbitrary edge of the graph G.

Remark A.1.5. Clearly Statement A.1.3 and A.1.4 simplify to

$$I(G, t) = I(G - u, t) - tI(G - N[u]; t)$$

and

$$I(G, t) = I(G - e, t) - t^2 I(G - N[v] - N[u], t)$$

in the case of the unweighted independence polynomial.

In what follows we show that $I((G, \underline{w}); t)$ has a real root. Let $\beta_w(G)$ denote the smallest real root of $I((G, \underline{w}); t)$; this is positive by the alternating sign of the coefficients of the polynomial $I((G, \underline{w}); t)$. We will also show that if H is a subgraph of G then $\beta_w(G) \leq \beta_w(H)$. This is a slight extension of the theorem of D. Fisher and J. Ryan [28]. They deduce their result from a counting problem where the reciprocal of the dependence polynomial was the generating function. We follow another way, our treatment resembles to that of H. Hajiabolhassan and M. L. Mehrabadi [38].

The key step of the proof of these statements is the following definition.

Definition A.1.6. Let $\beta(p)$ denote the smallest positive root of the polynomial p; if it does not exist set $\beta(p) = \infty$. Let $p \succ q$ if $q(x) \geq p(x)$ on the interval $[0, \beta(p)]$. Furthermore, we say that $(G_1, \underline{w}_1) \succ (G_2, \underline{w}_2)$ if $I((G_1, \underline{w}_1); t) \succ I((G_2, \underline{w}_2); t)$. If $(G_1, \underline{w}_1) \succ (G_2, \underline{w}_2)$ and $\underline{w}_1 = \underline{w}_2$ or one is the extension of the other we simply write $G_1 \succ G_2$.

We need the following observation about the relation $\succ$.

Statement A.1.7. *Let $p(0) = q(0) = r(0) = 1$ and assume that $p \succ q \succ r$. Then $\beta(p) \leq \beta(q)$ and $p \succ r$.*

Proof. Since $p(0) = 1$ we have $p(t) > 0$ on the interval $[0, \beta(p))$. Thus $q(t) \geq p(t) > 0$ on the interval $[0, \beta(p))$ giving that $\beta(q) \geq \beta(p)$. If $p \succ q \succ r$ then $\beta(r) \geq \beta(q) \geq \beta(p)$ and $r(t) \geq q(t) \geq p(t)$ on the interval $[0, \min(\beta(p), \beta(q))) = [0, \beta(p))$ thus $p \succ r$. ☐

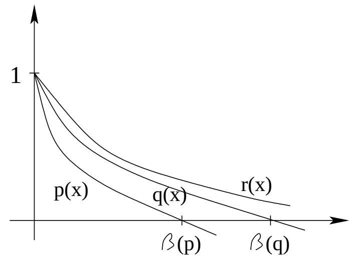

Figure 6.1: The functions $p(x), q(x)$ and $r(x)$.

Remark A.1.8. Note that if $q(t) \geq p(t)$ on the interval $[0, \beta(q)]$ where $\beta(q) < \infty$ then we have $\beta(p) \leq \beta(q)$ and so $p \succ q$.

Clearly, we can apply this lemma to the polynomials $I((G, \underline{w}); t)$ since their values are 1 at 0. Now we are ready to prove the statements mentioned above.

Statement A.1.9. *For every weighted graph $(G, \underline{w})$ we have $\beta_w(G) < \infty$ and if G_2 is an induced subgraph of G_1 then $G_1 \succ G_2$.*

Proof. We prove the two statements together. We prove them by induction on the number of vertices of G_1. For the graph consisting of only one node we have $\beta_w(G) = \frac{1}{w_u} < \infty$. For the sake of simplicity let us use the notation $G_1 = G$. By the transitivity of the relation $\succ$ (Statement A.1.7) it is enough to prove that $G \succ G - v$. The statement is true if $|V(G)| = 2$.

Since $G - N[v]$ is an induced subgraph of $G - v$, by the induction hypothesis we have

$$I((G - v, \underline{w}); t) \succ I((G - N[v], \underline{w}); t)$$

and $\beta_w(G - v) \leq \beta_w(G - N[v]) < \infty$. This means that

$$I((G - N[v], \underline{w}); t) \geq I((G - v, \underline{w}); t)$$

on the interval $[0, \beta_w(G - v)]$. Thus $I((G - N[v], \underline{w}); t) \geq 0$ on the interval $[0, \beta_w(G - v)]$. Hence by Statement A.1.3 we have $I((G, \underline{w}); t) \leq I((G - v, \underline{w}); t)$ on the interval $[0, \beta_w(G - v)]$. This implies that $\beta_w(G) \leq \beta_w(G - v)$. Indeed, since $I((G, \underline{w}); 0) = 1$ and $I((G, \underline{w}), \beta_w(G - v)) \leq 0$ so $I((G, \underline{w}); t)$ has a root in the interval $[0, \beta_w(G - v)]$. Hence $I((G, \underline{w}); t) \leq I((G - v, \underline{w}); t)$ on the interval $[0, \beta_w(G)]$, i.e., $G \succ G - v$. $\square$

Statement A.1.10. *If G_2 is a subgraph of G_1 then $G_1 \succ G_2$.*

Proof. Clearly, it is enough to prove the statement when $G_1 = G$ and $G_2 = G - e$ for some $e = (u, v) \in E(G)$. We need to prove that $G \succ G - e$. Let us use the recursion formula of Statement A.1.4 to G:

$$I((G, \underline{w}); t) = I((G - e, \underline{w}); t) - w_u w_v t^2 I((G - N[u] - N[v], \underline{w}); t).$$

By Statement A.1.9 we have $G \succ G - N[u] - N[v]$ and so $I((G - N[u] - N[v], \underline{w}); t) \geq I((G, \underline{w}); t) \geq 0$ on the interval $[0, \beta_w(G)]$. Hence $I((G - e, \underline{w}); t) \geq I((G, \underline{w}); t)$ on this interval, i.e. , $G \succ G - e$. □

⋆ ⋆ ⋆

Our next goal is to prove Alex Scott and Alan Sokal's extension of the Lovász local lemma. In fact, we modify the statement a bit in order to get a version that is easier to use, but which is clearly just a special case of the original Scott-Sokal theorem.

Theorem A.1.11. *(Scott-Sokal [60]) Assume that given a graph G and there is an event A_i assigned to each node i. Assume that A_i is totally independent of the events $\{A_k \mid (i,k) \in E(\overline{G})\}$. Set $\mathbb{P}r(A_i) = p_i$.*

(a) Assume that $I((G, \underline{p}), t) > 0$ for $t \in [0,1]$, i.e., $\beta_p(G) > 1$. Then we have

$$\mathbb{P}r(\cap_{i \in V(G)} \overline{A_i}) \geq I((G, \underline{p}), 1) > 0.$$

(b) Assume that $I((G, \underline{p}), t) = 0$ for some $t \in [0,1]$. Then there exist a probability space and a family of events B_i with $\mathbb{P}r(B_i) \geq p_i$ and with dependency graph G such that

$$\mathbb{P}r(\cap_{i \in V(G)} \overline{B_i}) = 0.$$

Remark A.1.12. Hence the smallest root of $I(G,t)$, $\beta(G)$ has the following meaning. If the events A_i have the dependency graph G and $\mathbb{P}r(A_i) < \beta(G)$ for all i then $\mathbb{P}r(\cap_{i \in V(G)} \overline{A_i}) > 0$.

Proof. Let us define the events B_i on a new probability space as follows

$$\mathbb{P}r(\cap_{i \in S} B_i) = \begin{cases} \prod_{i \in S} p_i & \text{if S is independent in G,} \\ 0 & \text{otherwise.} \end{cases}$$

Consider the expression

$$\mathbb{P}r((\cap_{i \in S} B_i) \cap (\cap_{i \notin S} \overline{B_i})).$$

This is clearly 0 if S is not an independent set. So assume that S is an independent set. Then we have

$$\mathbb{P}r((\cap_{i \in S} B_i) \cap (\cap_{i \notin S} \overline{B_i})) =$$
$$= \sum_{S \subseteq I} (-1)^{|I|-|S|} \mathbb{P}r(\cap_{i \in I} B_i) =$$
$$= \sum_{\substack{S \subseteq I \\ I \in \mathcal{I}}} (-1)^{|I|-|S|} \prod_{i \in I} p_i = (\prod_{i \in S} p_i) \cdot I((G - N[S], \underline{p}), 1),$$

where $\mathcal{I}$ is the set of independent sets and $N[S]$ denote the set S together with all their neighbors. Note that $\beta_p(G) > 1$, so by Statement A.1.9 we have $\beta_p(G - N[S]) > 1$; this means that the last expression is non-negative for all S. Hence we have defined a probability measure on the generated σ-algebra $\sigma(B_i \mid i \in V(G))$.

As a next step we show that $(B_i)_{i\in V(G)}$ minimizes the expression $\mathbb{P}r(\cap_{i\in V(G)}\overline{B_i})$ among the families of events with dependency graph G. For $S \subset V(G)$, set

$$P_S = \mathbb{P}r(\cap_{i\in S}\overline{A_i})$$

and

$$Q_S = \mathbb{P}r(\cap_{i\in S}\overline{B_i}).$$

Now we prove by induction on $|S|$ that P_S/Q_S is monotone increasing in S. First of all,

$$Q_S = \sum_{I\subseteq S}(-1)^{|I|}\mathbb{P}r(\cap_{i\in I}B_i) =$$

$$= \sum_{\substack{I\subseteq S\\ I\in\mathcal{I}}}(-1)^{|I|}\prod_{i\in I}p_i = I((S,\underline{p});1) > 0.$$

Furthermore, for $j \notin S$ we have

$$Q_{S\cup\{j\}} = I((S\cup\{j\},\underline{p});1) =$$

$$= I((S,\underline{p});1) - p_j I((S-N[j],\underline{p});1) = Q_S - p_j Q_{S-N[j]}.$$

On the other hand,

$$P_{S\cup\{j\}} = P_S - \mathbb{P}r(A_j \cap (\cap_{i\in S}\overline{A_i})) \geq$$

$$\geq P_S - \mathbb{P}r(A_j \cap (\cap_{i\in S-N[j]}\overline{A_i})) \geq$$

$$\geq P_S - p_j P_{S-N[j]}.$$

Now we show that $P_{S\cup\{j\}}/Q_{S\cup\{j\}} \geq P_S/Q_S$, or equivalently that $P_{S\cup\{j\}}Q_S - Q_{S\cup\{j\}}P_S \geq 0$. We have

$$P_{S\cup\{j\}}Q_S - Q_{S\cup\{j\}}P_S \geq (P_S - p_j P_{S-N[j]})Q_S - (Q_S - p_j Q_{S-N[j]})P_S = p_j(P_S Q_{S-N[j]} - Q_S P_{S-N[j]}) \geq 0$$

since

$$\frac{P_S}{Q_S} \geq \frac{P_{S-N[j]}}{Q_{S-N[j]}}$$

by the induction hypothesis.

Since P_S/Q_S is monotone increasing in S we have $P_{V(G)}/Q_{V(G)} \geq P_\emptyset/Q_\emptyset = 1$. Hence we have proved part (a) of the theorem.

To prove part (b) it is enough to use the construction of the events B_i with probability $\beta_p(G)p_i$. Then this will define a probability measure again the same way. Now we have

$$\mathbb{P}r(\cap_{i\in V(G)}\overline{B_i}) = I((G,\beta_p(G)\underline{p});1) = I((G,\underline{p});\beta_p(G)) = 0.$$

□

A.1.2 Weighted matching polynomial

Definition A.1.13. Let G be a graph and assume that a positive weight function $w : E(G) \to \mathbb{R}^+$ is given. Then let

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

where the summation goes over the set $\mathcal{M}$ of all independent edge set S of the graph G including the empty set. In the case when $\underline{w} = \underline{1}$ we call the polynomial

$$M(G,t) = M((G,\underline{1});t)$$

the matching polynomial of G.

Remark A.1.14. First of all, it is clear that the weighted matching polynomial is just a simple transformation of the weighted independence polynomial of the line graph of G. Indeed, let L_G be the line graph of G then we have

$$M((G,\underline{w});t) = t^n I((L_G,\underline{w});\frac{1}{t^2}).$$

Thus we can apply the theorems concerning the weighted independence polynomials. As a particular case we get the following statement.

Statement A.1.15. *Let $t_w(G)$ denote the largest real root of the polynomial $M((G,\underline{w});t)$. Let G_1 be a subgraph of G then we have*

$$t_w(G_1) \le t_w(G).$$

For the sake of convenience, we repeat some of the arguments when the weights are 1.

Definition A.1.16. Let $t(G)$ be the largest root of the matching polynomial $M(G,x)$. Furthermore, let $G_1 \succ G_2$ if for all $x \ge t(G_1)$ we have $M(G_2,x) \ge M(G_1,x)$.

Statement A.1.17. *The relation $\succ$ is transitive and if $G_1 \succ G_2$ then $t(G_1) \ge t(G_2)$.*

Proof. Let $G_1 \succ G_2$. Since $M(G_1,x)$ has positive leading coefficient and $t(G_1)$ is the largest root we have $M(G_1,x) > 0$ for $x > t(G_1)$. Since $M(G_2,x) \ge M(G_1,x) > 0$ on the interval $(t(G_1),\infty)$ we have $t(G_2) \le t(G_1)$. If $G_1 \succ G_2 \succ G_3$ then $M(G_3,x) \ge M(G_2,x) \ge M(G_1,x)$ on the interval $[\max(t(G_2),t(G_1)),\infty) = [t(G_1),\infty)$, i.e., $G_1 \succ G_3$. □

The weighted matching polynomial also satisfies certain recursion formulas:

Statement A.1.18. *For the weighted matching polynomial we have*

$$M((G,\underline{w});t) = M((G-e,\underline{w});t) - w_e M((G-\{u,v\},\underline{w});t),$$

where $e=(u,v)\in E(G)$*. In particular, for the unweighted matching polynomial we have*

$$M(G;t) = M(G-e,t) - M(G-\{u,v\},t).$$

For a graph G *and vertex* u *we have*

$$M((G,\underline{w});t) = tM(G-u,\underline{w});t) - \sum_{v\in N(u)} w_{uv} M((G-\{u,v\},\underline{w});t).$$

Statement A.1.19. *If* G_2 *is a spanning subgraph of* G_1 *then* $G_1 \succ G_2$*.*

Proof. By the transitivity of the relation $\succ$ it is enough to prove the statement when $G_2 = G_1 - e$ for some edge $e=uv$. By Statement A.1.18 we have

$$M(G,x) = M(G-e,x) - M(G-\{u,v\},x).$$

Since $G-\{u,v\}$ is a subgraph of G we have $t(G-\{u,v\}) \le t(G)$ by Statement A.1.17. Since the main coefficient of $M(G-\{u,v\})$ is 1, this implies that for $x \ge t(G)$ we have $M(G-\{u,v\},x) \ge 0$. By the above identity we get $G \succ G-e$. □

⋆ ⋆ ⋆

Our next goal is to prove that all roots of the weighted matching polynomial are real. This is a straightforward extension of the classical result of Heilmann and Lieb [41] and this was proved by Bodo Lass [2]. Here we give another proof which goes on the line of the classical proof, namely it uses the path tree of the graph. The reason why we give this proof is that we need this connection between the graph and its weighted path tree.

Before we prove the general statement, we need to prove the statement for trees.

Theorem A.1.20. *(a) Let* T *be a forest with non-negative weights* w *on its edges. Let us define the following matrix of size* $n\times n$*. The entry* $a_{i,j}=0$ *if vertices* v_i *and* v_j *are not adjacent and* $a_{i,j}=\sqrt{w_e}$ *if* $e=v_iv_j\in E(T)$*. Let* $\phi((T,\underline{w}_e);t)$ *be the characteristic polynomial of this matrix. Then*

$$\phi((T,\underline{w}_e);t) = M((T,\underline{w}_e);t).$$

In particular, if $w_e=1$ *for all edge* e *we have*

$$\phi(T,x) = M(T,x).$$

(b) All the roots of the polynomial $M((G,\underline{w});t)$ *are real.*

Proof. (a) Indeed when we expand the $\det(tI - A)$ we only get non-zero terms when the cycle decomposition of the permutation consist of cycles of length at most 2; but these terms correspond to the terms of the matching polynomial.

(b) Since the above defined matrix is a real symmetric matrix, all of its eigenvalues are real. $\square$

Definition A.1.21. Let $(G, \underline{w})$ be a weighted graph with vertex u as a root. Let the tree $T_{w,u}(G)$ be defined as follows: its vertex set is the paths of G with starting node u. The path p and p' is connected if one is the extension of the other with one new vertex. Let $p = uv_1 \dots v_k$ and $p' = uv_1 \dots v_k v_{k+1}$ be two paths then we define the weight of the edge (p, p') to be the weight of the edge $v_k v_{k+1}$. We call the tree $T_{w,u}(G)$ the *weighted path tree* of the weighted graph $(G, \underline{w})$.

Remark A.1.22. We mention that if we allow the weights being not only positive, but equal to 0, then we have to deal with only one weighted graph, namely with the complete graph K_n. Indeed, if we assign 0 weights to the edges not in G then with this extension we have

$$M((K_n, \underline{w}); t) = M((G, \underline{w}); t).$$

On the other hand, the weighted path tree of G and K_n are different. Hence, in order to avoid confusion we will not use this extra observation.

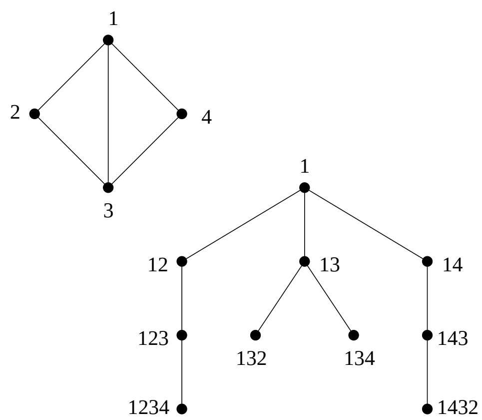

Figure 6.2: A path-tree of the diamond.

Now we prove that the weighted matching polynomial divides the weighted matching polynomial of its weighted path tree. For the sake of brevity we simplify our notation.

Let $S \subseteq V(G)$. Then set

$$M(S) = M((G|_S, \underline{w}); t)$$

the weighted matching polynomial of the induced subgraph. We also put

$$J(S, u) = M((T_{w,u}(S), \underline{w}); t)$$

for $u \in S$.

The next lemma is the main tool.

Lemma A.1.23. *For $u \in S$ we have*

$$J(S,u) = \frac{M(S)}{M(S-u)} \prod_{v \in N(u)} J(S-u,v).$$

Proof. We prove the statement by induction on $|S|$. Let $w_{u,v}$ be the weight of the edge $(u,v) \in E(S)$, equivalently this is the weight of the edge (u,uv) in the path tree $T_{w,u}(G)$. Let us decompose $J(S,u)$ according to the cases we do not select any edge (u,uv) or we select one of them (in this case we can select only one of them since they are adjacent edges)

$$J(S,u) = t \prod_{v \in N(u)} J(S-u,v) - \sum_{v \in N(u)} w_{u,v} \cdot \frac{\prod_{x \in N(u)} J(S-u,x)}{J(S-u,v)} \cdot \prod_{y \in N(v)-\{u\}} J(S-u-v,y) =$$

Now let us use the induction hypothesis for the last product.

$$= \prod_{v \in N(u)} J(S-u,v) \cdot \left(t - \sum_{v \in N(u)} \frac{w_{u,v}}{J(S-u,v)} \cdot J(S-u,v) \cdot \frac{M(S-u-v)}{M(S-u)} \right) =$$

$$= \prod_{v \in N(u)} J(S-u,v) \cdot \left(t - \sum_{v \in N(u)} w_{u,v} \frac{M(S-u-v)}{M(S-u)} \right) =$$

$$= \prod_{v \in N(u)} J(S-u,v) \cdot \frac{tM(S-u) - \sum_{v \in N(u)} w_{u,v} M(S-u-v)}{M(S-u)}.$$

Note that $tM(S-u) - \sum_{v \in N(u)} w_{u,v} M(S-u-v) = M(S)$ since we can decompose $M(S)$ according to the cases we do not select any edge (u,v) or we select one of them. Hence

$$J(S,u) = \frac{M(S)}{M(S-u)} \prod_{v \in N(u)} J(S-u,v).$$

□

An easy corollary of this result is the following theorem.

Theorem A.1.24. *There exist non-negative integers $\alpha(S)$ for all $S \subseteq V(G)$ such that*

$$M((T_{w,u}(G), \underline{w}), t) = \prod_{S \subseteq V(G)} M((S, \underline{w}), t)^{\alpha(S)}$$

and $\alpha(V(G)) = 1$.

Proof. We can prove the statement by induction on $|V(G)|$. The statement is trivial for $|V(G)| = 1, 2$. Hence we can assume that $|V(G)| \geq 3$. Let us use that

$$J(S,u) = \frac{M(S)}{M(S-u)} \prod_{v \in N(u)} J(S-u,v).$$

Let us choose some $v \in N(u)$. Then $\frac{J(S-u,v)}{M(S-u)}$ is the product of some $M(K)^{\alpha'(K)}$ for $K \subseteq S-u$. It is also true for other $J(S-u,v')$. Hence $J(S,u)$ is also the product of weighted matching polynomials of the induced subgraphs of G. Clearly, $\alpha(V(G)) = 1$. We are done. □

Corollary A.1.25. *All roots of the weighted matching polynomial are real.*

Proof. This is clear since the weighted matching polynomial divides the weighted matching polynomial of its path tree and according to Theorem A.1.20 the roots of this polynomial are real. □

Corollary A.1.26.

$$t_w(G) = t_w(T_{w,u}(G))$$

Proof. Since for $S \subseteq V(G)$ we have $t_w(S) \leq t_w(G)$ by Statement A.1.15, the claim follows from Theorem A.1.24. □

Corollary A.1.27. [41] *Assume that the largest degree in G is Δ. Then*

$$t(G) \leq 2\sqrt{\Delta - 1}.$$

Proof. Since the largest degree in G is Δ so is in the path tree. For the path tree we have

$$t(T_u(G)) = \mu(T_u(G)).$$

But for trees (and forests) it is well-known that $\mu(T) \leq 2\sqrt{\Delta_T - 1}$. (This last statement is again the result of Heilmann and Lieb [41], but it can be found in [30] and in [45] as well.) □

A.2 Laplacian characteristic polynomial

Definition A.2.1. Let $L(G)$ be the Laplacian matrix of G (so $L(G)_{ii} = d_i$ and $-L(G)_{ij}$ is the number of edges between i and j if $i \neq j$). We call the polynomial $L(G,x) = \det(xI - L(G))$ the Laplacian polynomial of the graph G, i.e., it is the characteristic polynomial of the Laplacian matrix of G.

Statement A.2.2. *The eigenvalues of $L(G)$ are non-negative real numbers, at least one of them is 0. Thus we can order them as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n = 0$.*

Proof. The Laplacian matrix is symmetric, thus its eigenvalues are real.

It is also positive semidefinite since

$$\underline{x}^T L(G)\underline{x} = \sum_{(i,j)\in E(G)} (x_i - x_j)^2 \geq 0.$$

Hence its eigenvalues are non-negative.

Finally, the vector $\underline{1}$ is an eigenvector of $L(G)$ belonging to the eigenvalue 0. □

Corollary A.2.3. *The Laplacian polynomial can be written as*

$$L(G,x) = x^n - a_{n-1}x^{n-1} + a_{n-2}x^{n-2} - \cdots + (-1)^{n-1}a_1 x,$$

where $a_1, a_2, \ldots, a_{n-1}$ *are positive integers.*

In what follows let $\tau(G)$ denote the number of spanning trees of the graph G. The following statement is the fundamental matrix-tree theorem.

Theorem A.2.4. *Let* $L(G)_i$ *be the matrix obtained from* $L(G)$ *by deleting the* i*-th row and column. Then* $\det L(G)_i = \tau(G)$.

Proof. We will prove the statement for an arbitrary multigraph G.

We begin with a simple observation, namely that for any edge e we have

$$\tau(G) = \tau(G - e) + \tau(G/e).$$

Indeed, we can decompose the set of spanning tree according to that a spanning tree contains the edge e or not. If it does not contain the edge e then it is also a spanning tree of $G - e$ and vice versa. If it contains the edge e then we can contract it, this way we obtain a spanning tree of G/e; this construction again works in the reversed way.

Now we can prove the statement by induction on the number of edges. For the empty graph the statement is clearly true. We can assume that we erased the row and column corresponding to the vertex v_n. We distinguish two cases according to that v_n was an isolated vertex of G or not.

Case 1. Assume that v_n is an isolated vertex of G. Then $\tau(G) = 0$. On the other hand, $\det(L(G)_n) = 0$, because the vector $\underline{1}$ is an eigenvector of $L(G)_n$ belonging to 0. Hence, in this case, we are done.

Case 2. Assume that v_n is not an isolated vertex, we can assume that $e = (v_{n-1}, v_n) \in E(G)$ (maybe there are more than one such edges since this is a multigraph). Let $\underline{l}_{n-1}$ be the $(n-1)$.th row vector of $L(G)_n$ and let $\underline{s} = (0, 0, \ldots, 0, 1)$ consisting of $(n-2)$ 0's and a 1 entry. Now we consider the matrices A_{n-1} and B_{n-1} where we exchange the last row of $L(G)_n$ to the vector $\underline{l}_{n-1} - \underline{s}$ and $\underline{s}$, respectively. Then

$$\det L(G)_n = \det A_{n-1} + \det B_{n-1}.$$

Observe that $A_{n-1} = L(G-e)_n$; since $G-e$ has less number of edges then G, we have by induction that $\det A_{n-1} = \det L(G-e)_n = \tau(G-e)$.

On the other hand, $\det B_{n-1} = \det A_{n-2}$, where $A_{n-2} = L(G)_{\{n-1,n\}}$. Observe that A_{n-2} is nothing else than $L(G/e)_{n-1=n}$. Since G/e has less number of edges than G, we have $\det A_{n-2} = \det L(G/e)_{n-1=n} = \tau(G-e)$. Hence

$$\det L(G)_n = \tau(G-e) + \tau(G/e) = \tau(G).$$

□

Corollary A.2.5. *The coefficient of x^1 in $L(G,x)$ is $n\tau(G)$. Furthermore,*

$$\tau(G) = \frac{1}{n}\prod_{j=1}^{n-1} \lambda_i.$$

Proof. Let $L(G,x) = x^n - a_{n-1}x^{n-1} + a_{n-2}x^{n-2} - \cdots + (-1)^{n-1}a_1x$. Then by the Viéte's formula we have

$$a_1 = \lambda_2\lambda_3\ldots\lambda_n + \lambda_1\lambda_3\ldots\lambda_n + \cdots + \lambda_1\lambda_2\ldots\lambda_{n-1}.$$

Since $\lambda_n = 0$ we have $a_1 = \lambda_1\lambda_2\ldots\lambda_{n-1}$. On the other hand, by expanding $\det(xI - L(G))$ we see that the coefficient of x is

$$a_1 = \sum_{i=1}^{n} \det(L(G)_i) = n\tau(G),$$

by Theorem A.2.4. Hence $\tau(G) = \frac{1}{n}a_1 = \prod_{i=1}^{n-1}\lambda_i$. □

Part (a) and (b) of Lemma A.2.9 is a well-known generalization of Corollary A.2.5. To state this lemma we need the following notation.

Definition A.2.6. For $I \subset V(G)$, let G/I denote the graph obtained from G by contracting all vertices of I, but erasing the loops at the vertex corresponding to I. (Hence G/I is a multigraph without loops.)

Definition A.2.7. Let $\mathcal{F}_k(G)$ denote the set of spanning forests of the graph G which have exactly k components. For $F = T_1 \cup \cdots \cup T_k \in \mathcal{F}_k$ let $\gamma(F) = \prod_{i=1}^{k} |T_i|$, where T_i's are the connected components of the forest F.

Definition A.2.8. For $S \subseteq V(G)$ let $\overline{\tau}(S) = |S|\tau(S)$ where $\tau(S)$ is the number of spanning trees of the induced subgraph of G on the vertex set S.

Lemma A.2.9. *Let $L(G,x) = \sum_{k=1}^{n} a_k(-1)^{n-k}x^k$. Then*

(a)

$$a_k = \sum_{\substack{I\subseteq V(G)\\ |I|=k}} \tau(G/I).$$

(b)

$$a_k = \sum_{F \in \mathcal{F}_k} \gamma(F).$$

(c)

$$a_k = \sum_{\{S_1, S_2, \dots, S_k\}} \overline{\tau}(S_1)\overline{\tau}(S_2)\dots\overline{\tau}(S_k),$$

where the summation goes over all partition of $V(G)$ into exactly k non-empty sets.

Proof. (a) Let $L(G)_I$ be the matrix obtained from $L(G)$ by erasing all rows and columns corresponding to I. Note that $\det L(G)_I = \tau(G/I)$, since if we erase the row and column corresponding to I from $L(G/I)$ we get exactly $L(G)_I$ and so the observation follows from Theorem A.2.4. On the other hand,

$$a_k = \sum_{|I|=k} \det L(G)_I$$

follows simply from expanding $\det(xI - L(G))$. By combining this with our previous observation we are done.

(b) For $F \in \mathcal{F}_k$ we can choose a set I with k elements exactly $\gamma(F)$ ways such that after the contraction of the set I, the contraction of F becomes the spanning tree of G/I. Indeed we have to choose an element of I from each component of F, but then no matter how we chose these elements, the contraction of these elements makes F become the spanning tree of G/I.

(c) We can decompose the sum in part (b) such that we consider those forest of $\mathcal{F}_k$ whose components span the sets $S_1, \dots, S_k$. For such a forest $\gamma(F) = |S_1||S_2|\dots|S_k|$. The number of such forests is clearly $\tau(S_1)\tau(S_2)\dots\tau(S_k)$. Altogether we have

$$a_k = \sum_{F \in \mathcal{F}_k} \gamma(F) = \sum_{\{S_1, S_2, \dots, S_k\}} \overline{\tau}(S_1)\overline{\tau}(S_2)\dots\overline{\tau}(S_k).$$

□

Recall that the Wiener-index of the graph G is $\sum_{u,v} d(u,v)$, where $d(u,v)$ denotes the distance of the vertices u and v.

Corollary A.2.10. [66] *Let T be a tree and $L(T,x) = \sum_{k=1}^{n} (-1)^{n-k} a_k(T) x^k$. Then $a_2(T)$ is the Wiener-index of the tree T.*

Proof. Observe that in a tree T we have $\tau(T/\{u,v\}) = d(u,v)$. Indeed, if u, v are adjacent then $T/\{u,v\}$ is again a tree. If u and v have distance greater than 1 then $T/\{u,v\}$ has $n-1$ vertices and edges and it contains a cycle of length $d(u,v)$ (possibly this cycle has only two edges). Hence every spanning tree of $T/\{u,v\}$ miss exactly one of the edge of the cycle. Thus $\tau(T/\{u,v\}) = d(u,v)$. Now the statement follows from part (a) of Lemma A.2.9. □

Remark A.2.11. We will see that the identity in part (c) reveals an interesting property of the Laplacian polynomial, namely it satisfies that

$$\sum_{\substack{S_1 \cup S_2 = V(G) \\ S_1 \cap S_2 = \emptyset}} L(S_1, x) L(S_2, y) = L(G, x + y).$$

⋆ ⋆ ⋆

In this part we collect some results on the eigenvalues of the Laplacian matrix.

Statement A.2.12. *If we add k isolated vertices to the graph G then the Laplacian spectra of the obtained graph consists of the Laplacian spectra of the graph G and k zeros.*

Statement A.2.13. [32] *If the Laplacian spectra of the graph G is $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n = 0$ then the Laplacian spectra of $\overline{G}$ is $n - \lambda_1, n - \lambda_2, \ldots, n - \lambda_{n-1}, 0$.*

Proof. Note that $L(G) + L(\overline{G}) = nI - J$. We know that $\underline{1}$ is both an eigenvector of $L(G)$ and $L(\overline{G})$ belonging to the eigenvalue 0. Since $L(G)$ is symmetric we can choose orthonormal eigenvectors $v_1, \ldots, v_n$ spanning $\mathbb{R}^n$ ($|V(G)| = n$) from which $v_n = \underline{1}$ and $L(G)v_i = \lambda_i v_i$. Then for $i \neq n$ we have

$$L(\overline{G})v_i = (nI - J - L(G))v_i = nv_i - \underline{0} - \lambda_i v_i = (n - \lambda_i)v_i.$$

Hence the Laplacian spectra of $\overline{G}$ is $n - \lambda_1, n - \lambda_2, \ldots, n - \lambda_{n-1}, 0$. □

Lemma A.2.14. *(Interlacing lemma,* [32]*) Let G be a graph and e an edge of it. Let $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_{n-1} \geq \lambda_n = 0$ be the roots of $L(G, x)$ and let $\tau_1 \geq \tau_2 \geq \ldots \tau_{n-1} \geq \tau_n = 0$ be the roots of $L(G - e, x)$. Then*

$$\lambda_1 \geq \tau_1 \geq \lambda_2 \geq \tau_2 \geq \cdots \geq \lambda_{n-1} \geq \tau_{n-1}$$

Proof. Let us direct the edges of the graph G arbitrarily. Let D be the incidence matrix of this directed graph. So D has size $|V(G) \times |E(G)|$ and

$$D_{v,e} = \begin{cases} 1 \text{ if } v \text{ is the head of the edge } e \\ -1 \text{ if } v \text{ is the tail of the edge } e \\ 0 \text{ otherwise} \end{cases}$$

It is easy to see that $DD^T = L(G)$. The spectrum of D^TD is the union of the spectrum of DD^T and $|E(G)| - |V(G)|$ 0's. (If $|V(G)| > |E(G)|$ then the spectrum of DD^T is the union of the spectrum of D^TD and $|V(G)| - |E(G)|$ 0's.) Let D' be the incidence matrix of $G - e$ then $D'D'^T = L(G - e)$ and D'^TD' is a minor of D^TD; we simply delete the row and column corresponding the edge e. Hence the eigenvalues of $D'D'^T$ interlace the eigenvalues of DD^T. After removing (adding) some 0's we obtain the statement. □

Corollary A.2.15. *Let G_2 be a subgraph of G_1 then $\theta(G_2) \leq \theta(G_1)$.*

Proof. First we delete all edges belonging to $E(G_1) \setminus E(G_2)$. This way we obtain that $\theta(G_1) \geq \theta(G_2')$ where $G_2' = (V(G_1), E(G_2))$. Then we delete the isolated vertices consisting of $V(G_1) \setminus V(G_2)$, this way we deleted some 0's from the Laplacian spectrum of G_2'. Clearly, this does not affect $\theta(G_2') = \theta(G_2)$. Hence $\theta(G_1) \geq \theta(G_2)$. □

Corollary A.2.16. *Let T_1 be a tree and T_2 be its subtree. Then $a(T_1) \leq a(T_2)$.*

Proof. It is enough to prove the statement for $T_1 - v = T_2$, where the degree of the vertex v is one. Let e be the pendant edge whose one of the endvertex is v. Then we can get T_2 by deleting the edge e and then the isolated vertex v. First we get that $\lambda_{n-2}(T_2 \cup \{v\}) \geq \lambda_{n-1}(T_1) \geq \lambda_{n-1}(T_2 \cup \{v\})$ by the interlacing lemma. After deleting the isolated vertex v we exactly delete the $\lambda_{n-1}(T_2 \cup \{v\}) = 0$ from the Laplacian spectra and we get that

$$a(T_2) = \lambda_{n-2}(T_2) = \lambda_{n-2}(T_2 \cup \{v\}) \geq \lambda_{n-1}(T_1) = a(T_1).$$

□

A.3 Exponential-type graph polynomials

Definition A.3.1. Let us say that the sequence of polynomials $p_0(x), p_1(x), p_2(x), \dots$ satisfy the binomial theorem if for any n

$$\sum_{k=0}^{n} \binom{n}{k} p_k(x) p_{n-k}(y) = p_n(x+y)$$

and $\deg p_k(x) = k$.

Remark A.3.2. Clearly, the polynomial sequence $p_n(x) = x^n$ motivates this definition. It is also well-known that the polynomials $p_n(x) = x^{\underline{n}} = x(x-1)\dots(x-n+1)$ and $x^{\overline{n}} = x(x+1)\dots(x+n-1)$ also satisfy the binomial theorem. Abel's identity implies that the polynomial sequence $p_n(x) = x(x+n)^{n-1}$ also satisfies the binomial theorem, i. e.,

$$\sum_{k=0}^{n} \binom{n}{k} x(x+k)^{k-1} y(y+n-k)^{n-k-1} = (x+y)(x+y+n)^{n-1}.$$

In this last identity we can write $-x$ and $-y$ instead of x and y and then by multiplying both side with $(-1)^n$ we obtain that the polynomials $p_n(x) = x(x-n)^{n-1}$ also satisfy the binomial theorem. On the other hand, we can recognize $x(x-n)^{n-1}$ as the Laplacian characteristic polynomial of the complete graph K_n. Thus the previous identity can be rewritten as

$$\sum_{\substack{S_1 \cup S_2 = V(G) \\ S_1 \cap S_2 = \emptyset}} L(S_1, x) L(S_2, y) = L(K_n, x+y),$$

where $L(S_i, x)$ is the Laplacian characteristic polynomial of the graph induced by the set S_i. We will see soon that we could have written arbitrary an graph G instead of K_n. This motivates the following definition.

Definition A.3.3. We say that the graph polynomial f is exponential-type if for every graph $G = (V(G), E(G))$ we have $\deg f(G,x) = |V(G)|$, $f(\emptyset, x) = 1$ and $f(G,x)$ satisfies that

$$\sum_{\substack{S_1 \cup S_2 = V(G) \\ S_1 \cap S_2 = \emptyset}} f(S_1, x) f(S_2, y) = f(G, x+y),$$

where $f(S_1, x) = f(G|_{S_1}, x), f(S_2, y) = f(G|_{S_2}, y)$ are the polynomials of the subgraphs of G induced by the sets S_1 and S_2, respectively.

Remark A.3.4. Gus Wiseman [65] calls the exponential-type graph polynomials "binomial-type". This section is partly motivated by his paper, although our treatment will be a bit different.

We will show that the Laplacian characteristic polynomial, the chromatic polynomial and a modified version of the matching polynomial belong to the class of the exponential-type graph polynomials.

A.3.1 Set-generating function

It is easy to give a characterisation of polynomial sequences satisfying the binomial theorem.

Theorem A.3.5. (Theorem 4.3.3. in [57]) *The polynomial sequence $p_0(x), p_1(x), p_2(x), \dots$ satisfies the binomial theorem if and only if there exist a generating function $f(z) = \sum_{k=1}^{\infty} b_k \frac{z^k}{k!}$ such that*

$$e^{xf(z)} = \sum_{k=1}^{\infty} p_n(x) \frac{z^n}{n!}.$$

Then the binomial identity simply follows from the identity $e^{xf(z)} e^{yf(z)} = e^{(x+y)f(z)}$. Note that we have written the function $f(z)$ as an exponential generating function; clearly, we could have written it as an ordinary generating function, but this form will be more convenient for us. Note that $p_0(x)$ must be the function 1 and for $k \geq 1$ the polynomial $p_k(x)$ has no constant term. Once we have a polynomial sequence $(p_n(x))$ satisfying the binomial theorem we can easily determine $f(z)$: the coefficient of x^1 in $p_n(x)$ is exactly b_n.

Now we will give the corresponding generalisation of this ideas to graph polynomials. First we introduce the set-generating function.

Let V be a set of n elements and let us consider the ring with elements

$$\mathbb{D} = \left\{ \sum_{S \subseteq V} a_S \nu^S \mid a_S \in \mathbb{R} \right\},$$

where $\nu^{S_1} \nu^{S_2} = 0$ if $S_1 \cap S_2 \neq \emptyset$ and $\nu^{S_1} \nu^{S_2} = \nu^{S_1 \cup S_2}$ if $S_1 \cap S_2 = \emptyset$. Note that the ring $\mathbb{D}$ is isomorphic with the ring

$$\mathbb{R}[a_1, \dots, a_n] / \langle a_i^2 = 0 \ (i = 1, \dots, n) \rangle$$

by $\prod_{i \in S} a_i$ corresponding to ν^S. If $F = \sum_{S \subseteq V} f_S \nu^S$ and $G = \sum_{S \subseteq V} g_S \nu^S$ are two elements of $\mathbb{D}$ then

$$F \cdot G = \sum_{S \subseteq V} \Big(\sum_{\substack{S_1 \cup S_2 = S \\ S_1 \cap S_2 = \emptyset}} f_{S_1} g_{S_2} \Big) \nu^S.$$

Now we are ready to give a description of exponential-type graph polynomials. Let b be a function from the isomorphism classes of graphs to $\mathbb{R}$ or $\mathbb{C}$ such that $b(\emptyset) = 0$. Let us fix a graph $G = (V, E)$ and let us consider the set-generating function

$$\exp(x \sum_{S \subseteq V} b(S) \nu^S) = \sum_{S \subseteq V} f_b(S, x) \nu^S,$$

where $b(S) = b(G|_S)$. The polynomial $f_b(V, x) = f_b(G, x)$ depends only on the isomorphism class of G and is exponential-type. Indeed, with the notation $B(\nu) = \sum_{S \subseteq V} b(S) \nu^S$ we have

$$\exp(xB(\nu)) \exp(yB(\nu)) = \exp((x+y)B(\nu))$$

and it exactly means that

$$\sum_{\substack{S_1 \cup S_2 = V(G) \\ S_1 \cap S_2 = \emptyset}} f_b(S_1, x) f_b(S_2, y) = f_b(G, x+y).$$

Note that since $(\nu^S)^k = 0$ if $k \geq 2$ we have

$$\exp(x \sum_{S \subseteq V} b(S) \nu^S) = \prod_{S \subseteq V} \exp(x b(S) \nu^S) = \prod_{S \subseteq V} (1 + x b(S) \nu^S).$$

From this we can immediately see the following important corollary.

Theorem A.3.6. *Let*

$$\exp(x \sum_{S \subseteq V} b(S) \nu^S) = \sum_{S \subseteq V} f_b(S, x) \nu^S.$$

Furthermore, let $f_b(S, x) = \sum_{k=1}^{n} a_k(S) x^k$. *Then*

$$a_k(S) = \sum_{\{S_1, S_2, \dots, S_k\} \in \mathcal{P}_k} b(S_1) b(S_2) \dots b(S_k),$$

where the summation goes over the set $\mathcal{P}_k$ *of all partitions of* S *into exactly* k *sets.*

Now we prove that every exponential-type graph polynomial arise this way.

Theorem A.3.7. *Let* f *be a graph polynomial satisfying that for every graph* G *we have*

$$\sum_{\substack{S_1 \cup S_2 = V(G) \\ S_1 \cap S_2 = \emptyset}} f(S_1, x) f(S_2, y) = f(G, x+y).$$

Then there exist a graph function b *such that* $f(G, x) = f_b(G, x)$. *More precisely, if* $b(G)$ *is the coefficient of* x^1 *in* $f(G, x)$ *then* $f = f_b$.

Proof. Let

$$f(G,x)=\sum_{k=0}^{|V(G)|}a_k(G)x^k.$$

First of all, we prove that the coefficient of x^0 in $f(G,x)$ is 0 unless $G=\emptyset$. We prove it by induction on $|V(G)|$. If $|V(G)|=1$ then let $f(K_1,x)=ax+c$. Then

$$a(x+y)+c=f(K_1,x+y)=f(K_1,x)f(\emptyset,y)+f(\emptyset,x)f(K_1,y)=$$

$$=(ax+c)\cdot 1+(ay+c)\cdot 1=a(x+y)+2c.$$

Hence $c=0$. Now assume that $|V(G)|\geq 2$ and we know the statement for every graph H with $|V(H)|<|V(G)|$, $H\neq\emptyset$. Now comparing the coefficient of x^0y^0 in

$$\sum_{\substack{S_1\cup S_2=V(G)\\ S_1\cap S_2=\emptyset}} f(S_1,x)f(S_2,y)=f(G,x+y)$$

we obtain that

$$a_0(G)=a_0(G)\cdot 1+1\cdot a_0(G)+\sum_{\substack{S_1\cup S_2=V(G),\ S_1\cap S_2=\emptyset\\ S_1,S_2\neq\emptyset}} a_0(S_1)a_0(S_2)=2a_0(G)$$

by the induction hypothesis. From this we obtain that $a_0(G)=0$ as well.

Now let $b(G)$ be the coefficient of x^1 in the polynomial $f(G,x)$. We will show that

$$a_k(G)=\sum_{\{S_1,S_2,\dots,S_k\}\in\mathcal{P}_k} b(S_1)b(S_2)\dots b(S_k).$$

We prove it by induction on $k+|V(G)|$. For $k=1$ this is exactly the definition so we can assume that $k\geq 2$. Since $f(.,x)$ is exponential-type we have

$$\sum_{\substack{S_1\cup S_2=V(G)\\ S_1\cap S_2=\emptyset}}\left(\sum_{r=1}^{|S_1|}a_r(S_1)x^r\right)\left(\sum_{t=1}^{|S_2|}a_t(S_2)y^t\right)=\sum_{k=1}^{|V(G)|}a_k(G)(x+y)^k.$$

By comparing the coefficient of x^ry^{k-r} we obtain that

$$a_k(G)\binom{k}{r}=\sum_{\substack{S_1\cup S_2=V(G),\ S_1\cap S_2=\emptyset\\ |S_1|=r,\ |S_2|=k-r}} a_r(S_1)a_{k-r}(S_2).$$

Now we can apply the induction hypothesis to all terms of the sum unless $S_1=V(G), r=k$ or $S_2=V(G), r=0$. To avoid this we simply choose $r=k-1$ to get that

$$a_k(G)k=\sum_{\substack{S_1\cup S_2=V(G),\ S_1\cap S_2=\emptyset\\ |S_1|=k-1,\ |S_2|=1}} a_{k-1}(S_1)a_1(S_2)=$$

$$= \sum_{S_2} b(S_2) \sum_{\{T_1,\dots,T_{k-1}\}\in\mathcal{P}_{k-1}(S_1)} b(T_1)\dots b(T_{k-1}) =$$

$$= k \sum_{\{T_1,\dots,T_{k-1},T_k\}\in\mathcal{P}_k(V(G))} b(T_1)\dots b(T_{k-1})b(T_k).$$

Hence

$$a_k(G) = \sum_{\{S_1,S_2,\dots,S_k\}\in\mathcal{P}_k} b(S_1)b(S_2)\dots b(S_k).$$

Hence $f(G,x) = f_b(G,x)$. ☐

Remark A.3.8. In the "nice cases" we have $f(K_1,x) = x$ or in other words, $b(K_1) = 1$ implies that $f(G,x)$ is a monic polynomial for every graph G, but it is not necessarily true in general.

We can prove some simple consequences of the previous two theorems. Many graph polynomials have the following multiplicativity property.

Definition A.3.9. We say that a graph polynomial is multiplicative if

$$f(G_1 \cup G_2, x) = f(G_1,x)f(G_2,x),$$

where $G_1 \cup G_2$ denotes the disjoint union of the graphs G_1 and G_2 and $f(\emptyset) = 1$.

Theorem A.3.10. *Let $f_b(G,x)$ be an exponential-type graph polynomial. Then f_b is multiplicative if and only if $b(H) = 0$ for all disconnected graphs.*

Proof. Since the constant term of an exponential type polynomial is 0 for every non-empty graph the condition is necessary: if $H = H_1 \cup H_2$ then $f_b(H) = f_b(H_1)f_b(H_2)$ implies that $b(H) = 0$.

On the other hand, if $b(H) = 0$ for all disconnected graphs then from Theorem A.3.6 we see that

$$a_k(H_1 \cup H_2) = \sum_{j=1}^{k} a_j(H_1)a_{k-j}(H_2)$$

which means that $f(H_1 \cup H_2, x) = f(H_1,x)f(H_2,x)$. ☐

The following identity connects the classical theory with the theory of the exponential-type graph polynomials.

Theorem A.3.11.

$$\sum_{k=0}^{\infty} f_b(K_n,x)\frac{z^n}{n!} = \exp(x\sum_{n=1}^{\infty} b(K_n)\frac{z^n}{n!})$$

A.3.2 Examples of exponential-type polynomials

In this section we prove that some well-known graph polynomials are exponential-type. For the chromatic polynomial this is almost trivial and was already observed by Tutte [62].

Theorem A.3.12. *The chromatic polynomial $ch(.,x)$ is exponential-type.*

Proof. Let $G = (V, E)$ be a graph. We need to prove that

$$\sum_{\substack{S_1 \cup S_2 = V(G) \\ S_1 \cap S_2 = \emptyset}} ch(S_1, x) ch(S_2, y) = ch(G, x + y).$$

Since there are polynomials on both sides it is enough to prove that there is equality for all positive integers x, y. But this is trivial: if we color G with $x + y$ colors then we can decompose $V(G)$ to $S_1 \cup S_2$ according we used a color from the first x colors or from the last y colors; such a decomposition provides a term $ch(S_1, x)ch(S_2, y)$. □

Theorem A.3.13. *The Laplacian polynomial $L(., x)$ is exponential-type with*

$$b(G) = (-1)^{|V(G)|-1}\overline{\tau}(G) = (-1)^{|V(G)|-1}|V(G)|\tau(G).$$

Proof. Indeed, by part (c) of the Lemma A.2.9 we have $L(G, x) = f_b(G, x)$, where

$$b(G) = (-1)^{|V(G)|-1}\overline{\tau}(G) = (-1)^{|V(G)|-1}|V(G)|\tau(G).$$

□

Theorem A.3.14. *Let $M(G, x) = \sum_{k=0}^{n} m_k(G)x^{n-k}$ be the modified matching polynomial. Then $M(G, x)$ is exponential-type.*

Proof. Let $b(K_1) = b(K_2) = 1$ and $b(H) = 0$ otherwise. Then $M(G, x) = f_b(G, x)$; indeed, this time we can easily check that

$$\sum_{S \subseteq V} M(G, x)\nu^S = \prod_{i=1}^{n}(1 + x\nu^{\{v_i\}}) \prod_{e=(v_i,v_j)\in E(G)} (1 + x\nu^{\{v_i,v_j\}}).$$

□

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Abstract

The thesis consists of two parts. In the first part we study two graph transformations, namely the Kelmans transformation and the generalized tree shift. In the second part of this thesis we study an extremal graph theoretic problem and its relationship with algebraic graph theory. The main results of this thesis are the following.

- We show that the Kelmans transformation is a very effective tool in many extremal algebraic graph theoretic problems. Among many other things, we attain a breakthrough in a problem of Eva Nosal by the aid of this transformation.
- We define the generalized tree shift which turns out to be a powerful tool in many extremal graph theoretic problems concerning trees. With the aid of this transformation we prove a conjecture of V. Nikiforov. We give a strong method for attacking extremal graph theoretic problems involving graph polynomials and trees. By this method we give new proofs for several known results and we attain some new results.
- We completely solve the so-called density Turán problem for trees and we give sharp bounds for the critical edge density in terms of the largest degree for every graphs. We establish connection between the problem and algebraic graph theory. By the aid of this connection we construct integral trees of arbitrarily large diameters. This was an open problem for more than 30 years.

Összefoglalás

Az értekezés két részből áll. Az első felében két gráftranszformáció, az ún. Kelmans-transzformáció valamint az általánosított fa transzformációval foglalkozunk. A tézis másik felében egy extremális gráfelméleti problémával foglalkozunk, valamint ezen problémának az algebrai gráfelmélettel való kapcsolatával. Az értekezés fő eredményei a következők.

- Megmutatjuk, hogy a Kelmans-transzformáció hatékony eszköz számos extremális algebrai gráfelméleti problémában. Többek között segítségével áttörést érünk el Eva Nosal egy régi problémájában.
- Definiáljuk az általánosított fa transzformációt, amely hatékony eszköznek bizonyul fákra vonatkozó extremális gráfelméleti problémákban. Segítségével bebizonyítjuk V. Nikiforov egy sejtését. Megadunk egy erős módszert gráfpolinomokkal kapcsolatos, fákon értelmezett extremális algebrai gráfelméleti problémák megtámadására. Segítségével új bizonyítást adunk számos ismert tételre és néhány új eredményt is elérünk.
- Az ún. sűrűségi Turán problémát teljesen megoldjuk fákra valamint minden gráfra éles becslést adunk a kritikus élsűrűségre a legnagyobb fokszám függvényében. Kapcsolatot teremtünk a probléma és az algebrai gráfelmélet között. Ezen kapcsolat segítségével konstruálunk tetszőlegesen nagy átmérőjű fákat melyek minden sajátértéke egész szám. Ez utóbbi probléma több, mint 30 évig megoldatlan volt.